

# BAYESUVIUS

A VISUAL DICTIONARY OF BAYESIAN  
NETWORKS AND CAUSAL INFERENCE



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**Bayesuvius,**  
a visual dictionary of Bayesian Networks and  
Causal Inference

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This book is constantly being expanded and improved. To download the latest version, go to <https://github.com/rrtucci/Bayesuvius>

**Bayesuvius**

by Robert R. Tucci

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Figure 1: View of Mount Vesuvius from Pompeii



Figure 2: Mount Vesuvius and Bay of Naples

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# Foreword

Welcome to Bayesuvius! a proto-book uploaded to github.

A different Bayesian network is discussed in each chapter. Each chapter title is the name of a Bnet. Chapter titles are in alphabetical order.

This is a volcano in its early stages. First version uploaded to a github repo called Bayesuvius on June 24, 2020. First version only covers 2 Bnets (Linear Regression and GAN). I will add more chapters periodically. Remember, this is a moon-lighting effort so I can't do it all at once.

For any questions about notation, please go to Notational Conventions section.  
Requests and advice are welcomed.

Thanks for reading this

Robert R. Tucci

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## ADDENDA

- **August 15, 2021:** At this point in time, the book has grown to 67 Chapters and 433 pages. Today, I am self-publishing it as an ebook at Amazon and similar outlets. It will still be free.

# Appendices

# Appendix A

## Navigating the ocean of Judea Pearl's Books

Many of the greatest ideas in the bnet field were invented by Judea Pearl and his collaborators. Thus, this book is heavily indebted to those great scientists. Those ideas have had no clearer and more generous expositor than Judea Pearl himself.

Pearl has written 4 books that I have used in writing Bayesuvius. His 1988 book Ref.[50] dates back to his pre-causal period. That book I used to learn about topics such as d-separation, belief propagation, Markov-blankets, and noisy-ORs. 3 other books that he wrote later, in his causal period, are:

1. In 2000 (1st ed.), and 2013 (2nd ed.), Pearl published what is so far his most technical and exhaustive book on the subject of causality, Ref.[52].
2. In 2016, he released together with Glymour and Jewell, a less advanced "primer" on causality, Ref.[55].
3. In 2018, he released together with Mackenzie his lovely "The Book of Why", Ref.[56].

Those 3 books I used to learn about causality topics such as Do Calculus, backdoor and frontdoor adjustment formulae, linear deterministic bnets with exogenous noise, and counterfactuals.

A micro poem written by me to celebrate Judea Pearl and his work:

### I, Robot

Let other robots `talk()`,  
while I,  
`talk()`, `do()` and `imagine()`.

# Appendix B

## CI-2-3 track

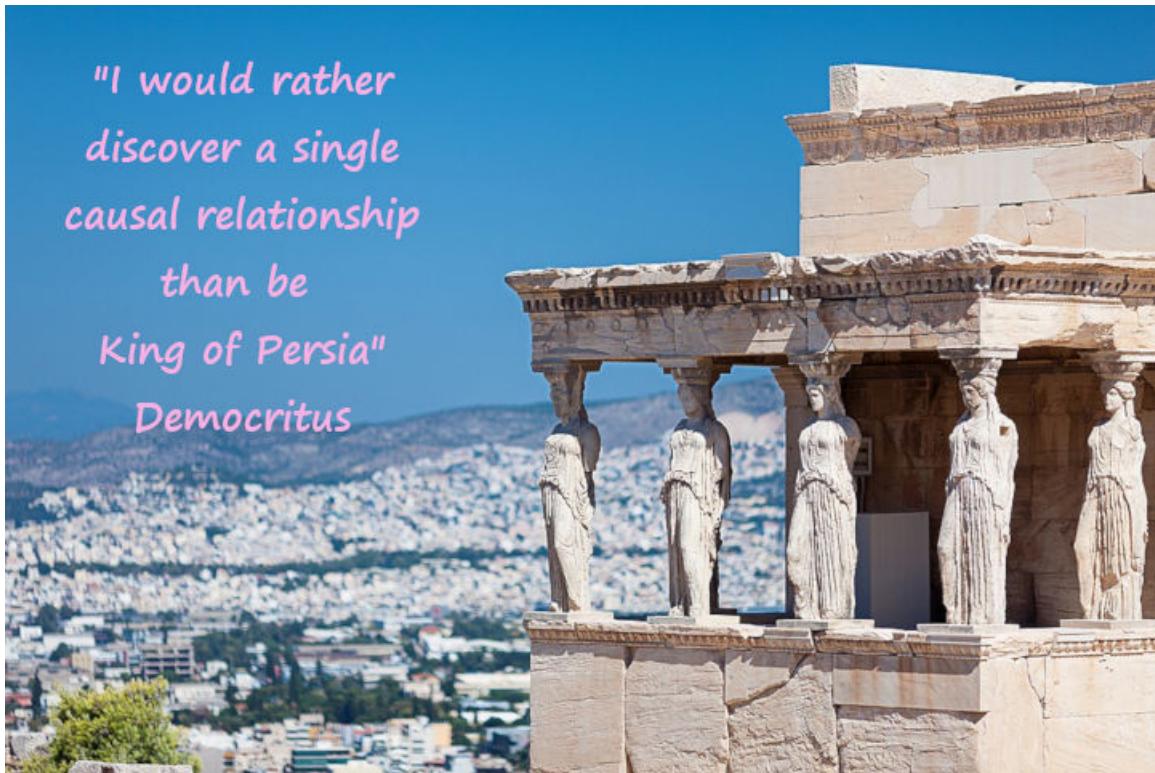


Figure B.1: Democritus quote, Acropolis Caryatids background

As discussed in Chapter 12, Judea Pearl has proposed 3 rungs of Causal Inference (CI). This book covers all 3 rungs.

Confusingly, it has become common to use the term CI to refer to only the highest 2 rungs of the CI hierarchy; i.e, rung 2 (do operations) and rung 3 (imaging/counterfactual thinking). Also confusingly, rung 1 uses causal diagrams and is often referred to as "inference", so it could reasonably have been defined as the whole of CI, but Pearl has defined the CI hierarchy to include two more rungs. To



Figure B.2: CI meme

patch over this linguistic confusion, I sometimes refer to rung 1 as “prediction”, or as “predictive inference” instead of calling it merely “inference”. Also, when I want to be precise, I use the term “CI-2-3” to refer to CI restricted to only rungs 2 and 3.

Here is a subset of chapters that I call the CI-2-3 track, that are devoted mostly to rungs 2 and 3.

1. Backdoor Adjustment Formula
2. Berkson’s Paradox
3. Counterfactual Reasoning
4. Decisions Based on Rungs 2 and 3: COMING SOON
5. Difference-in-Differences
6. Do Calculus



Figure B.3: Slide from Pearl talk at IJCAI-2022. Putting the joking of Fig.B.2 aside, let me emphasize that CI advocates are not trying to vanish NNs from AI. To us, NNs and bnets are different tools, like hammer and saw. We believe AI should use both tools. For those who are trying to do CI using a NN instead of a bnet, it looks to me like you are trying to use a hammer to cut wood. Why don't you cut with a saw instead? As Pearl says in this slide, CI elevates Data Science from Deep Learning (curve-fitting) to Deep Understanding.

7. Do Calculus proofs
8. D-Separation
9. Frisch-Waugh-Lovell (FWL) theorem
10. Frontdoor Adjustment Formula
11. G-formula (Sequential Backdoor Adjustment Formula)
12. Goodness of Causal Fit
13. Granger Causality
14. Identification of do queries via LDEN diagrams
15. Instrumental Inequality and beyond
16. Instrumental Variables
17. LATE (Local Average Treatment Effect)
18. LDEN with feedback loops
19. Linear Deterministic Bnets with External Noise

- 20. Mediation Analysis
- 21. Mendelian Randomization
- 22. Meta-learners for estimating ATE
- 23. Modified Treatment Policy
- 24. Omitted Variable Bias
- 25. Personalized Expected Utility
- 26. Personalized Treatment Effects
- 27. Potential Outcomes and Beyond
- 28. Regression Discontinuity Design
- 29. Selection Bias Removal
- 30. Simpson's Paradox
- 31. Survival Analysis
- 32. Synthetic Controls
- 33. Targeted Estimator
- 34. Transportability of Causal Knowledge
- 35. Uplift Modelling

# Appendix C

## Notational Conventions and Preliminaries

### C.1 Some abbreviations frequently used throughout this book

- AI/ML = Artificial Intelligence/Machine Learning
- bnet= Bnet= Bayesian Network
- CPT = Conditional Probabilities Table, same as TPM
- DAG = Directed Acyclic Graph
- i.i.d.= independent identically distributed.
- RCT= Randomized Controlled Trial, a.k.a. A/B testing.
- TPM= Transition Probability Matrix, same as CPT

### C.2 $\mathcal{N}(!a)$

$\mathcal{N}(!a)$  will denote a normalization constant that does not depend on  $a$ . For example,  $P(x) = \mathcal{N}(!x)e^{-x}$  where  $\int_0^\infty dx P(x) = 1$ .

### C.3 Indicator function (a.k.a. Truth function)

$$\mathbb{1}(\mathcal{S}) = \begin{cases} 1 & \text{if } \mathcal{S} \text{ is true} \\ 0 & \text{if } \mathcal{S} \text{ is false} \end{cases} \quad (\text{C.1})$$

For example,  $\delta(x, y) = \mathbb{1}(x = y)$ .

## C.4 One hot vector

A **one hot vector** is a vector with all entries equal to zero with the exception of a single entry which is one. A **one cold vector** is a vector with all entries equal to one with the exception of a single entry which is zero. For example, if  $x^n = (x_0, x_1, \dots, x_{n-1})$  and  $x_i = \delta(i, 0)$  then  $x^n$  is one hot.

Two types of sets that one frequently encounters are **categorical sets** (a.k.a. “nominal sets”, i.e., sets with “named” elements, with elements given a “nomme”) and **numerical sets** (a.k.a. “ordinal sets”, i.e., sets with “ordered” elements). For example,  $\{1, 2, 5\}$  is a numerical set because its elements have a natural order, and  $\{\text{cat, dog, bird}\}$  is a categorical set because its elements don’t have a natural order.

In Machine Learning (ML), one often encodes categorical sets as one-hot vectors. For example, suppose we have 4 binary registers (i.e., nodes)  $x_3, x_2, x_1, x_0$  and the categorical set  $\{\text{cat, dog, canary}\}$ . Then a possible **one-hot encoding** of the set is cat=0001, dog=0010 and canary=0100. This differs from a **binary encoding** of the set such as cat=0000, dog=0001, canary=0011. Clearly, a binary encoding requires fewer registers than a one-hot encoding to encode the same set, and the one-hot encoding of a set with  $n$  elements requires  $n$  or more registers.

## C.5 $L^p$ norm

For  $p \in [0, \infty]$  and  $\vec{x} \in \mathbb{R}^n$  or  $\vec{x} \in \mathbb{C}^n$  (note that  $n$  and  $p$  are generally not the same), the  $L^p$  **norm**  $\|\vec{x}\|_p$  of  $\vec{x}$  is defined as

$$\|\vec{x}\|_p = \left( \sum_{i=1}^n |x_i|^p \right)^{\frac{1}{p}} \quad (\text{C.2})$$

For example,

$$\|\vec{x}\|_0 = \sum_{i=1}^n \mathbb{1}(|x_i| > 0) = \text{number of non-zero } x_i \quad (\text{C.3})$$

$$\|\vec{x}\|_1 = \sum_{i=1}^n |x_i| \quad (\text{C.4})$$

$$\|\vec{x}\|_2 = \sqrt{\sum_{i=1}^n (x_i)^2} \quad (\text{C.5})$$

$$\|\vec{x}\|_3 = \left( \sum_{i=1}^n |x_i|^3 \right)^{\frac{1}{3}} \quad (\text{C.6})$$

$$\|\vec{x}\|_\infty = \lim_{p \rightarrow \infty} \|\vec{x}\|_p \quad (\text{C.7})$$

$$= \lim_{p \rightarrow \infty} ((\max_i |x_i|)^p)^{\frac{1}{p}} \quad (\text{because one } |x_i|^p \text{ dominates the rest}) \quad (\text{C.8})$$

$$= \max_i |x_i| \quad (\text{C.9})$$

Note that as  $\lim_{p \rightarrow 0} \|\vec{x}\|_p \neq \|\vec{x}\|_0$ . In fact, as  $p \rightarrow 0$ ,

$$\|\vec{x}\|_p \rightarrow (\text{number of non-zero } x_i)^{\frac{1}{p}} \quad (\text{because } |x|^0 = 1 \text{ for } x \neq 0) \quad (\text{C.10})$$

$$\rightarrow \|\vec{x}\|_0^{\frac{1}{p}} \rightarrow \infty \quad (\text{C.11})$$

When  $n$  is large and only a few of the  $n$  components of  $\vec{x} \in \mathbb{C}^n$  are non-zero, we say  $\vec{x}$  is **sparse**.  $\|\vec{x}\|_0$  is used to measure the **sparsity** of vectors.

Fig.C.1 shows the **unit balls**  $\{\vec{x} \in \mathbb{R}^n : \|\vec{x}\|_p \leq 1\}$  for various values of  $p$  and for  $n = 2$ .  $\{\vec{x} \in \mathbb{R}^2 : \|\vec{x}\|_0 \leq 1\}$  is not shown. It equals all the  $x$  and  $y$  axes, because, by definition, it contains all  $(x, y) \in \mathbb{R}^2$  such that  $x = 0$  or  $y = 0$  or both (i.e., 0 or 1 non-zero components).

$$\mathcal{C}_p = \{(x, y) \mid (|x|^p + |y|^p)^{1/p} \leq 1\}$$

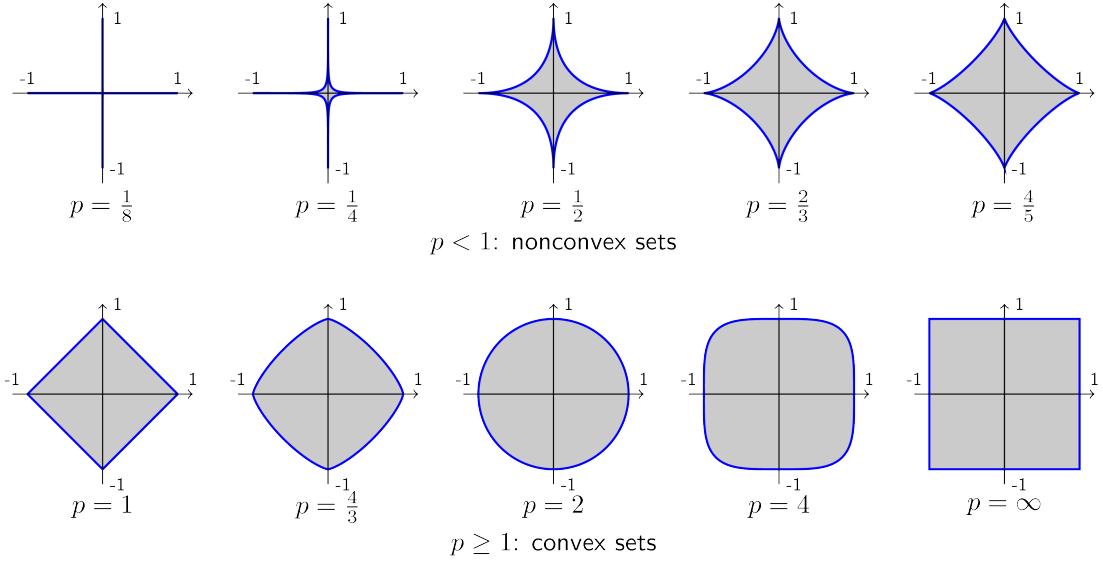


Figure C.1: Unit Balls  $\{\vec{x} \in \mathbb{R}^n : \|\vec{x}\|_p \leq 1\}$  for various values of  $p$  and for  $n = 2$ .

## C.6 Special sets

Define  $\mathbb{Z}, \mathbb{R}, \mathbb{C}$  to be the integers, real numbers and complex numbers, respectively.

For  $a < b$ , define  $\mathbb{Z}_I$  to be the integers in the interval  $I$ , where  $I = [a, b], [a, b), (a, b], (a, b)$  (i.e.,  $I$  can be closed or open on either side).

$$A_{>0} = \{k \in A : k > 0\} \text{ for } A = \mathbb{Z}, \mathbb{R}.$$

## C.7 Kronecker delta function

For  $x, y$  in discrete set  $S$ ,

$$\delta(x, y) = \begin{cases} 1 & \text{if } x = y \\ 0 & \text{if } x \neq y \end{cases} \quad (\text{C.12})$$

## C.8 Dirac delta function

For  $x, y \in \mathbb{R}$ ,

$$\int_{-\infty}^{+\infty} dx \delta(x - y) f(x) = f(y) \quad (\text{C.13})$$

## C.9 Majority function

The **majority function** is defined as follows.

$$\text{majority}(L) = \begin{array}{l} \text{most common element of list } L \\ \text{(ties resolved by chance)} \end{array} \quad (\text{C.14})$$

Note that the majority function acts on lists, not sets. By definition, all elements of a set appear only once in the set.  $\text{majority}(L)$  is usually used when the elements of  $L$  are categorical (i.e., not real numbers). When they are real numbers, it makes more sense to use, instead of  $\text{majority}(L)$ , a simple average of the elements of  $L$ .

## C.10 Underlined letters indicate random variables

Random variables will be indicated by underlined letters and their values by non-underlined letters. Each node of a bnet will be labelled by a random variable. Thus,  $\underline{x} = x$  means that node  $\underline{x}$  is in state  $x$ .

It is more conventional to use an upper case letter to indicate a random variable and a lower case letter for its state. Thus,  $X = x$  means that random variable  $X$  is in state  $x$ . However, we have opted in this book to avoid that notation, because we often want to define certain lower case letters to be random variables or, conversely, define certain upper case letters to be non-random variables.

## C.11 Probability distributions

$P_{\underline{x}}(x) = P(\underline{x} = x) = P(x)$  is the probability that random variable  $\underline{x}$  equals  $x \in S_{\underline{x}}$ .  $S_{\underline{x}}$  is the set of states (i.e., values) that  $\underline{x}$  can assume and  $n_{\underline{x}} = |S_{\underline{x}}|$  is the size (a.k.a. cardinality) of that set. Hence,

$$\sum_{x \in S_{\underline{x}}} P_{\underline{x}}(x) = 1 \quad (\text{C.15})$$

$$P_{\underline{x},y}(x,y) = P(\underline{x} = x, \underline{y} = y) = P(x,y) \quad (\text{C.16})$$

$$P_{\underline{x}|y}(x|y) = P(\underline{x} = x | \underline{y} = y) = P(x|y) = \frac{P(x,y)}{P(y)} \quad (\text{C.17})$$

## C.12 Discretization of continuous probability distributions

The TPM of a node of a bnet can be either a discrete or a continuous probability distribution. To go from continuous to discrete, one replaces integrals over states of a node by sums over new states, and Dirac delta functions by Kronecker delta functions. More precisely, consider a function  $f : [a, b] \rightarrow \mathbb{R}$ . Express  $[a, b]$  as a union of small, disjoint (except for one point) closed sub-intervals (bins) of length  $\Delta x$ . Name one point in each bin to be the representative of that bin, and let  $S_{\underline{x}}$  be the set of all the bin representatives. This is called discretization or binning. Then

$$\frac{1}{(b-a)} \int_{[a,b]} dx f(x) \rightarrow \frac{\Delta x}{(b-a)} \sum_{x \in S_{\underline{x}}} f(x) = \frac{1}{n_{\underline{x}}} \sum_{x \in S_{\underline{x}}} f(x) . \quad (\text{C.18})$$

Both sides of last equation are 1 when  $f(x) = 1$ . Furthermore, if  $y \in S_{\underline{x}}$ , then

$$\int_{[a,b]} dx \delta(x - y) f(x) = f(y) \rightarrow \sum_{x \in S_{\underline{x}}} \delta(x, y) f(x) = f(y) . \quad (\text{C.19})$$

As usual in this book, let  $S_{\underline{x}}$  denote the set of values that the random variable  $\underline{x}$  can take. When  $S_{\underline{x}} \subset \mathbb{R}$ , we will assume that  $S_{\underline{x}}$  for a probability distribution  $P(x)$  can be either a discrete or a continuous subset of  $\mathbb{R}$ .<sup>1</sup> When  $S_{\underline{x}}$  is a discrete subset of  $\mathbb{R}$ ,  $P(x)$  will denote a probability distribution for which  $\sum_{x \in S_{\underline{x}}} P(x) = 1$ , whereas when  $S_{\underline{x}}$  is continuous,  $P(x)$  will denote a probability density for which  $\int_{x \in S_{\underline{x}}} dx P(x) = 1$ .

<sup>1</sup>By a “continuous set” we mean a finite set of intervals each of which has non-zero length.

## C.13 Samples, i.i.d. variables

$$\vec{x} = (x[0], x[1], x[2] \dots, x[n_{sam}(\vec{x}) - 1]) = x[:] \quad (\text{C.20})$$

$n_{sam}(\vec{x})$  is the number of samples of  $\vec{x}$ .  $x[\sigma] \in S_{\underline{x}}$  are i.i.d. (independent identically distributed) samples with

$$x[\sigma] \sim P_{\underline{x}} \quad (\text{i.e. } P_{\underline{x}[\sigma]} = P_{\underline{x}}) \quad (\text{C.21})$$

$$P(\underline{x} = x) = \frac{1}{n_{sam}(\vec{x})} \sum_{\sigma} \mathbb{1}(x[\sigma] = x) \quad (\text{C.22})$$

Hence, for any  $f : S_{\underline{x}} \rightarrow \mathbb{R}$ ,

$$\sum_x P(\underline{x} = x) f(x) = \frac{1}{n_{sam}(\vec{x})} \sum_{\sigma} f(x[\sigma]) \quad (\text{C.23})$$

If we use two sampled variables, say  $\vec{x}$  and  $\vec{y}$ , in a given bnet, their number of samples  $n_{sam}(\vec{x})$  and  $n_{sam}(\vec{y})$  need not be equal.

---

$$P(\vec{x}) = \prod_{\sigma} P(x[\sigma]) \quad (\text{C.24})$$

$$\sum_{\vec{x}} = \prod_{\sigma} \sum_{x[\sigma]} \quad (\text{C.25})$$

$$\partial_{\vec{x}} = [\partial_{x[0]}, \partial_{x[1]}, \partial_{x[2]}, \dots, \partial_{x[n_{sam}(\vec{x})-1]}] \quad (\text{C.26})$$


---

$$P(\vec{x}) \approx [\prod_x P(x)^{P(x)}]^{n_{sam}(\vec{x})} \quad (\text{C.27})$$

$$= e^{n_{sam}(\vec{x}) \sum_x P(x) \ln P(x)} \quad (\text{C.28})$$

$$= e^{-n_{sam}(\vec{x}) H(P_{\underline{x}})} \quad (\text{C.29})$$

## C.14 Expected Value and Variance

Given a random variable  $\underline{x}$  with states  $S_{\underline{x}}$  and a function  $f : S_{\underline{x}} \rightarrow \mathbb{R}$ , define

$$E_{\underline{x}}[f(\underline{x})] = E_{x \sim P(x)}[f(x)] = \sum_x P(x) f(x) \quad (\text{C.30})$$

$$Var_{\underline{x}}[f(\underline{x})] = E_{\underline{x}}[(f(\underline{x}) - E_{\underline{x}}[f(\underline{x})])^2] \quad (\text{C.31})$$

$$= E_{\underline{x}}[f(\underline{x})^2] - (E_{\underline{x}}[f(\underline{x})])^2 \quad (\text{C.32})$$

$$E[\underline{x}] = E_{\underline{x}}[\underline{x}] \quad (\text{C.33})$$

$$Var[\underline{x}] = Var_{\underline{x}}[\underline{x}] \quad (\text{C.34})$$

## C.15 Conditional Expected Value

Given a random variable  $\underline{x}$  with states  $S_{\underline{x}}$ , a random variable  $\underline{y}$  with states  $S_{\underline{y}}$ , and a function  $f : S_{\underline{x}} \times S_{\underline{y}} \rightarrow \mathbb{R}$ , define

$$E_{\underline{x}|\underline{y}}[f(\underline{x}, \underline{y})] = \sum_x P(x|\underline{y}) f(x, \underline{y}), \quad (\text{C.35})$$

$$E_{\underline{x}|\underline{y}=y}[f(\underline{x}, y)] = E_{\underline{x}|y}[f(\underline{x}, y)] = \sum_x P(x|y) f(x, y). \quad (\text{C.36})$$

Note that

$$E_{\underline{y}}[E_{\underline{x}|\underline{y}}[f(\underline{x}, \underline{y})]] = \sum_{x,y} P(x|y) P(y) f(x, y) \quad (\text{C.37})$$

$$= \sum_{x,y} P(x, y) f(x, y) \quad (\text{C.38})$$

$$= E_{\underline{x}, \underline{y}}[f(\underline{x}, \underline{y})]. \quad (\text{C.39})$$

## C.16 Notation for covariances

Consider two random variables  $\underline{x}, \underline{y}$ .

- Mean value of  $\underline{x}$

$$\langle \underline{x} \rangle = E_{\underline{x}}[\underline{x}] \quad (\text{C.40})$$

- Signed distance of  $\underline{x}$  to its mean value

$$\Delta \underline{x} = \underline{x} - \langle \underline{x} \rangle \quad (\text{C.41})$$

- Covariance of  $(\underline{x}, \underline{y})$

$$Cov(\underline{x}, \underline{y}) = \langle \underline{x}, \underline{y} \rangle = \langle \Delta \underline{x} \Delta \underline{y} \rangle = \langle \underline{x} \underline{y} \rangle - \langle \underline{x} \rangle \langle \underline{y} \rangle \quad (\text{C.42})$$

$\langle \underline{x}, \underline{y} \rangle$  is symmetric (i.e.,  $\langle \underline{x}, \underline{y} \rangle = \langle \underline{y}, \underline{x} \rangle$ ) and bilinear (i.e.,  $\langle \sum_i \alpha_i \underline{x}_i, \underline{y} \rangle = \sum_i \alpha_i \langle \underline{x}_i, \underline{y} \rangle$ , where  $\alpha_i \in \mathbb{R}$  are non-random scalars and  $\underline{x}_i, \underline{y} \in \mathbb{R}$  are real-valued random variables.)

- Variance of  $\underline{x}$

$$Var(\underline{x}) = \langle \underline{x}, \underline{x} \rangle \quad (\text{C.43})$$

- Standard deviation or  $\underline{x}$

$$\sigma_{\underline{x}} = \sqrt{\langle \underline{x}, \underline{x} \rangle} \quad (\text{C.44})$$

- Correlation Coefficient of  $(\underline{x}, \underline{y})$

$$\rho_{\underline{x}, \underline{y}} = \frac{\langle \underline{x}, \underline{y} \rangle}{\sqrt{\langle \underline{x}, \underline{x} \rangle \langle \underline{y}, \underline{y} \rangle}} \quad (\text{C.45})$$

- Partial derivative of  $\underline{y}$  wrt (i.e., with respect to)  $\underline{x}$

$$\partial_{\underline{x}} \underline{y} = \frac{\partial \underline{y}}{\partial \underline{x}} = \frac{\langle \underline{x}, \underline{y} \rangle}{\langle \underline{x}, \underline{x} \rangle} = \rho_{\underline{x}, \underline{y}} \frac{\sigma_y}{\sigma_x} \quad (\text{C.46})$$

## C.17 Conditional Covariance

Let  $\underline{x}, \underline{y}, \underline{a}$  be random variables. The covariance  $Cov(\underline{x}, \underline{y} | \underline{a} = a)$  of  $\underline{x}$  and  $\underline{y}$  given  $\underline{a} = a$ , is defined the same way as  $Cov(\underline{x}, \underline{y})$ , except that all expected values are conditioned on  $\underline{a} = a$ .

$$Cov(\underline{x}, \underline{y} | \underline{a} = a) = \langle \underline{x}, \underline{y} \rangle^{|a} = \left\langle (\underline{x} - \langle \underline{x} \rangle^{|a})(\underline{y} - \langle \underline{y} \rangle^{|a}) \right\rangle^{|a} \quad (\text{C.47})$$

where

$$\langle \underline{x} \rangle^{|a} = E_{\underline{x}|a}[\underline{x}] . \quad (\text{C.48})$$

In this book, we will use the following notation for conditional averages. For any random variables  $\underline{x}, \underline{y}, \underline{a}$ , let

$$E_a[\underline{x}] = \langle \underline{x} \rangle^{|a} \quad (\text{mean}) \quad (\text{C.49})$$

$$\langle \underline{x}, \underline{y} \rangle^{|a} = \langle \underline{x} \underline{y} \rangle^{|a} - \langle \underline{x} \rangle^{|a} \langle \underline{y} \rangle^{|a} \quad (\text{covariance}) \quad (\text{C.50})$$

$$\sigma_{\underline{x}}^{|a} = \sqrt{\langle \underline{x}, \underline{x} \rangle^{|a}} \quad (\text{standard deviation}) \quad (\text{C.51})$$

$$\rho_{\underline{x}, \underline{y}}^{|a} = \frac{\langle \underline{x}, \underline{y} \rangle^{|a}}{\sigma_{\underline{x}}^{|a} \sigma_{\underline{y}}^{|a}} = \left[ \frac{\langle \underline{x}, \underline{y} \rangle}{\sigma_{\underline{x}} \sigma_{\underline{y}}} \right]^{|a} \quad (\text{correlation}) \quad (\text{C.52})$$

$$\partial_{\underline{x}}^{|a} \underline{y} = \left[ \frac{\partial}{\partial \underline{x}} \right]^{|a} \underline{y} = \frac{\langle \underline{x}, \underline{y} \rangle^{|a}}{\langle \underline{x}, \underline{x} \rangle^{|a}} = \rho_{\underline{x}, \underline{y}}^{|a} \frac{\sigma_{\underline{y}}^{|a}}{\sigma_{\underline{x}}^{|a}} = \left[ \rho_{\underline{x}, \underline{y}} \frac{\sigma_{\underline{y}}}{\sigma_{\underline{x}}} \right]^{|a} \quad (\text{partial derivative}) \quad (\text{C.53})$$

“ $|a$ ” means that the variable  $\underline{a}$  is held fixed to  $a$  when taking all averages.

## C.18 Normal Distribution

For  $x, \mu, \sigma \in \mathbb{R}$ ,  $\sigma > 0$ , we define the Normal Distribution (see Fig.C.2) by

$$\mathcal{N}(x; \mu, \sigma^2) = \frac{1}{\sigma\sqrt{2\pi}} e^{-\frac{1}{2}\left(\frac{x-\mu}{\sigma}\right)^2}. \quad (\text{C.54})$$

For a **standard deviation**  $\sigma$ , the **precision**  $\tau$  is defined as  $\tau = \frac{1}{\sigma^2}$ .

**Claim 1** *If*

$$\underline{x}_1 \sim \mathcal{N}(\mu_1, \sigma_1^2) \quad (\text{C.55})$$

and

$$\underline{x}_2 \sim \mathcal{N}(\mu_2, \sigma_2^2) \quad (\text{C.56})$$

then

$$\underline{x} = \underline{x}_1 + \underline{x}_2 \sim \mathcal{N}(\mu_1 + \mu_2, \sigma_1^2 + \sigma_2^2). \quad (\text{C.57})$$

**proof:**

$$P(\underline{x} = x) = \mathcal{N}(!x) \int_{-\infty}^{+\infty} dx_2 P(\underline{x}_1 + \underline{x}_2 = x | \underline{x}_2 = x_2) P(x_2) \quad (\text{C.58})$$

$$= \mathcal{N}(!x) \int_{-\infty}^{+\infty} dx_2 \mathcal{N}(x - x_2; \mu_1, \sigma_1^2) \mathcal{N}(x_2; \mu_2, \sigma_2^2) \quad (\text{C.59})$$

$$= \mathcal{N}(x; \mu_1 + \mu_2; \sigma_1^2 + \sigma_2^2) \quad (\text{C.60})$$

**QED**

The **Standard Normal Distribution**  $P_{SND}(x)$  and its cumulative distribution  $\Phi(x)$  are defined by

$$P_{SND}(x) = \mathcal{N}(x; \mu = 0, \sigma = 1) \quad (\text{C.61})$$

$$\Phi(x) = \int_{-\infty}^x dx' P_{SND}(x') \quad (\text{C.62})$$

The **error function**  $\text{erf} : \mathbb{R} \rightarrow [-1, 1]$  is defined by

$$\text{erf}(x) = \frac{2}{\sqrt{\pi}} \int_0^x du e^{-\frac{u^2}{2}} \quad (\text{C.63})$$

Note that

$$\Phi(x) = \frac{1}{2} + \frac{1}{2}\text{erf}(x) \quad (\text{C.64})$$

Eq.(C.64) is interpreted geometrically in Fig.C.3.

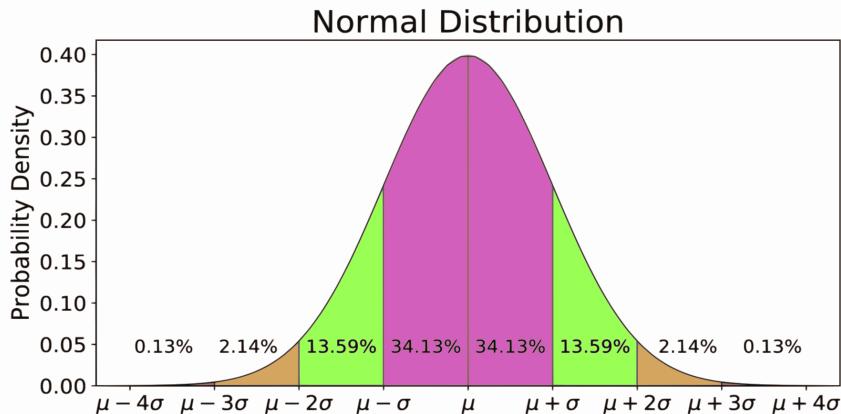


Figure C.2: Normal Distribution  $\mathcal{N}(x; \mu, \sigma^2)$ .

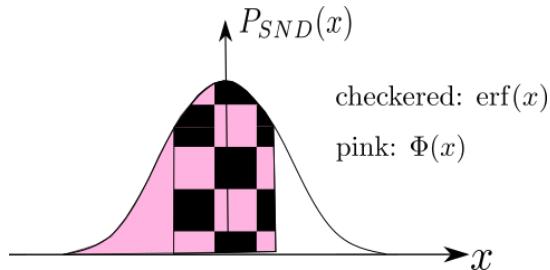


Figure C.3: Plot of Standard Normal Distribution  $P_{SND}(x)$ . Values of  $\text{erf}(x)$  and  $\Phi(x)$  equal indicated areas.

## C.19 Uniform Distribution

For  $a < b$ ,  $x \in [a, b]$

$$\mathcal{U}(x; a, b) = \frac{1}{b - a} \quad (\text{C.65})$$

## C.20 Softmax function (a.k.a. Boltzmann Distribution)

The Softmax function is defined by

$$P(x_i | x.) = \frac{e^{x_i}}{\sum_i e^{x_i}} = \text{softmax}(x.)(i) \quad (\text{C.66})$$

The Boltzmann distribution is defined as

$$P(\underline{E}_a = E_a) = \frac{\exp(-\frac{E_a}{kT})}{\sum_a \exp(-\frac{E_a}{kT})} = P(\frac{-E_a}{kT} | E.) \quad (\text{C.67})$$

for a system with energies  $E_a$  and temperature  $T$ , where  $k$  is Boltzmann's constant.

The function softmax() is called softmax because if we approximate the exponentials, both in the numerator and denominator of Eq.(C.66), by the largest one of them or zero, we get

$$\text{softmax}(x.)(i) \approx \delta(i, \underset{k}{\operatorname{argmax}} x_k) . \quad (\text{C.68})$$

Thus, softmax( $x.$ )( $i$ ) returns a continuous function that approximates a Kronecker delta function. The softmax function doesn't really return the soft maximum of a finite set, so its name is a bit of a misnomer. A better name for it would have been "soft Kronecker delta function".

Note that

$$\frac{\partial \ln P(x_i|x)}{\partial x_a} = \frac{\partial}{\partial x_a} \ln \left[ \frac{e^{x_i}}{\sum_i e^{x_i}} \right] = \delta(a, i) - P(x_a|x) \quad (\text{C.69})$$

For 2 variables  $x_0, x_1$ ,

$$P(x_0|x.) = \frac{e^{x_0}}{e^{x_0} + e^{x_1}} \quad (\text{C.70})$$

$$= \text{smoid}(x_0 - x_1) , \quad (\text{C.71})$$

$$P(x_1|x.) = \text{smoid}(x_1 - x_0) . \quad (\text{C.72})$$

## C.21 Sigmoid and log-odds functions

The **sigmoid (a.k.a. exp-it, logistic) function** smoid: $\mathbb{R} \rightarrow [0, 1]$  is defined by

$$\text{smoid}(x) = \frac{1}{1 + e^{-x}} \quad (\text{C.73})$$

smoid() is monotonically increasing with  $\text{smoid}(-\infty) = 0$ ,  $\text{smoid}(0) = 1/2$  and  $\text{smoid}(+\infty) = 1$ . Note that for  $x \ll 0$ ,  $\text{smoid}(x) \approx e^x$ , which is why "smoid" is also called "expit".

$$\text{smoid}(x) + \text{smoid}(-x) = \frac{1}{1 + e^{-x}} + \frac{1}{1 + e^x} \quad (\text{C.74})$$

$$= \frac{2 + e^x + e^{-x}}{2 + e^x + e^{-x}} \quad (\text{C.75})$$

$$= 1 \quad (\text{C.76})$$

The **log-odds (a.k.a. log-it) function**  $\text{lodds}:[0, 1] \rightarrow \mathbb{R}$  is defined by

$$\text{lodds}(p) = \ln \frac{p}{1-p} \quad (\text{C.77})$$

Note that for  $0 < p \ll 1$ ,  $\text{lodds}(x) \approx \ln p$ , which is why "lodds" is also called "logit".

Note that for  $x \ll 1$ ,  $\text{smoid}(x) \approx e^x \ll 1$ , so  $\text{lodds}(e^x) \approx \ln(e^x) = x$ . More generally, it is easy to check that for any  $p \in [0, 1]$  and  $x \in \mathbb{R}$ ,

$$\text{lodds}[\text{smoid}(x)] = x \quad (\text{C.78})$$

$$\text{smoid}[\text{lodds}(p)] = p \quad (\text{C.79})$$

Hence,  $\text{lodds}()$  is the inverse of  $\text{smoid}()$  and vice-versa.

### Claim 2

$$\text{smoid}'(x) = \text{smoid}(x)[1 - \text{smoid}(x)] \quad (\text{C.80})$$

$$\text{smoid}''(x) = \text{smoid}'(x)[1 - 2\text{smoid}(x)] \quad (\text{C.81})$$

#### proof:

In this proof, we will abbreviate  $\text{smoid}(x)$  by  $s(x)$ .

$$1 - s(x) = 1 - \frac{1}{1 + e^{-x}} = \frac{e^{-x}}{1 + e^{-x}} \quad (\text{C.82})$$

$$s'(x) = \frac{e^{-x}}{(1 + e^{-x})^2} = s(x)[1 - s(x)] \quad (\text{C.83})$$

$$s''(x) = s'(x)[1 - s(x)] + s(x)(-1)s'(x) \quad (\text{C.84})$$

$$= s'(x)[1 - 2s(x)] \quad (\text{C.85})$$

$$= s(x)[1 - s(x)][1 - 2s(x)] \quad (\text{C.86})$$

**QED**

## C.22 Estimand, Estimator (curve-fit), Estimate, Bias

For an **estimand**  $\theta$ , an **estimator (a.k.a. curve-fit)**  $\hat{\theta}$  gives **estimate**  $E[\hat{\theta}(\theta)] = \theta + b$  with **bias**  $b$ . We say this estimate is an **unbiased estimate** if  $b = 0$ .

Note that, strictly speaking, an estimator is a function waiting to be averaged over and denoted by a letter with a hat, whereas an estimate is a real number denoted

by a letter without a hat. Unfortunately, the words “estimator” and “estimate” are often used interchangeably, as if they were synonyms. And often the estimate  $\theta + b$  is denoted by a letter with a hat too. In some sense, an estimator is an estimate of a curve, so it’s understandable that the terms “estimator” and “estimate” are used synonymously. In this book, we will bow to traditional practice and also use the terms “estimator” and “estimate” synonymously, and use a letter with a hat to denote either of them. This is not ambiguous as long as we don’t use the same letter with a hat to denote two different quantities, of course. When we need to distinguish semantically between the real value and the function, we will call the function a curve-fit, and the real value the estimate.

## C.23 Maximum Likelihood Estimate, Likelihood Ratio Test

Given a bnet, let  $P(x|\theta)$  be its full joint probability distribution, where  $x$  denotes the joint state of all the nodes and  $\theta$  denotes all the parameters.  $P(x|\theta)$  is often called the **likelihood function of  $\theta$**  and is denoted by

$$L(\theta) = P(x|\theta) \quad (\text{C.87})$$

It’s called a likelihood of  $\theta$  because, even though it’s a probability, it isn’t the probability of  $\theta$ , but rather of  $x$ .

The value of  $\theta$  that we obtain by maximizing  $L(\theta)$  over  $\theta$  is called the **maximum likelihood estimate (MLE) of  $\theta$** . Let us denote it by  $\hat{\theta}$ . Note that<sup>2</sup>

$$\sup_{\theta \in S} L(\theta) = L(\hat{\theta}) \quad (\text{C.88})$$

Let  $S_0, S_1$  be disjoint sets such that  $S = S_0 \cup S_1$ . We’ll say the **null hypothesis**  $H_0$  holds if  $\theta \in S_0$ , and the **alternative hypothesis**  $H_1$  holds if  $\theta \in S_1$ . The **likelihood ratio (LR) test statistic** is defined by

$$R = -2 \ln \left( \frac{\sup_{\theta \in S_0} L(\theta)}{\sup_{\theta \in S} L(\theta)} \right) \quad (\text{C.89})$$

$R \geq 0$  and  $R = 0$  if  $S_0 = S$ . For some small  $c > 0$ , if  $R < c$ , then we reject the alternative hypothesis, and if  $R > c$ , we accept it.

If  $S_0 = \{\theta_0\}$ , then

$$R = -2[\ln L(\theta_0) - \ln L(\hat{\theta})] \quad (\text{C.90})$$

---

<sup>2</sup>“sup” stands for supremum. It’s a generalization of the function `max()` to arbitrary sets that might not be discrete or finite. If  $S$  is a finite set, then  $\sup_{\theta \in S} f(\theta) = \max_{\theta \in S} f(\theta)$  for any function  $f : S \rightarrow \mathbb{R}$ . Likewise, “inf” stands for infimum, and it generalizes the `min()` function.

## C.24 Mean Square Error (MSE)

Suppose we are given  $nsam$  samples  $y^\sigma \in \mathbb{R}$  labeled by an index  $\sigma$ , and a curve-fit  $\hat{y}^\sigma(a) \in \mathbb{R}$  that depends on a parameter  $a \in \mathbb{R}$ . Define the **Mean Square Error (MSE)** by

$$MSE(a) = \frac{1}{nsam} \sum_{\sigma} (y^\sigma - \hat{y}^\sigma(a))^2. \quad (\text{C.91})$$

For example, in Linear Regression (LR), we have  $\hat{y}^\sigma = a_0 + a_1 x^\sigma$  where  $a = (a_0, a_1)$  is a deterministic parameter. If the samples  $y^\sigma$  are i.i.d, then we can also write

$$MSE(a) = E_{|a}[(\underline{y} - \hat{y}(a))^2]. \quad (\text{C.92})$$

and for LR,  $\hat{y}(a) = a_0 + a_1 \underline{x}$ .

Define the **residual**  $\Delta\underline{y}$  by:

$$\Delta\underline{y}(a) = \underline{y} - \hat{y}(a) \quad (\text{Hence } \underline{y} = \hat{y} + \Delta\underline{y}) \quad (\text{C.93})$$

In the rest of this section, we will discuss the case that  $\hat{y}^\sigma(a)$  is independent of  $x^\sigma$ . I call this the **deterministic MSE (D-MSE)** model. Note that this is different from the LR case where  $\hat{y}^\sigma(a)$  does depend on  $x^\sigma$ . In LR, we are trying to fit a line to a cigar-shaped 2-D scatter plot. Here, we are just trying to estimate the mean value (center of mass) of a scatter plot.

**Claim 3** *MSE is minimized over all functions  $\hat{y}$  if*

$$\hat{y} = E_{|a}[\underline{y}] \quad (\text{C.94})$$

**proof:**

$$MSE = E_{|a}[\underline{y}^2] - 2\hat{y}E_{|a}[\underline{y}] + \hat{y}^2 \quad (\text{C.95})$$

$$0 = \frac{d}{d\hat{y}} MSE = 2(-E_{|a}[\underline{y}] + \hat{y}) \quad (\text{C.96})$$

Hence,

$$\hat{y} = E_{|a}[\underline{y}] \quad (\text{C.97})$$

**QED**

Sometimes, we will use the notation

$$\hat{y}_{MSE} = E_{|a=a_{MSE}}[\underline{y}]. \quad (\text{C.98})$$

**Claim 4** Suppose  $f(a)$  is a function of  $a$ . If  $\hat{y} = E_{|a}[\underline{y}]$ , then

$$E_{|a}[\Delta\underline{y}] = E[\Delta\underline{y}] = 0 \quad (\text{C.99})$$

$$E_{|a} [\Delta\underline{y}f(\underline{a})] = E [\Delta\underline{y}f(\underline{a})] = 0 \quad (\text{C.100})$$

**proof:**

$$E_{|a}[\Delta\underline{y}] = E_{|a} [y - E_{|a}[\underline{y}]] = E_{|a}[y] - E_{|a}[\underline{y}] = 0 \quad (\text{C.101})$$

$$E[\Delta\underline{y}] = E_{\underline{a}}[E_{|\underline{a}}[\Delta\underline{y}]] = 0 \quad (\text{C.102})$$

$$E_{|\underline{a}} [\Delta\underline{y}f(\underline{a})] = f(\underline{a}) \underbrace{E_{|\underline{a}}[\Delta\underline{y}]}_{=0} \quad (\text{C.103})$$

$$E[\Delta\underline{y}f(\underline{a})] = E_{\underline{a}}[E_{|\underline{a}}[\Delta\underline{y}f(\underline{a})]] = 0 \quad (\text{C.104})$$

**QED**

**Claim 5** If  $\hat{y} = E_{|a}[\underline{y}]$ , then

$$\langle \Delta\underline{y}, \hat{y} \rangle_{|a} = 0 \quad (\text{C.105})$$

$$Var_{|a}[\underline{y}] = Var_{|a}[\hat{y}] + Var_{|a}[\Delta\underline{y}] \quad (\text{C.106})$$

The same results hold without the conditioning on  $a$ .

**proof:**

$$\langle \Delta\underline{y}, \hat{y} \rangle_{|a} = \underbrace{E_{|a}[\Delta\underline{y} \underbrace{\hat{y}}_{f(\underline{a})}]}_{=0} - \underbrace{E_{|a}[\Delta\underline{y}] E_{|a}[\hat{y}]}_{=0} \quad (\text{C.107})$$

$$Var_{|a}[\underline{y}] = \langle \hat{y} + \Delta\underline{y}, \hat{y} + \Delta\underline{y} \rangle_{|a} \quad (\text{C.108})$$

$$= \langle \hat{y}, \hat{y} \rangle_{|a} + \langle \Delta\underline{y}, \Delta\underline{y} \rangle_{|a} \quad (\text{by Eq.(C.105)}) \quad (\text{C.109})$$

$$= Var_{|a}[\hat{y}] + Var_{|a}[\Delta\underline{y}] \quad (\text{C.110})$$

The same proof holds if we remove all the  $|a$  subscripts.

**QED**

Fig.C.4 illustrates how  $\underline{y} = \hat{y} + \Delta\underline{y}$  and the variances of these quantities add.

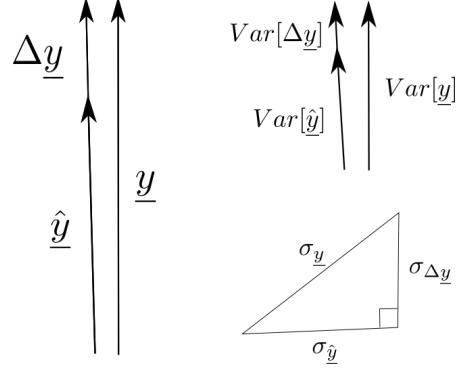


Figure C.4:  $\underline{y} = \hat{y} + \Delta\underline{y}$  and the variances (not standard deviations) of these quantities add.

## C.25 Cramer-Rao Bound

This discussion of the Cramer-Rao (CR) bound is based on Ref.[105].

Suppose  $\underline{x}$  is a random variable with values  $x \in S_{\underline{x}}$  and  $\theta \in \mathbb{R}$  is a parameter. For any function  $f_{\underline{x},\theta} : S_{\underline{x}} \times \mathbb{R} \rightarrow \mathbb{R}$ , define

$$\langle f_{\underline{x},\theta} \rangle = \sum_x P(x|\theta) f_{x,\theta} \quad (\text{C.111})$$

$$\Delta f_{\underline{x},\theta} = f_{\underline{x},\theta} - \langle f_{\underline{x},\theta} \rangle \quad (\text{C.112})$$

$$\langle f_{\underline{x},\theta}, f_{\underline{x},\theta} \rangle = \langle \Delta f_{\underline{x},\theta} \Delta f_{\underline{x},\theta} \rangle \quad (\text{C.113})$$

Define the **log likelihood function** by

$$LL_\theta = \ln P(x|\theta) \quad (\text{C.114})$$

Define the **Fisher information** by

$$I_\theta = \langle \partial_\theta LL_\theta, \partial_\theta LL_\theta \rangle \quad (\text{C.115})$$

Note that  $LL_\theta \leq 0$ . Let  $\theta^*$  be the value of  $\theta$  that maximizes  $LL_\theta$ .

Note that  $I_\theta \geq 0$  and  $I_\theta = 0$  when  $\theta = \theta^*$  because  $\partial_\theta LL_\theta|_{\theta=\theta^*} = 0$ . This suggests that  $I_\theta$  measures the distance between  $\theta$  and  $\theta^*$ .

Note that

$$\langle \partial_\theta LL_\theta \rangle = \sum_x P(x|\theta) \frac{1}{P(x|\theta)} \partial_\theta P(x|\theta) \quad (\text{C.116})$$

$$= \partial_\theta \sum_x P(x|\theta) \quad (\text{C.117})$$

$$= 0 \quad (\text{C.118})$$

Therefore

$$I_\theta = \langle [\partial_\theta LL_\theta]^2 \rangle - \langle \partial_\theta LL_\theta \rangle^2 \quad (\text{C.119})$$

$$= \langle [\partial_\theta LL_\theta]^2 \rangle \quad (\text{C.120})$$

**Claim 6**

$$I_\theta = -\langle \partial_\theta^2 LL_\theta \rangle \quad (\text{C.121})$$

**proof:**

$$I_\theta = \langle [\partial_\theta LL_\theta]^2 \rangle \quad (\text{C.122})$$

$$= \sum_x P(x|\theta) \frac{1}{P(x|\theta)} \partial_\theta P(x|\theta) \partial_\theta \ln P(x|\theta) \quad (\text{C.123})$$

$$= -\sum_x P(x|\theta) \partial_\theta^2 \ln P(x|\theta) + \partial_\theta \sum_x P(x|\theta) \partial_\theta \ln P(x|\theta) \quad (\text{C.124})$$

$$= -\langle \partial_\theta^2 LL_\theta \rangle + \partial_\theta^2 \sum_x P(x|\theta) \quad (\text{C.125})$$

$$= -\langle \partial_\theta^2 LL_\theta \rangle \quad (\text{C.126})$$

**QED**

**Claim 7** If  $x = [x_i]_{i=1,2,\dots,\nu} \in \mathbb{R}^\nu$  are i.i.d., then

$$I_\theta = \nu \langle [\partial_\theta LL_{\theta,i}]^2 \rangle \quad (\text{C.127})$$

where

$$LL_{\theta,i} = \ln P(x_i|\theta) \quad (\text{C.128})$$

**proof:**

$$LL_\theta = \ln \prod_i P(x_i|\theta) \quad (\text{C.129})$$

$$= \sum_i LL_{\theta,i} \quad (\text{C.130})$$

$$I_\theta = \sum_i \sum_j \langle \partial_\theta LL_{\theta,i} \partial_\theta LL_{\theta,j} \rangle \quad (\text{C.131})$$

$$= \sum_i \langle [\partial_\theta LL_{\theta,i}]^2 \rangle \quad (\text{C.132})$$

$$= \nu \langle [\partial_\theta LL_{\theta,i}]^2 \rangle \quad (\text{C.133})$$

**QED**

A function  $t_{\underline{x}} : S_{\underline{x}} \rightarrow \mathbb{R}$  is called a **test statistic** of random variable  $\underline{x}$ .

**Claim 8** (*Cramer-Rao bound for single parameter  $\theta \in \mathbb{R}$* )

$$\langle t_{\underline{x}}, t_{\underline{x}} \rangle I_{\theta} \geq [\partial_{\theta} \langle t_{\underline{x}} \rangle]^2 \quad (\text{C.134})$$

**proof:**

Cauchy-Schwartz inequality

For two vectors  $\vec{a}, \vec{b} \in \mathbb{R}^n$ :

$$\vec{a} \cdot \vec{b} = |\vec{a}| |\vec{b}| \cos \phi \leq |\vec{a}| |\vec{b}| \quad (\text{C.135})$$

For two real valued random variables  $\underline{a}, \underline{b}$ :

$$\langle \underline{a}, \underline{a} \rangle \langle \underline{b}, \underline{b} \rangle \geq |\langle \underline{a}, \underline{b} \rangle|^2 \quad (\text{C.136})$$

Replace

$$\underline{a} \rightarrow t_{\underline{x}}, \quad \underline{b} \rightarrow \partial_{\theta} LL_{\theta} \quad (\text{C.137})$$

Then

$$\langle t_{\underline{x}}, \partial_{\theta} LL_{\theta} \rangle = \langle t_{\underline{x}} \partial_{\theta} LL_{\theta} \rangle - \underbrace{\langle t_{\underline{x}} \rangle}_{=0} \langle \partial_{\theta} LL_{\theta} \rangle \quad (\text{C.138})$$

$$= \sum_x P(x|\theta) t_{\underline{x}} \frac{1}{P(x|\theta)} \partial_{\theta} P(x|\theta) \quad (\text{C.139})$$

$$= \partial_{\theta} \sum_x t_{\underline{x}} P(x|\theta) \quad (\text{C.140})$$

$$= \partial_{\theta} \langle t_{\underline{x}} \rangle \quad (\text{C.141})$$

**QED**

See Fig.C.5 for a pictorial representation of Eq.(C.134).

Now suppose the test statistic  $t_{\underline{x}}$  equals an **estimator**  $\hat{\theta}$  of  $\theta$  with bias  $b_{\underline{x}}$  :  $S_{\underline{x}} \rightarrow \mathbb{R}$ .

$$t_{\underline{x}} = \hat{\theta}(\underline{x}) = \theta + b_{\underline{x}} \quad (\text{C.142})$$

$\hat{\theta}$  is said to be a **biased estimator** if  $b_{\underline{x}} \neq 0$  and an **unbiased estimator** if  $b_{\underline{x}} = 0$ .

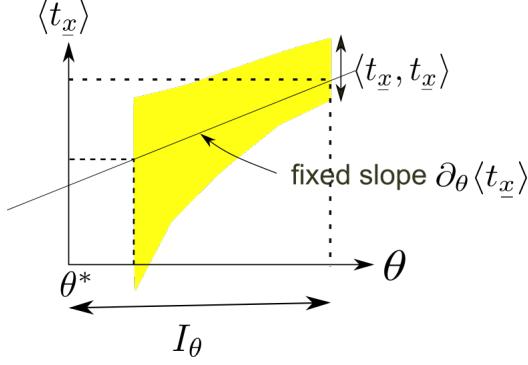


Figure C.5: In this drawing,  $\theta^*$  is the value of  $\theta$  that maximizes  $LL_\theta$ . According to the CR bound, the product of the variance  $\langle t_{\underline{x}}, t_{\underline{x}} \rangle$  and the distance  $I_\theta$  must be greater or equal to  $[\partial_\theta \langle t_{\underline{x}} \rangle]^2$ . At fixed  $[\partial_\theta \langle t_{\underline{x}} \rangle]^2$ , if the variance increases, the distance decreases, and vice versa.

**Claim 9**

$$\langle \widehat{\theta} \rangle = \theta + \langle b_{\underline{x}} \rangle \quad (\text{C.143})$$

$$\langle \widehat{\theta}, \widehat{\theta} \rangle \geq \frac{[1 + \partial_\theta \langle b_{\underline{x}} \rangle]^2}{I_\theta} \quad (\text{C.144})$$

$$\langle [\widehat{\theta} - \theta]^2 \rangle \geq \frac{[1 + \partial_\theta \langle b_{\underline{x}} \rangle]^2}{I_\theta} + \langle b_{\underline{x}} \rangle^2 \quad (\text{C.145})$$

**proof:**

$$\partial_\theta \langle t_{\underline{x}} \rangle = \partial_\theta \langle \theta + b_{\underline{x}} \rangle \quad (\text{C.146})$$

$$= \partial_\theta [\theta + \langle b_{\underline{x}} \rangle] \quad (\text{C.147})$$

$$= 1 + \partial_\theta \langle b_{\underline{x}} \rangle \quad (\text{C.148})$$

Eq.(C.144) follows from Eq.(C.134) once we replace  $t_{\underline{x}}$  by  $\widehat{\theta}$ .

Let

$$\Delta\widehat{\theta} = \widehat{\theta} - \langle \widehat{\theta} \rangle = \underbrace{(\widehat{\theta} - \theta)}_{\xi} - \langle b_{\underline{x}} \rangle \quad (\text{C.149})$$

Then

$$0 = \langle \Delta\widehat{\theta} \rangle = \langle \xi \rangle - \langle b_{\underline{x}} \rangle \quad (\text{C.150})$$

$$\frac{[1 + \partial_\theta \langle b_{\underline{x}} \rangle]^2}{I_\theta} \leq \langle [\Delta\widehat{\theta}]^2 \rangle \quad (\text{C.151})$$

$$= \langle \xi^2 - 2\xi \langle b_{\underline{x}} \rangle + \langle b_{\underline{x}} \rangle^2 \rangle \quad (\text{C.152})$$

$$= \langle \xi^2 \rangle - \langle b_{\underline{x}} \rangle^2 \quad (\text{C.153})$$

**QED**

Multi-dimensional case: parameter  $\theta = [\theta_1, \theta_2, \dots, \theta_n]^T \in \mathbb{R}^n$  and test statistic  $t_{\underline{x}} = [t_{\underline{x},1}, t_{\underline{x},2}, \dots, t_{\underline{x},n}]^T \in \mathbb{R}^n$  are column vectors.

Define **Fisher information matrix** by

$$[I_\theta]_{i,j} = \langle \partial_{\theta_i} LL_\theta, \partial_{\theta_j} LL_\theta \rangle = \langle \partial_{\theta_i} LL_\theta \partial_{\theta_j} LL_\theta \rangle \quad (\text{C.154})$$

CR bound for multi-dimensional parameter  $\theta \in \mathbb{R}^n$ :

$$\text{matrix} [\langle t_{\underline{x},i}, t_{\underline{x},j} \rangle] \geq \text{matrix} [\partial_{\theta_i} \langle t_{\underline{x},a} \rangle [I_\theta]_{a,b}^{-1} \partial_{\theta_j} \langle t_{\underline{x},b} \rangle] \quad (\text{C.155})$$

where we are using the Einstein summation convention (repeated indices are summed over). For two matrices  $A, B \in \mathbb{R}^n$ ,  $A \geq B$  means  $A - B$  has non-negative eigenvalues.

## C.26 Bayes Rule, Bayesian Updating And Conjugate Priors

Bayes Rule says:

$$P(\theta|x)P(x) = P(x|\theta)P(\theta) \quad (\text{C.156})$$

Expressed diagrammatically<sup>3</sup>, we have for  $\underline{x} \in \mathbb{R}$ :

$$\underline{\theta} \xleftarrow{} \underline{x} = \underline{\theta} \xrightarrow{} \underline{x} \quad (\text{C.157})$$

and for  $\underline{x} = (x_1, \underline{x}_2) \in \mathbb{R}^2$ :

$$\begin{array}{ccc} \begin{array}{c} \theta \\ \swarrow \quad \searrow \\ x_1 \\ \downarrow \\ x_2 \end{array} & = & \begin{array}{c} \theta \\ \swarrow \quad \searrow \\ x_1 \\ \downarrow \\ x_2 \end{array} \end{array} \quad (\text{C.158})$$

Note how Bayes rule allows us to reverse the direction of the arrows impinging on  $\theta$ . We see from Bayes Rule that even though the directions of the arrows in a bnet can have causal motivation, a bnet with arrows reversed from their causally motivated directions can still be very useful as a calculation tool.

Another way of stating Bayes Rule is

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<sup>3</sup>Two bnets are equated if their full probability distributions (i.e., their full instantiations) are equal numerically. For example,

$$\underline{a} \rightarrow \underline{b} \rightarrow \underline{c} = P(c|b)P(b|a)P(a) = \underline{a} \leftarrow \underline{b} \leftarrow \underline{c}$$

$$\underbrace{P(\theta|x)}_{\text{posterior}} = \mathcal{N}(!\theta) \underbrace{P(x|\theta)}_{\text{likelihood}} \underbrace{P(\theta)}_{\text{prior}} . \quad (\text{C.159})$$

If, for a given likelihood, the prior and posterior distributions belong to the same family (for instance, they are both Beta distributions), then we say that the prior is the **conjugate prior** of that likelihood.

For example,  $\text{Beta} \sim \text{Bernoulli}^* \text{Beta}$ . Hence, the Beta distribution<sup>4</sup> is the conjugate prior of the Bernoulli distribution<sup>5</sup>. More explicitly, if

$$p_1 \sim \text{Beta}(p_1; \alpha, \beta) \quad (\text{C.160})$$

and

$$x|p_1 \sim \text{Bernoulli}(x; p_1) , \quad (\text{C.161})$$

where  $p_1 = P(x = 1)$ , then

$$p_1|x \sim \text{Beta}(p_1; \alpha', \beta') \quad (\text{C.162})$$

where

$$\alpha' = \alpha + x \quad (\text{C.163})$$

$$\beta' = \beta + (1 - x) \quad (\text{C.164})$$

Ref.[103] has a table of conjugate priors.

Conjugate priors facilitate Bayesian updating of the prior to posterior in a feedback loop(see Fig.C.6).

## C.27 Linear regression, Ordinary Least Squares (OLS)

Wikipedia articles

### 1. Linear Regression (LR)

- linear regression, Ref.[134]
- simple linear regression, Ref.[153]
- errors in variable, Ref.[109]

### 2. Least squares (LS)

- least squares, Ref.[131]

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<sup>4</sup>See Ref.[94] for a discussion of the Beta distribution.

<sup>5</sup>See Ref.[93] for a discussion of the Bernoulli distribution

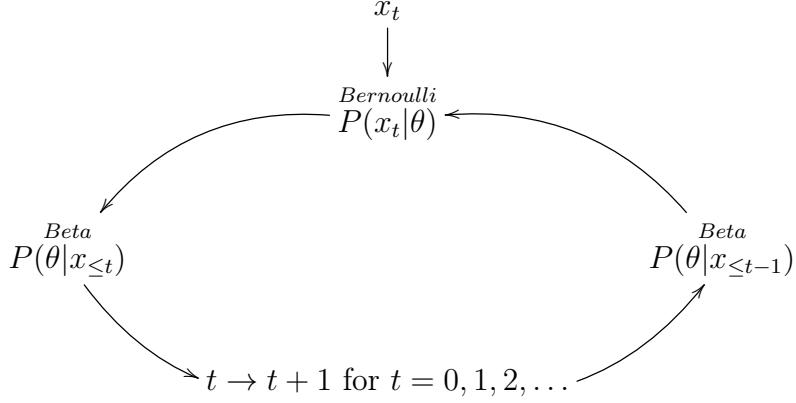


Figure C.6: Bayesian updating facilitated by conjugate prior. In this figure,  $x_{\leq t} = (x_0, x_1, \dots, x_{t-1}, x_t)$ .

- ordinary least squares (OLS), Ref.[146]

Some nomenclature: In LR, the data consists of **independent x-variables**  $x_1^\sigma, x_2^\sigma, \dots, x_n^\sigma$  and a **dependent y-variable**  $y^\sigma$ . We find a linear fit  $\hat{y}^\sigma = \beta_0 + \sum_{i=1}^n \beta_i x_i^\sigma$  to the data.  $\hat{y}^\sigma$  is called the **estimate** of  $y^\sigma$ . The coefficients  $\beta_0, \beta_i$  are called **regression coefficients**.  $y^\sigma - \hat{y}^\sigma = \epsilon^\sigma$  are called the **residuals**.  $\mathcal{E} = \sum_\sigma (\epsilon^\sigma)^2$  is called the **error or cost**. We choose the regression coefficients so as to minimize the error.

Below, we consider two types of LR:

1. LR in which the independent x-variables are non-random.
2. LR in which the independent x-variables are random and i.i.d.

The term OLS is often used to refer to LR of type 1.

For LR of type 2, there is randomness in  $y$  coming from the randomness in  $x$  and in the residuals. For LR of type 1, there is randomness in  $y$  too, but it comes from the residuals only.

Once one assumes that certain variables are random, a “model” (i.e., a bnet, with probabilities expressed as TPMs) must be specified.

### C.27.1 LR, assuming $x_\sigma$ are non-random

Let

$$\sigma \in \{0, 1, 2, \dots, nsam - 1\} : \text{sample index}$$

$$i_0 \in \{0, 1, 2, \dots, n\} : \text{index that can assume values 0 to } n$$

$$i \in \{1, 2, \dots, n\} : \text{index that can assume values 1 to } n. i \text{ is never equal to 0.}$$

- $y_\sigma \in \mathbb{R}$ : dependent y-variables
- $x_{\sigma i} \in \mathbb{R}$ : independent x-variables
- $\epsilon_\sigma \in \mathbb{R}$ : residuals
- $\beta_0, \beta_i \in \mathbb{R}$ : regression coefficients

$$y_\sigma = \beta_0 + \sum_{i=1}^n x_{\sigma i} \beta_i + \epsilon_\sigma \quad (\text{C.165})$$

If we define

$$x_{\sigma 0} = 1 \quad (\text{C.166})$$

for all  $\sigma$ , then

$$y_\sigma = \sum_{i_0=0}^n x_{\sigma i_0} \beta_{i_0} + \epsilon_\sigma . \quad (\text{C.167})$$

If  $y$  and  $\epsilon$  are  $nsam$  dimensional column vectors and  $\beta$  is an  $n+1$  dimensional column vector, and  $X$  is an  $nsam \times (n+1)$  matrix, then we can write the previous equation in matrix form as:

$$y = X\beta + \epsilon . \quad (\text{C.168})$$

### Derivation of LR From Minimization of Error

Let  $W = [W_{\sigma,\sigma'}]$  be a symmetric matrix with non-negative diagonal elements  $W_{\sigma,\sigma} \geq 0$  for all  $\sigma$ .  $W$  is called the **weight matrix**. The following claim describes the method of **Weighted LR** when  $W \neq 1$  and of simple LR when  $W = 1$ .

**Claim 10** *Assume the Einstein summation convention; i.e., implicit sum over repeated indices. The error function  $\mathcal{E}$  given by*

$$\mathcal{E} = \underbrace{(y_\sigma - X_{\sigma,j_0} \beta_{j_0})}_{\text{residual } \epsilon_\sigma} W_{\sigma,\sigma'} \underbrace{(y_{\sigma'} - X_{\sigma',k_0} \beta_{k_0})}_{\epsilon_{\sigma'}} , \quad (\text{C.169})$$

*is minimized over  $\beta_{k_0}$  for all  $k_0 \in \{0, 1, \dots, n\}$ , if  $\beta_{k_0}$  is given by:*

$$\hat{\beta} = (X^T W X)^{-1} X^T W y . \quad (\text{C.170})$$

*When  $W = 1$ ,*

$$\hat{\beta} = (X^T X)^{-1} X^T y . \quad (\text{C.171})$$

#### proof:

At the minimum of  $\mathcal{E}$ , the variation  $\delta\mathcal{E}$  must vanish:

$$0 = \delta\mathcal{E} = -2X_{\sigma j_0}(\delta\beta_{j_0})W_{\sigma,\sigma'}(y_{\sigma'} - X_{\sigma',k_0}\beta_{k_0}) . \quad (\text{C.172})$$

Thus,

$$X^T W y - X^T W X \beta = 0 \quad (\text{C.173})$$

which implies Eq.(C.170).

**QED**

**Geometry of LR with non-random  $x_\sigma$ .**

Recall that

$$y = X\beta + \epsilon . \quad (\text{C.174})$$

Define the **projection matrices**

$$I_X = X(X^T X)^{-1} X^T , \quad A_X = 1 - I_X \quad (\text{C.175})$$

A square matrix  $M$  is symmetric if  $M^T = M$  and is idempotent if  $M^2 = M$ .  $I_X$  is symmetric and idempotent and so is  $A_X$ . Note that  $I_X$  and  $A_X$  also satisfy:

$$A_X I_X = I_X A_X = 0 \quad (\text{C.176})$$

and

$$I_X X = X , \quad A_X X = 0 . \quad (\text{C.177})$$

$I_X$  acts as the identity on  $X$ , and  $A_X$  annihilates  $X$ .

One has

$$\beta = (X^T X)^{-1} X^T (y - \epsilon) . \quad (\text{C.178})$$

Define

$$\boxed{\widehat{\beta} = \underbrace{(X^T X)^{-1} X^T}_B y ,} \quad (\text{C.179a})$$

$$\widehat{y} = X\widehat{\beta} = I_X y , \quad (\text{C.179b})$$

and

$$\widehat{\epsilon} = y - X\widehat{\beta} = y - \widehat{y} = (1 - I_X)y = A_X y . \quad (\text{C.179c})$$

$I_X$  is sometimes called the **hat matrix**, because it gives  $y$  a hat.

Given any function  $f = f(y, X, \epsilon)$  and a scalar factor  $\xi \in \mathbb{R}$ , suppose  $f(\xi y, \xi X, \xi \epsilon) = \xi^{\mathcal{O}} f(y, X, \epsilon)$ . Then we will say that  $f(\cdot)$  is of **order  $\mathcal{O}$  under scaling**. Note that  $\{\widehat{y}, \widehat{\epsilon}\}$  are all of order 1 under scaling,  $\{\beta, \widehat{\beta}, I_X, A_X\}$  are all of order 0 under scaling, and  $B$  is of order  $-1$  under scaling. Thus, each curve-fit (i.e., symbol with a hat)

scales the same way as its estimand (i.e., same symbol without a hat). Furthermore,  $\beta$ , its curve-fit  $\hat{\beta}$ , and the projection matrices  $I_X, A_X$  are invariant ( $\mathcal{O} = 0$ ) under scaling.

Note that  $y$  can be expressed as a sum of 2 orthogonal estimates:

$$y = \underbrace{\hat{y}}_{I_X y} + \underbrace{\hat{\epsilon}}_{A_X y}. \quad (\text{C.180})$$

Fig.C.7 shows triangles representing  $y = X\beta + \epsilon$  and  $y = \hat{y} + \hat{\epsilon}$ .

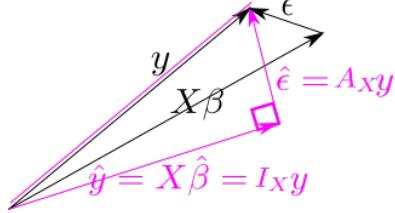


Figure C.7: Triangles representing  $y = X\beta + \epsilon$  and  $y = \hat{y} + \hat{\epsilon}$ .

## LR Goodness of Fit, $R^2$

Assume the components of  $\epsilon$  are random with zero mean:

$$E[\epsilon] = \langle \epsilon \rangle = 0 \quad (\text{C.181})$$

Assume  $X$  and  $\beta$  are not random. This makes  $\underline{y} = X\beta + \underline{\epsilon}$  and  $\hat{\beta} = (X^T X)^{-1} X^T \underline{y}$  random. One finds that

$$\langle \underline{y} \rangle = X\beta \quad (\text{C.182a})$$

$$\langle \hat{y} \rangle = I_X \underbrace{\langle \underline{y} \rangle}_{X\beta} = \langle \underline{y} \rangle \quad (\text{C.182b})$$

$$\langle \hat{\epsilon} \rangle = A_X \underbrace{\langle \underline{y} \rangle}_{X\beta} = 0 \quad (\text{C.182c})$$

$$\langle \hat{\beta} \rangle = \beta \quad (\text{C.182d})$$

So far, we have assumed a zero mean value for  $\epsilon$ . Next, assume “**homoscedasticity**” (**homo-spread**)<sup>6</sup>, which means that

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<sup>6</sup>I find the word “homoscedasticity” unnecessarily long, cryptic and easy to misspell so I like to replace it by “homo-spread”. The opposite of “homoscedasticity” is “heteroscedasticity”, which I like to replace with “hetero-spread”.

$$\langle \underline{\epsilon}, \underline{\epsilon}^T \rangle = \xi^2 I_{nsam} \quad (\text{C.182e})$$

where  $\xi \geq 0$ , and  $I_{nsam}$  is the  $nsam \times nsam$  identity matrix. It follows that

$$\langle \underline{y}, \underline{y}^T \rangle = \langle \underline{\epsilon}, \underline{\epsilon}^T \rangle = \xi^2 I_{nsam}, \quad (\text{C.183a})$$

$$\langle \widehat{\underline{\epsilon}}, \widehat{\underline{\epsilon}}^T \rangle = A_X \langle \underline{y}, \underline{y}^T \rangle A_X^T = \xi^2 A_X, \quad (\text{C.183b})$$

$$\langle \widehat{\underline{y}}, \widehat{\underline{y}}^T \rangle = I_X \langle \underline{y}, \underline{y}^T \rangle I_X^T = \xi^2 I_X \quad (\text{C.183c})$$

and

$$\langle \widehat{\underline{\beta}}, \widehat{\underline{\beta}}^T \rangle = B \langle \underline{y}, \underline{y}^T \rangle B^T = \xi^2 (X^T X)^{-1}. \quad (\text{C.183d})$$

For any random column vector  $\underline{a}$ , let

$$\| \underline{a} \|^2 = \underline{a}^T \underline{a} = \text{tr}(\underline{a} \underline{a}^T) \quad (\text{C.184})$$

and

$$\langle \| \underline{a} - \langle \underline{a} \rangle \|^2 \rangle = \langle \underline{a}^T \underline{a} \rangle - \langle \underline{a}^T \rangle \langle \underline{a} \rangle = \text{tr} \langle \underline{a}, \underline{a}^T \rangle. \quad (\text{C.185})$$

Define the following sums of squares (SS):

$$SS_{\underline{y}} = \langle \| \underline{y} - \langle \underline{y} \rangle \|^2 \rangle = \langle \underline{y}^T \underline{y} \rangle - \langle \underline{y}^T \rangle \langle \underline{y} \rangle = \text{tr} \langle \underline{y}, \underline{y}^T \rangle \quad (\text{C.186a})$$

$$SS_{\widehat{\underline{y}}} = \langle \| \widehat{\underline{y}} - \langle \widehat{\underline{y}} \rangle \|^2 \rangle = \langle \widehat{\underline{y}}^T \widehat{\underline{y}} \rangle - \langle \widehat{\underline{y}}^T \rangle \langle \widehat{\underline{y}} \rangle = \text{tr} \langle \widehat{\underline{y}}, \widehat{\underline{y}}^T \rangle \quad (\text{C.186b})$$

$$SS_{res} = \langle \| \underline{y} - \widehat{\underline{y}} \|^2 \rangle = \langle \| \widehat{\underline{\epsilon}} \|^2 \rangle = \text{tr} \langle \widehat{\underline{\epsilon}}, \widehat{\underline{\epsilon}}^T \rangle \quad (\text{C.186c})$$

**Claim 11** *The following is true without homo-spread:*

$$\underbrace{\text{tr} \langle \underline{y}, \underline{y}^T \rangle}_{SS_{\underline{y}}} = \underbrace{\text{tr} \langle \widehat{\underline{y}}, \widehat{\underline{y}}^T \rangle}_{SS_{\widehat{\underline{y}}}} + \underbrace{\text{tr} \langle \widehat{\underline{\epsilon}}, \widehat{\underline{\epsilon}}^T \rangle}_{SS_{res}} \quad (\text{C.187})$$

*This is like the Pythagorean Theorem for the magenta right triangle in Fig. C.7.*

**proof:**

From Eqs.C.183 and C.186, we see that

$$SS_{\underline{y}} = \text{tr} \langle \underline{y}, \underline{y}^T \rangle \quad (\text{C.188})$$

$$SS_{\hat{y}} = \text{tr} \langle \hat{y}, \hat{y}^T \rangle = \text{tr} \langle I_X \underline{y}, \underline{y}^T \rangle \quad (\text{C.189})$$

$$SS_{res} = \text{tr} \langle \underline{\epsilon}, \underline{\epsilon}^T \rangle = \text{tr} \langle A_X \underline{y}, \underline{y}^T \rangle \quad (\text{C.190})$$

Now use  $I_X + A_X = 1$ .

**QED**

The goodness of fit for this model is often measured using the **coefficient of determination**  $R^2$ .  $R^2$  is defined by

$$R^2 = 1 - \frac{SS_{res}}{SS_{\underline{y}}} = \frac{SS_{\hat{y}}}{SS_{\underline{y}}} = \frac{\text{tr} \langle \hat{y}, \hat{y}^T \rangle}{\text{tr} \langle \underline{y}, \underline{y}^T \rangle} \quad (\text{C.191})$$

If homo-spread holds, then  $R^2$  reduces to

$$R^2 = \frac{\text{tr} I_X}{nsam} . \quad (\text{C.192})$$

See Fig.C.8 for a pictorial explanation of  $R^2$ .

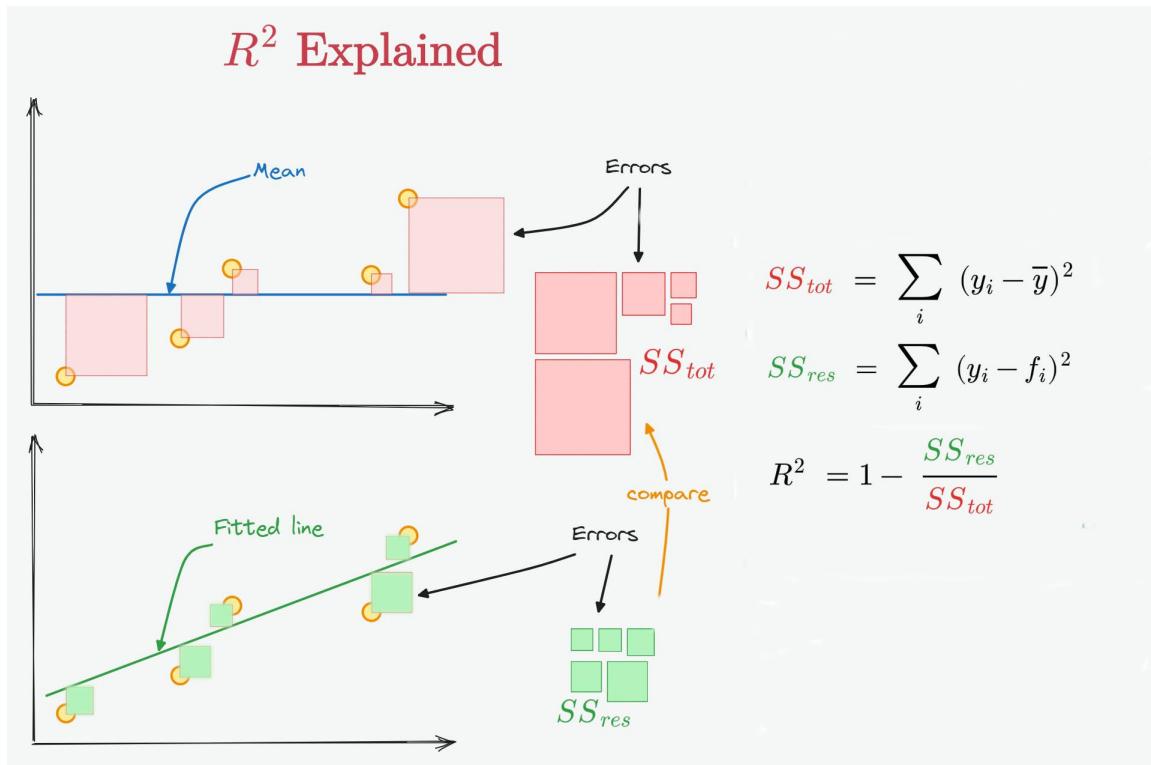


Figure C.8: Pictorial explanation of  $R^2$ .

## C.27.2 LR, assuming $x_\sigma$ are random

Let

- $i_0 \in \{0, 1, 2, \dots, n\}$  : index that can assume values 0 to  $n$
- $i \in \{1, 2, \dots, n\}$  : index that can assume values 1 to  $n$ .  $i$  is never equal to 0.
- $y \in \mathbb{R}$ : true value of dependent y-variable
- $\hat{y} \in \mathbb{R}$ : curve-fit of dependent y-variable
- $\epsilon \in \mathbb{R}$ : residual
- $\underline{x}_i \in \mathbb{R}$ : independent x-variables for  $i \in \{1, \dots, n\}$
- $\beta_0, \beta_i \in \mathbb{R}$ : regression coefficients

$$\hat{y} = \beta_0 + \sum_{j=1}^n \beta_j \underline{x}_j \quad (\text{C.193})$$

$$= \sum_{j_0=0}^n \beta_{j_0} \underline{x}_{j_0} \quad (\text{Assume } \underline{x}_0 = 1.) \quad (\text{C.194})$$

$$y = \hat{y} + \epsilon \quad (\text{C.195})$$

Fitting  $y$  with a hyperplane in the variables  $x^n = (x_i)_{i=1}^n$  (i.e., finding the best coefficients  $\beta^n = (\beta_i)_{i=1}^n$ ) is called **regressing  $y$  on  $x^n$** .

**Transforming expressions from non-random to random  $x_\sigma$**

Define the following population averages:

$$E_\sigma[x^\sigma] = \frac{1}{nsam} \sum_\sigma x^\sigma, \quad (\text{C.196})$$

$$E_\sigma[x^\sigma y^\sigma] = \frac{1}{nsam} \sum_\sigma x^\sigma y^\sigma, \quad (\text{C.197})$$

$$\langle x^\sigma, y^\sigma \rangle_\sigma = E_\sigma[x^\sigma y^\sigma] - E_\sigma[x^\sigma] E_\sigma[y^\sigma]. \quad (\text{C.198})$$

**Claim 12** If the  $x_\sigma$  are i.i.d. random variables,

$$E_\sigma[x^\sigma] = \langle \underline{x} \rangle \quad (\text{C.199})$$

$$E_\sigma[x^\sigma y^\sigma] = \langle \underline{x} \underline{y} \rangle \quad (\text{C.200})$$

$$\langle x^\sigma, y^\sigma \rangle_\sigma = \langle \underline{x}, \underline{y} \rangle \quad (\text{C.201})$$

**proof:**

$$\frac{1}{nsam} \sum_{\sigma} x^{\sigma} = \frac{1}{nsam} \sum_{x \in S_{\underline{x}}} x \underbrace{\sum_{\sigma} \mathbb{1}(x^{\sigma} = x)}_{N(x^{\sigma} = x)} \quad (\text{C.202})$$

$$= \sum_{x} x P(x) \quad (\text{C.203})$$

$$= \langle \underline{x} \rangle \quad (\text{C.204})$$

$$\frac{1}{nsam} \sum_{\sigma} x^{\sigma} y^{\sigma} = \frac{1}{nsam} \sum_{x \in S_{\underline{x}}} \sum_{y \in S_{\underline{y}}} xy \underbrace{\sum_{\sigma} \mathbb{1}(x^{\sigma} = x, y^{\sigma} = y)}_{N(x^{\sigma} = x, y^{\sigma} = y)} \quad (\text{C.205})$$

$$= \sum_{x,y} xy P(x,y) \quad (\text{C.206})$$

$$= \langle \underline{xy} \rangle \quad (\text{C.207})$$

Eq.(C.201) follows from Eq.(C.199) and Eq.(C.200).

**QED**

Recall that

$$Y_{\sigma} = \beta_0 + \sum_{j=1}^n X_{\sigma,j} \beta_j + \epsilon_{\sigma} . \quad (\text{C.208})$$

Assume

$$E_{\sigma}[X_{\sigma,k} \epsilon_{\sigma}] = E_{\sigma}[X_{\sigma,k}] \underbrace{E_{\sigma}[\epsilon_{\sigma}]}_{=0} = 0 . \quad (\text{C.209})$$

Then we have

$$E_{\sigma}[X_{\sigma,k} Y_{\sigma}] = E_{\sigma}[X_{\sigma,k}] \beta_0 + \sum_{j=1}^n E_{\sigma}[X_{\sigma,k} X_{\sigma,j}] \beta_j + \underbrace{E_{\sigma}[X_{\sigma,k} \epsilon_{\sigma}]}_{=0} \quad (\text{C.210})$$

and

$$E_{\sigma'}[X_{\sigma',k}] E_{\sigma}[Y_{\sigma}] = E_{\sigma'}[X_{\sigma',k}] \beta_0 + \sum_{j=1}^n E_{\sigma'}[X_{\sigma',k}] E_{\sigma}[X_{\sigma,j}] \beta_j + \underbrace{E_{\sigma'}[X_{\sigma',k}] E_{\sigma}[\epsilon_{\sigma}]}_{=0} . \quad (\text{C.211})$$

Subtracting Eq.(C.211) from Eq.(C.210), we get

$$\langle X_{\sigma,k}, Y_\sigma \rangle_\sigma = \sum_{j=1}^n \langle X_{\sigma,k}, X_{\sigma,j} \rangle_\sigma \beta_j . \quad (\text{C.212})$$

Define the  $n$  dimensional covariance matrix  $C$  by

$$C_{k,j} = \langle X_{\sigma,k}, X_{\sigma,j} \rangle_\sigma . \quad (\text{C.213})$$

Then Eq.(C.212) implies

$$\beta_j = \sum_{k=1}^n C_{j,k}^{-1} \langle X_{\sigma,k}, Y_\sigma \rangle_\sigma \quad (\text{C.214})$$

for all  $j = 1, 2, \dots, n$ .

If we assume that the  $x_\sigma$  are i.i.d., then, by virtue of Claim 12, the matrix  $C$  tends to

$$C_{k,j} \rightarrow \langle \underline{x}_k, \underline{x}_j \rangle \quad (\text{C.215})$$

and Eq.(C.214) implies

$$\beta_j = \sum_{k=1}^n C_{j,k}^{-1} \langle \underline{x}_k, \underline{y} \rangle . \quad (\text{C.216})$$

### LR with random $x_\sigma$ , expressed in derivative notation

Recall our notation for *conditional* averages. For any random variables  $\underline{x}, \underline{y}, \underline{a}$ , let

$$E_{|\underline{a}}[\underline{x}] = \langle \underline{x} \rangle^{|\underline{a}} \quad (\text{mean}) \quad (\text{C.217})$$

$$\langle \underline{x}, \underline{y} \rangle^{|\underline{a}} = \langle \underline{x}\underline{y} \rangle^{|\underline{a}} - \langle \underline{x} \rangle^{|\underline{a}} \langle \underline{y} \rangle^{|\underline{a}} \quad (\text{covariance}) \quad (\text{C.218})$$

$$\sigma_{\underline{x}}^{|\underline{a}} = \sqrt{\langle \underline{x}, \underline{x} \rangle^{|\underline{a}}} \quad (\text{standard deviation}) \quad (\text{C.219})$$

$$\rho_{\underline{x}, \underline{y}}^{|\underline{a}} = \frac{\langle \underline{x}, \underline{y} \rangle^{|\underline{a}}}{\sigma_{\underline{x}}^{|\underline{a}} \sigma_{\underline{y}}^{|\underline{a}}} = \left[ \frac{\langle \underline{x}, \underline{y} \rangle}{\sigma_{\underline{x}} \sigma_{\underline{y}}} \right]^{|\underline{a}} \quad (\text{correlation}) \quad (\text{C.220})$$

$$\partial_{\underline{x}}^{|\underline{a}} \underline{y} = \left[ \frac{\partial}{\partial \underline{x}} \right]^{|\underline{a}} \underline{y} = \frac{\langle \underline{x}, \underline{y} \rangle^{|\underline{a}}}{\langle \underline{x}, \underline{x} \rangle^{|\underline{a}}} = \rho_{\underline{x}, \underline{y}}^{|\underline{a}} \frac{\sigma_{\underline{y}}^{|\underline{a}}}{\sigma_{\underline{x}}^{|\underline{a}}} = \left[ \rho_{\underline{x}, \underline{y}} \frac{\sigma_{\underline{y}}}{\sigma_{\underline{x}}} \right]^{|\underline{a}} \quad (\text{partial derivative}) \quad (\text{C.221})$$

“ $|\underline{a}$ ” means that the variable  $\underline{a}$  is held fixed to  $a$  when taking all averages.

Recall that

$$\underline{y} = \beta_0 + \underbrace{\sum_{j=1}^n \beta_j \underline{x}_j}_{\hat{y}} + \underline{\epsilon}. \quad (\text{C.222})$$

Assume

$$\langle \underline{\epsilon} \rangle = 0 \quad (\text{C.223})$$

and

$$\langle \underline{x}_j, \underline{\epsilon} \rangle = 0 \quad (\text{C.224})$$

for all  $j$ .

For  $k = 1, \dots, n$ ,

$$\langle \underline{x}_k, \underline{y} \rangle = \sum_{j=1}^n \beta_j \langle \underline{x}_k, \underline{x}_j \rangle. \quad (\text{C.225})$$

Define the linear operator

$$\frac{\partial \cdot}{\partial \underline{a}} = \frac{\langle \underline{a}, \cdot \rangle}{\langle \underline{a}, \underline{a} \rangle} \quad (\text{C.226})$$

for any random variable  $\underline{a}$ . Then Eq.(C.225), after dividing both of its sides by  $\langle \underline{x}_k, \underline{x}_k \rangle$ , can be written as

$$\frac{\partial \underline{y}}{\partial \underline{x}_k} = \sum_{j=1}^n \beta_j \frac{\partial \underline{x}_j}{\partial \underline{x}_k} \quad (\text{C.227})$$

Let  $\underline{x}^n$  and  $\beta^n$  be  $n$ -dimensional column vectors. If we further define the gradient

$$\nabla_{\underline{x}^n} \underline{y} = \left[ \frac{\partial \underline{y}}{\partial \underline{x}_1}, \frac{\partial \underline{y}}{\partial \underline{x}_2}, \dots, \frac{\partial \underline{y}}{\partial \underline{x}_n} \right]^T \quad (\text{C.228})$$

and the Jacobian matrix

$$J_{j,k} = \frac{\partial \underline{x}_j}{\partial \underline{x}_k} \quad (\text{C.229})$$

then

$$\nabla_{\underline{x}^n} \underline{y} = J^T \beta^n \quad (\text{C.230})$$

so

$$\boxed{\beta^n = (J^T)^{-1} \nabla_{\underline{x}^n} \underline{y}} \quad (\text{C.231})$$

Note that  $J_{k,k} = 1$  for all  $k$ . Eq.(C.216) and Eq.(C.231) are equivalent. Whereas the matrix  $C$  has the nice property that it is symmetric, the matrix  $J$  has the nice property that its diagonal entries are 1.

Next, we will write Eq.(C.231) for the special cases  $n = 1, 2, 3$ , where  $n$  is the number of independent x-variables  $\underline{x}_j$ .

1.  $n = 1$  ( $\underline{y}$  fitted by a line)

$$\underline{y} = \beta_0 + \beta_1 \underline{x} + \epsilon \quad (\text{C.232})$$

Eq.(C.231) becomes

$$\beta_1 = \frac{\partial \underline{y}}{\partial \underline{x}} = \frac{\langle \underline{x}, \underline{y} \rangle}{\langle \underline{x}, \underline{x} \rangle} = \rho_{\underline{x}, \underline{y}} \frac{\sigma_{\underline{y}}}{\sigma_{\underline{x}}} \quad (\text{C.233})$$

2.  $n = 2$  ( $\underline{y}$  fitted by a plane)

$$\underline{y} = \beta_0 + \beta_1 \underline{x}_1 + \beta_2 \underline{x}_2 + \epsilon \quad (\text{C.234})$$

Eq.(C.231) becomes<sup>7</sup>

$$\begin{bmatrix} \beta_1 \\ \beta_2 \end{bmatrix} = (J^T)^{-1} \begin{bmatrix} \partial_{\underline{x}_1} \underline{y} \\ \partial_{\underline{x}_2} \underline{y} \end{bmatrix} \quad (\text{C.235})$$

$$= \frac{1}{\det J^T} \begin{bmatrix} J_{22} & -J_{21} \\ -J_{12} & J_{11} \end{bmatrix} \begin{bmatrix} \partial_{\underline{x}_1} \underline{y} \\ \partial_{\underline{x}_2} \underline{y} \end{bmatrix} \quad (\text{C.236})$$

Hence,

$$\beta_1 = \frac{J_{22} \partial_{\underline{x}_1} \underline{y} - J_{21} \partial_{\underline{x}_2} \underline{y}}{J_{11} J_{22} - J_{21} J_{12}} = \frac{\partial_{\underline{x}_1} \underline{y} - J_{21} \partial_{\underline{x}_2} \underline{y}}{1 - J_{21} J_{12}} \quad (\text{C.237})$$

We can express Eq.(C.237) in terms of variances and correlations as follows.

$$\beta_1 = \left[ \frac{1}{\langle \underline{x}_1, \underline{x}_1 \rangle} \right] \frac{\langle \underline{x}_1, \underline{y} \rangle - \langle \underline{x}_2, \underline{x}_1 \rangle \langle \underline{x}_2, \underline{y} \rangle \langle \underline{x}_2, \underline{x}_2 \rangle^{-1}}{1 - \rho_{\underline{x}_1, \underline{x}_2}^2} \quad (\text{C.238})$$

$$= \left[ \frac{1}{\sigma_{\underline{x}_1}^2} \right] \frac{\rho_{\underline{x}_1, \underline{y}} \sigma_{\underline{y}} \sigma_{\underline{x}_1} - \rho_{\underline{x}_1, \underline{x}_2} \rho_{\underline{x}_2, \underline{y}} \sigma_{\underline{x}_1} \sigma_{\underline{y}}}{1 - \rho_{\underline{x}_1, \underline{x}_2}^2} \quad (\text{C.239})$$

$$= \left[ \frac{\sigma_{\underline{y}}}{\sigma_{\underline{x}_1}} \right] \frac{\rho_{\underline{x}_1, \underline{y}} - \rho_{\underline{x}_1, \underline{x}_2} \rho_{\underline{x}_2, \underline{y}}}{1 - \rho_{\underline{x}_1, \underline{x}_2}^2} \quad (\text{C.240})$$

Eq.(C.240) agrees with the value of  $\beta_{YX,Z}$  in Ref.[46] by Pearl, if we replace in Pearl's formulae  $X \rightarrow \underline{x}_1$ ,  $Y \rightarrow \underline{y}$ ,  $Z \rightarrow \underline{x}_2$ .

Note that Eq.(C.237) can also be written as

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<sup>7</sup>Recall that if  $M = \begin{bmatrix} a & b \\ c & d \end{bmatrix}$  then  $M^{-1} = \frac{1}{\det M} \begin{bmatrix} d & -b \\ -c & a \end{bmatrix}$

$$\beta_1 = \frac{\partial_{\underline{x}_1} \underline{y} - J_{21} \partial_{\underline{x}_2} \underline{y}}{1 - J_{21} J_{12}} \quad (\text{C.241})$$

$$= \partial_{\underline{x}_1} \underline{y} + \underbrace{\frac{J_{21} J_{12} \partial_{\underline{x}_1} - J_{21} \partial_{\underline{x}_2}}{1 - J_{21} J_{12}}}_{-A_{\underline{x}_1}} \underline{y} \quad (\text{C.242})$$

The linear operator  $A_{\underline{x}_1}$  satisfies

$$A_{\underline{x}_1}(\underline{x}_1) = 0 \quad (A_{\underline{x}_1} \text{ annihilates } \underline{x}_1) \quad (\text{C.243})$$

and

$$A_{\underline{x}_1}(\underline{x}_2) = J_{21} = \partial_{\underline{x}_1} \underline{x}_2 \quad (\text{C.244})$$

Therefore

$$A_{\underline{x}_1} = \partial_{\underline{x}_1}^{|x_1} \quad (\text{C.245})$$

and

$$\beta_1 = \partial_{\underline{x}_1} \underline{y} - \partial_{\underline{x}_1}^{|x_1} \underline{y} \quad (\text{C.246})$$

If we define

$$I_{\underline{x}_1} = 1 - A_{\underline{x}_1} \quad (\text{C.247})$$

then

$$\beta_1 = \partial_{\underline{x}_1}(I_{\underline{x}_1} \underline{y}) \quad (\text{C.248})$$

3.  $n = 3$  ( $\underline{y}$  fitted by a volume)

$$\underline{x}^3 = [\underline{x}_1, \underline{x}_2, \underline{x}_3]^T \quad (\text{C.249})$$

$$\beta^3 = [\beta_1, \beta_2, \beta_3]^T \quad (\text{C.250})$$

$$\underline{y} = [\beta^3]^T \underline{x}^3 + \underline{\epsilon} \quad (\text{C.251})$$

$$J_{i,j} = \frac{\partial x_i}{\partial \underline{x}_j} \quad (\text{C.252})$$

$$\beta^3 = (J^T)^{-1} \nabla_{\underline{x}^3} \underline{y} \quad (\text{C.253})$$

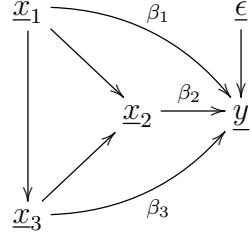


Figure C.9: Bnet for Linear Regression of  $\underline{y}$  with a 3 dimensional feature vector  $\underline{x} = (\underline{x}_1, \underline{x}_2, \underline{x}_3)$ .  $\langle \underline{x}_j, \epsilon \rangle = 0$  because the path from  $\underline{x}_j$  to  $\epsilon$  is blocked by a collider node. Note that even though node  $y$  is deterministic, nodes  $\underline{x}_j$  may be probabilistic. Hence, this is only a partial LDEN (LDEN are discussed in Chapter 48)

$$J^T = \begin{bmatrix} 1 & a_{12} & a_{13} \\ a_{21} & 1 & a_{23} \\ a_{31} & a_{32} & 1 \end{bmatrix} = A \quad (\text{C.254})$$

$$a_{i,j} = \frac{\partial \underline{x}_j}{\partial \underline{x}_i} \quad (\text{C.255})$$

Using Figs.C.10 and C.11, we get

$$\beta_1 = \frac{1}{\det A} \left( \det \begin{bmatrix} 1 & a_{23} \\ a_{32} & 1 \end{bmatrix} \partial_{\underline{x}_1} \underline{y} + \det \begin{bmatrix} a_{13} & a_{12} \\ 1 & a_{32} \end{bmatrix} \partial_{\underline{x}_2} \underline{y} + \det \begin{bmatrix} a_{12} & a_{13} \\ 1 & a_{23} \end{bmatrix} \partial_{\underline{x}_3} \underline{y} \right) \quad (\text{C.256})$$

$$\mathbf{A} \equiv \begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{bmatrix},$$

Figure C.10: Arbitrary 3 dimensional matrix  $A$

### Double regression of $y$

Recall that

$$\underline{y} = \beta_0 + \sum_{j=1}^n \underline{x}_j \beta_j + \underline{\epsilon}. \quad (\text{C.257})$$

Therefore,

$$\mathbf{A}^{-1} = \frac{1}{|\mathbf{A}|} \begin{bmatrix} \begin{vmatrix} a_{22} & a_{23} \\ a_{32} & a_{33} \end{vmatrix} & \begin{vmatrix} a_{13} & a_{12} \\ a_{33} & a_{32} \end{vmatrix} & \begin{vmatrix} a_{12} & a_{13} \\ a_{22} & a_{23} \end{vmatrix} \\ \begin{vmatrix} a_{23} & a_{21} \\ a_{33} & a_{31} \end{vmatrix} & \begin{vmatrix} a_{11} & a_{13} \\ a_{31} & a_{33} \end{vmatrix} & \begin{vmatrix} a_{13} & a_{11} \\ a_{23} & a_{21} \end{vmatrix} \\ \begin{vmatrix} a_{21} & a_{22} \\ a_{31} & a_{32} \end{vmatrix} & \begin{vmatrix} a_{12} & a_{11} \\ a_{32} & a_{31} \end{vmatrix} & \begin{vmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{vmatrix} \end{bmatrix}.$$

Figure C.11: Inverse of the 3 dimensional matrix  $A$  given by Fig.C.10.

$$\langle \underline{x}_i, \underline{y} \rangle = \sum_{j=1}^n \langle \underline{x}_i, \underline{x}_j \rangle \beta_j \quad (\text{C.258})$$

$$= \langle \underline{x}_i, \underline{x}_i \rangle \beta_i + \sum_{j=1}^n \mathbb{1}(j \neq i) \langle \underline{x}_i, \underline{x}_j \rangle \beta_j. \quad (\text{C.259})$$

Hence,

$$\beta_i = \frac{\langle \underline{x}_i, \underline{y} \rangle}{\langle \underline{x}_i, \underline{x}_i \rangle} - \sum_{j=1}^n \mathbb{1}(j \neq i) \frac{\langle \underline{x}_i, \underline{x}_j \rangle}{\langle \underline{x}_i, \underline{x}_i \rangle} \beta_j. \quad (\text{C.260})$$

Eq.(C.260) can be expressed in derivative notation as:

$$\beta_i = \frac{\partial \underline{y}}{\partial \underline{x}_i} - \sum_{j=1}^n \mathbb{1}(j \neq i) \frac{\partial \underline{x}_j}{\partial \underline{x}_i} \beta_j \quad (\text{C.261})$$

Note that, because of the linearity of the derivative operator, Eq.(C.261) implies:

$$\beta_i = \frac{\partial}{\partial \underline{x}_i} \left( \underline{y} - \underbrace{\sum_{j=1}^n \mathbb{1}(j \neq i) \underline{x}_j \beta_j}_{\underline{y} - \underline{x}_i \beta_i} \right) \quad (\text{C.262})$$

$$= \left[ \partial_{\underline{x}_i} - \partial_{\underline{x}_i}^{|\underline{x}_i} \right] \underline{y}. \quad (\text{C.263})$$

Eq.(C.263) can be used to find  $\hat{\beta}_i$  in two steps:

STEP 1: Regress  $\underline{y} - \underline{x}_i \beta_i$  on  $(\underline{x}_j)_{j \in \{1, 2, \dots, n\} - \{i\}}$ . Get estimates  $(\widehat{\beta}_j)_{j \in \{1, 2, \dots, n\} - \{i\}}$ .

STEP 2: Regress  $\underline{y} - \sum_{j \neq i} \underline{x}_j \widehat{\beta}_j$  on  $\underline{x}_i$ . Get estimate  $\widehat{\beta}_i$ .

Of course, one can also find  $\widehat{\beta}_i$  by regressing  $\underline{y}$  on  $(\underline{x}_j)_{j \in \{1, 2, \dots, n\}}$ , to get estimates  $(\widehat{\beta}_j)_{j \in \{1, 2, \dots, n\}}$ .

## $R^2$ with random $x_\sigma$

Recall that

$$\underline{y} = \beta_0 + \underbrace{\sum_{j=1}^n \beta_j \underline{x}_j}_{\widehat{y}} + \underline{\epsilon}. \quad (\text{C.264})$$

Assume

$$\langle \underline{\epsilon} \rangle = 0 \quad (\text{C.265})$$

and

$$\langle \underline{x}_j, \underline{\epsilon} \rangle = 0 \quad (\text{C.266})$$

for all  $j$ .

$$\widehat{y} = \underline{y} - \underline{\epsilon} \quad (\text{C.267})$$

$$\langle \widehat{y}, \widehat{y} \rangle = \langle \widehat{y}, \underline{y} - \underline{\epsilon} \rangle \quad (\text{C.268})$$

$$= \langle \widehat{y}, \underline{y} \rangle \quad (\text{C.269})$$

$$\langle \underline{y}, \underline{y} \rangle = \langle \widehat{y} - \underline{\epsilon}_y, \widehat{y} - \underline{\epsilon}_y \rangle \quad (\text{C.270})$$

$$= \langle \widehat{y}, \widehat{y} \rangle + \langle \underline{\epsilon}, \underline{\epsilon} \rangle \quad (\text{C.271})$$

The goodness of fit measure  $R^2$  for this model is defined by

$$R_{\underline{y} \sim \widehat{y}}^2 = \frac{\langle \widehat{y}, \widehat{y} \rangle}{\langle \underline{y}, \underline{y} \rangle} = 1 - \frac{\langle \underline{\epsilon}, \underline{\epsilon} \rangle}{\langle \underline{y}, \underline{y} \rangle} \quad (\text{C.272})$$

where we are using Eq.(C.271). By Eq.(C.269), we also have

$$R_{\underline{y} \sim \widehat{y}}^2 = \frac{\langle \underline{y}, \widehat{y} \rangle}{\langle \underline{y}, \underline{y} \rangle} = \frac{\partial \widehat{y}}{\partial \underline{y}} = \rho_{\underline{y}, \widehat{y}} \frac{\sigma_{\widehat{y}}}{\sigma_{\underline{y}}} \quad (\text{C.273})$$

$$R_{\underline{y} \sim \widehat{y}}^2 R_{\widehat{y} \sim \underline{y}}^2 = \rho_{\underline{y}, \widehat{y}}^2 \quad (\text{C.274})$$

## C.28 Logistic Regression (LoR)

Suppose  $x_\sigma \in \mathbb{R}^n$ ,  $y_\sigma \in \mathbb{R}$ , and  $\Sigma$  is a population of individuals  $\sigma$ . In general, a **regression** is when we curve-fit a dataset  $\{(x_\sigma, y_\sigma) : \sigma \in \Sigma\}$  with a function  $\hat{y} = f(x)$ . In **Linear Regression (LR)**, which we discussed earlier,  $f(x)$  is a hyperplane in  $x$ . On the other hand, in **Logistic Regression (LoR)**,  $y_\sigma \in [0, 1]$  and  $f(x)$  is the sigmoid of a hyperplane in  $x$ .

More specifically, for LR we have Eq.(C.165) which reads as follows:

$$y_\sigma = \beta_0 + \underbrace{\sum_{i=1}^n x_{\sigma i} \beta_i}_{\hat{y}_\sigma} + \epsilon_\sigma \quad (\text{LR}) . \quad (\text{C.275})$$

For LoR, we have instead

$$p_\sigma = \text{smoid} \left( \beta_0 + \sum_{i=1}^n x_{\sigma i} \beta_i + \epsilon_\sigma \right) \quad (\text{LoR}) , \quad (\text{C.276})$$

or, equivalently,

$$\underbrace{\text{lodds}(p_\sigma)}_{\ln \frac{p_\sigma}{1-p_\sigma}} = \beta_0 + \underbrace{\sum_{i=1}^n x_{\sigma i} \beta_i}_{\hat{y}_\sigma} + \epsilon_\sigma \quad (\text{LoR}) , \quad (\text{C.277})$$

where we have used the fact that  $\text{lodds}()$  is the inverse function of  $\text{smoid}()$ . Hence, an LoR fit can be calculated by collecting a dataset  $\{(x_\sigma, p_\sigma) : \sigma \in \Sigma\}$ , transforming that dataset to the dataset  $\{(x_\sigma, \text{lodds}(p_\sigma)) : \sigma \in \Sigma\}$ , and fitting the latter dataset with a hyperplane. Let  $P(\underline{Y}_\sigma = 1) = p_\sigma \in [0, 1]$ . LoR can be used for binary classification if we define the binary class variable  $c_\sigma \in \{0, 1\}$  by

$$c_\sigma = \mathbb{1}(P(\underline{Y}_\sigma = 1) > \alpha) \quad (\text{C.278})$$

for some  $0 < \alpha < 1$ .

## C.29 Entropy, Kullback-Leibler divergence, Cross-Entropy

For probability distributions  $p(x), q(x)$  of  $x \in S_x$

- Entropy:

$$H(p) = - \sum_x p(x) \ln p(x) \geq 0 \quad (\text{C.279})$$

- Kullback-Leibler divergence:

$$D_{KL}(p \parallel q) = \sum_x p(x) \ln \frac{p(x)}{q(x)} \geq 0 \quad (\text{C.280})$$

- Cross entropy:

$$CE(p \parallel q) = - \sum_x p(x) \ln q(x) \quad (\text{C.281})$$

$$= H(p) + D_{KL}(p \parallel q) \quad (\text{C.282})$$

## C.30 Definition of various entropies used in Shannon Information Theory

- (plain) Entropy of  $\underline{x}$

$$H(\underline{x}) = - \sum_x P(x) \ln P(x) \quad (\text{C.283})$$

This quantity measures the spread of  $P_{\underline{x}}$ .  $H(\underline{x}) \geq 0$  and it vanishes iff  $P(x) = \delta(x, x_0)$  (deterministic case)

- Conditional Entropy of  $\underline{y}$  given  $\underline{x}$

$$H(\underline{y}|\underline{x}) = - \sum_{x,y} P(x,y) \ln P(y|x) \quad (\text{C.284})$$

$$= H(\underline{y}, \underline{x}) - H(\underline{x}) \quad (\text{C.285})$$

This quantity measures the conditional spread of  $\underline{y}$  given  $\underline{x}$ .  $H(\underline{y}|\underline{x}) \geq 0$ .

- Mutual Information (MI) of  $\underline{x}$  and  $\underline{y}$ .

$$H(\underline{y} : \underline{x}) = \sum_{x,y} P(x,y) \ln \frac{P(x,y)}{P(x)P(y)} \quad (\text{C.286})$$

$$= H(\underline{x}) + H(\underline{y}) - H(\underline{y}, \underline{x}) \quad (\text{C.287})$$

This quantity measures the correlation between  $\underline{x}$  and  $\underline{y}$ .  $H(\underline{y} : \underline{x}) \geq 0$  and it vanishes iff  $P(x,y) = P(x)P(y)$ .

- Conditional Mutual Information (CMI)<sup>8</sup> of  $\underline{x}$  and  $\underline{y}$  given  $\lambda$

$$H(\underline{y} : \underline{x} | \lambda) = \sum_{x,y,\lambda} P(x,y,\lambda) \ln \frac{P(x,y|\lambda)}{P(x|\lambda)P(y|\lambda)} \quad (\text{C.288})$$

$$= H(\underline{x} | \lambda) + H(\underline{y} | \lambda) - H(\underline{y}, \underline{x} | \lambda) \quad (\text{C.289})$$

This quantity measures the conditional correlation of  $\underline{x}$  and  $\underline{y}$  given  $\lambda$ .  $H(\underline{y} : \underline{x} | \lambda) \geq 0$  and it vanishes iff  $P(x,y|\lambda) = P(x|\lambda)P(y|\lambda)$ .

An interesting special case occurs when  $P(\lambda) = \delta(\lambda, \lambda_0)$  (the frequentist case of no  $\lambda$  prior.) In that case CMI reduces to

$$H(\underline{y} : \underline{x} | \lambda_0) = \sum_{x,y} P(x,y|\lambda_0) \ln \frac{P(x,y|\lambda_0)}{P(x|\lambda_0)P(y|\lambda_0)} \geq 0 \quad (\text{C.290})$$

- Kullback-Leibler Divergence from  $P_{\underline{x}}$  to  $P_{\underline{y}}$ .

Assume random variables  $\underline{x}$  and  $\underline{y}$  have the same set of states  $S_x = S_y$ . Then

$$D_{KL}(P_{\underline{x}} \| P_{\underline{y}}) = \sum_x P_{\underline{x}}(x) \ln \frac{P_{\underline{x}}(x)}{P_{\underline{y}}(x)} \quad (\text{C.291})$$

This quantity measures a non-symmetric distance between the probability distributions  $P_{\underline{x}}$  and  $P_{\underline{y}}$ .  $D_{KL}(P_{\underline{x}} \| P_{\underline{y}}) \geq 0$  and it equals zero iff  $P_{\underline{x}} = P_{\underline{y}}$ .

## C.31 Mean log likelihood asymptotic behavior

Define the log likelihood by

$$LL_{y|\theta} = \ln P(y|\theta) . \quad (\text{C.292})$$

In this section, we will represent averages over  $y|\theta$  by angular brackets:

$$\langle f(y) \rangle = \sum_y P(y|\theta) f(y) = E_{y|\theta}[f(y)] . \quad (\text{C.293})$$

Note that the mean log likelihood equals minus the entropy:

$$H(\underline{y} | \theta) = - \langle LL_{y|\theta} \rangle \quad (\text{C.294})$$

---

<sup>8</sup>CMI can be read as “see me”.

**Claim 13**

$$\langle \partial_\theta LL_{y|\theta} \rangle = 0 \quad (\text{C.295})$$

$$\langle \partial_\theta^2 LL_{y|\theta} \rangle = -\langle (\partial_\theta LL_{y|\theta})^2 \rangle \quad (\text{C.296})$$

**proof:**

$$\langle \partial_\theta LL_{y|\theta} \rangle = \sum_y P(y|\theta) \partial_\theta \ln P(y|\theta) \quad (\text{C.297})$$

$$= \sum_y \partial_\theta P(y|\theta) \quad (\text{C.298})$$

$$= 0 \quad (\text{C.299})$$

$$\langle \partial_\theta^2 LL_{y|\theta} \rangle = \sum_y P(y|\theta) \partial_\theta \left[ \frac{1}{P(y|\theta)} \partial_\theta P(y|\theta) \right] \quad (\text{C.300})$$

$$= -\sum_y P(y|\theta) \frac{1}{P(y|\theta)^2} [\partial_\theta P(y|\theta)]^2 + \underbrace{\sum_y \partial_\theta^2 P(y|\theta)}_{=0} \quad (\text{C.301})$$

$$= -\sum_y P(y|\theta) [\partial_\theta \ln P(y|\theta)]^2 \quad (\text{C.302})$$

$$= -\langle (\partial_\theta LL_{y|\theta})^2 \rangle \quad (\text{C.303})$$

**QED**

Define

$$\Delta\theta = \theta' - \theta \quad (\text{C.304})$$

and

$$-\Delta H(\underline{y}|\theta) = \Delta \langle LL_{y|\theta} \rangle = \langle LL_{y|\theta'} \rangle - \langle LL_{y|\theta} \rangle \quad (\text{C.305})$$

If we expand  $\langle LL_{y|\theta'} \rangle$  as a Taylor series to second order about the point  $\theta' = \theta$ , we get

$$\langle LL_{y|\theta'} \rangle = \langle LL_{y|\theta} \rangle + \Delta\theta \underbrace{\langle \partial_\theta LL_{y|\theta} \rangle}_{=0} + \frac{(\Delta\theta)^2}{2} \underbrace{\langle \partial_\theta^2 LL_{y|\theta} \rangle}_{-\langle (\partial_\theta LL_{y|\theta})^2 \rangle} + \mathcal{O}((\Delta\theta)^3) \quad (\text{C.306})$$

$$-\Delta H(\underline{y}|\theta) = \Delta \langle LL_{y|\theta} \rangle = -\frac{(\Delta\theta)^2}{2} \langle (\partial_\theta LL_{y|\theta})^2 \rangle + \mathcal{O}((\Delta\theta)^3) \quad (\text{C.307})$$

Thus,  $\theta' = \theta$  maximizes the mean log likelihood  $\langle LL_{y|\theta} \rangle$  (and minimizes the entropy  $H(\underline{y}|\theta)$ ).

Note that

$$\Delta \langle LL_{y|\theta} \rangle = \left\langle \ln \frac{P(y|\theta')}{P(y|\theta)} \right\rangle . \quad (\text{C.308})$$

If we approximate the ratio of these 2 probabilities by a Gaussian,

$$\frac{P(y|\theta')}{P(y|\theta)} \approx \exp \left( - \frac{(\Delta\theta)^2}{2\sigma_\theta^2} \right) , \quad (\text{C.309})$$

then

$$\sigma_\theta^2 = \langle (\partial_\theta LL_{y|\theta})^2 \rangle^{-1} . \quad (\text{C.310})$$

## C.32 Arc Strength (Arc Force)

Given a bnet with an arc (i.e., arrow)  $\underline{x} \rightarrow \underline{y}$ , we define the **arc strength or arc force** of arc  $\underline{x} \rightarrow \underline{y}$  to be  $H(\underline{x} : \underline{y})$  (i.e., the mutual information between  $\underline{x}$  and  $\underline{y}$ ). Evaluation of  $H(\underline{x} : \underline{y})$  requires knowing  $P(y|x)$ ,  $P(x)$  and  $P(y)$ .  $P(y|x)$  is the TPM of node  $\underline{y}$ , so it is immediately available from the specification of the bnet. Calculating  $P(x)$  and  $P(y)$  is more involved, and requires marginalizing the full probability distribution of the bnet. Such marginalizations can be done using the junction tree algorithm described in Chapter 43.

## C.33 Pearson Chi-Squared Test

The **Pearson divergence** (a.k.a. **Pearson Chi-squared test statistic**) for two probability distributions  $PO(x)$  and  $PE(x)$ , where  $x \in S_{\underline{x}}$ , is defined as follows:

$$D_{\chi^2} = \sum_x \frac{[PO(x) - PE(x)]^2}{PE(x)} = \sum_x \frac{PO^2(x)}{PE(x)} - 1 . \quad (\text{C.311})$$

Usually  $PO$  is the observed probability distribution and  $PE$  is the expected, theoretical one.

As the following claim shows, the Pearson divergence is closely related to the Kullback-Leibler divergence.

**Claim 14** *If  $\left| \frac{PO(x)}{PE(x)} - 1 \right| << 1$  for all  $x \in S_{\underline{x}}$ , then*

$$D_{KL}(PO \parallel PE) \approx D_{\chi^2} . \quad (\text{C.312})$$

**proof:**

$$D_{KL}(PO \parallel PE) = \sum_x PO(x) \ln \frac{PO(x)}{PE(x)} \quad (\text{C.313})$$

$$= \sum_x PO(x) \ln \left( 1 + \frac{PO(x)}{PE(x)} - 1 \right) \quad (\text{C.314})$$

$$\approx \sum_x PO(x) \left( \frac{PO(x)}{PE(x)} - 1 \right) \quad (\text{C.315})$$

$$= \sum_x \frac{PO^2(x)}{PE(x)} - 1 \quad (\text{C.316})$$

$$= D_{\chi^2} \quad (\text{C.317})$$

**QED**

Let  $nx = |S_{\underline{x}}|$ . Let  $P_{\chi^2}(y)$  be the  $\chi^2$  (with  $nx - 1$  degrees of freedom) probability distribution, and let  $F_{\chi^2}(\alpha)$  be its cumulative distribution. Find  $\alpha$  such that

$$95\% = \int_0^\alpha dy P_{\chi^2}(y) = F_{\chi^2}(\alpha) \quad (\text{C.318})$$

If  $D_{\chi^2} < \alpha$ , then we say that  $PO = PE$  to 95% significance level (SL), whereas if  $D_{\chi^2} > \alpha$ , we say that  $PO \neq PE$  to 95% SL (i.e., SL = 95%). The higher SL becomes, the higher  $\alpha$  becomes, and the bigger the divergence  $D_{\chi^2}$  has to be, before we are willing to declare that  $PO \neq PE$ .

## C.34 Demystifying Population and Sample Variances

Let  $x[\sigma] = x^\sigma$ . Given i.i.d.real variables  $(x^\sigma)_{\sigma=0,1,\dots,n-1}$ , let<sup>9</sup>

$$\hat{\mu} = \bar{x} = \frac{1}{n} \sum_{\sigma} x^\sigma \quad (\text{C.319})$$

$$(\hat{\sigma}^2)_{\infty} = \frac{1}{n} \sum_{\sigma} (x^\sigma - \mu)^2 \quad (\text{C.320})$$

$$\hat{\sigma}^2 = \frac{1}{n-1} \sum_{\sigma} (x^\sigma - \hat{\mu})^2 \quad (\text{C.321})$$

---

<sup>9</sup>Do not confuse the sample index  $\sigma$  and the standard deviation  $\sigma$ .

Statisticians<sup>10</sup> call  $(\hat{\sigma}^2)_\infty$  the “population variance”. I will call it the **population variance for fixed  $\mu$** . Note that it depends on the fixed parameter  $\mu$ . Statisticians call  $\hat{\sigma}^2$  the “sample variance”. Instead, I will call  $\hat{\sigma}^2$  the **population variance for random  $\mu$** .

If one treats  $\underline{x}^\sigma$  as a random variable, then one must treat  $\hat{\mu}$  as a random variable too. Let

$$E[\underline{x}^\sigma] = \mu \quad (\text{C.322})$$

and

$$\langle \underline{x}^\sigma, \underline{x}^{\sigma'} \rangle = \delta(\sigma, \sigma')\sigma^2. \quad (\text{C.323})$$

Then one can show that

$$E[(\hat{\sigma}^2)_\infty] = \frac{1}{n} E \left[ \sum_{\sigma} (\underline{x}^\sigma - \mu)^2 \right] \quad (\text{C.324})$$

$$= \sigma^2 \quad (\text{C.325})$$

and

$$E[\hat{\sigma}^2] = \frac{1}{n-1} E \left[ \sum_{\sigma} (\underline{x}^\sigma - \hat{\mu})^2 \right] \quad (\text{C.326})$$

$$= \sigma^2 \quad (\text{C.327})$$

This is the reason why we use an  $n - 1$  instead of an  $n$  in  $\hat{\sigma}^2$ . Because it makes  $E[\hat{\sigma}^2] = \sigma^2$  so  $\hat{\sigma}^2$  is an unbiased estimator of the single individual variance  $\sigma^2$ .

The intuitive reason for why  $\hat{\sigma}^2$  is divided by  $n - 1$  instead of  $n$  is that whereas  $\mu$  in  $(\hat{\sigma}^2)_\infty$  is kept fixed and is “quiet”, the  $\hat{\mu}$  in  $\hat{\sigma}^2$  is a random variable, noisy instead of quiet. The fluctuations in  $\hat{\mu}$  are strongly correlated with the fluctuations of the  $\underline{x}^\sigma$ , so they decrease the fluctuations in  $\hat{\sigma}^2$  compared to those in  $(\hat{\sigma}^2)_\infty$ . By dividing by  $n - 1$  instead of  $n$ , we compensate for this decrease in fluctuations so that the ratio of the numerator and denominator of  $\hat{\sigma}^2$  equals  $\sigma^2$ , instead of something *smaller* than  $\sigma^2$ , as would happen if were to divide by  $n$  instead of  $n - 1$ . In terms of “degrees of freedom”(DOFs),  $(\hat{\sigma}^2)_\infty$  has  $n$  DOFs (namely one for each  $\underline{x}^\sigma$ ), whereas  $\hat{\sigma}^2$  has  $n - 1$  DOFs. (the presence of  $\hat{\mu}$  subtracts one DOF). In both  $(\hat{\sigma}^2)_\infty$  and  $\hat{\sigma}^2$ , one divides by the number of DOFs.

---

<sup>10</sup>In the language of Statisticians, a “population” is supposed to be so large that its  $\mu$  does not fluctuate, and a “sample” is supposed to be a small subset of that population for which the  $\mu$  is assumed to fluctuate. In this book, I use the word “population” to mean a set of any size containing individuals, I use the word “sub-population” to refer to a subset of the population, and I use the word “sample” (a.k.a. individual, observation, unit, record) to mean a single individual of the population.

### C.35 Independence of $\hat{\mu}$ and $\hat{\sigma}^2$

Let  $x[\sigma] = x^\sigma$ . Consider i.i.d.real variables  $(x^\sigma)_{\sigma=0,1,\dots,n-1}$  such that<sup>11</sup>

$$E[\underline{x}^\sigma] = \mu \quad (\text{C.328})$$

$$\langle \underline{x}^\sigma, \underline{x}^{\sigma'} \rangle = \delta(\sigma, \sigma') \sigma^2 . \quad (\text{C.329})$$

$$\hat{\mu} = \bar{x} = \frac{1}{n} \sum_{\sigma} x^\sigma \quad (\text{C.330})$$

$$(\hat{\sigma}^2)_\infty = \frac{1}{n} \sum_{\sigma} (x^\sigma - \mu)^2 \quad (\text{C.331})$$

$$\hat{\sigma}^2 = \frac{1}{n-1} \sum_{\sigma} (x^\sigma - \hat{\mu})^2 \quad (\text{C.332})$$

**Claim 15** *Let*

$$\underline{\Delta}^\sigma = \underline{x}^\sigma - \mu . \quad (\text{C.333})$$

*For any  $\sigma_1, \sigma_2, \sigma_3$ ,*

$$\langle \underline{\Delta}^{\sigma_1} \underline{\Delta}^{\sigma_2}, \underline{\Delta}^{\sigma_3} \rangle = 0 . \quad (\text{C.334})$$

**proof:**

Suppose  $\sigma_2 \neq \sigma_3$ . Then

$$\langle \underline{\Delta}^{\sigma_1} \underline{\Delta}^{\sigma_2}, \underline{\Delta}^{\sigma_3} \rangle = \underbrace{\langle \underline{\Delta}^{\sigma_2} \rangle}_0 \langle \underline{\Delta}^{\sigma_1}, \underline{\Delta}^{\sigma_3} \rangle = 0 . \quad (\text{C.335})$$

So assume  $\sigma_2 = \sigma_3 = \sigma$  and evaluate  $\langle \underline{\Delta}^{\sigma_1} \underline{\Delta}^{\sigma}, \underline{\Delta}^{\sigma} \rangle$ .

Suppose  $\sigma_1 \neq \sigma$ . Then

$$\langle \underline{\Delta}^{\sigma_1} \underline{\Delta}^{\sigma}, \underline{\Delta}^{\sigma} \rangle = \underbrace{\langle \underline{\Delta}^{\sigma_1} \rangle}_0 \langle \underline{\Delta}^{\sigma}, \underline{\Delta}^{\sigma} \rangle = 0 . \quad (\text{C.336})$$

So suppose  $\sigma_1 = \sigma$  and evaluate  $\langle (\underline{\Delta}^{\sigma})^2, \underline{\Delta}^{\sigma} \rangle$ .

$$\langle (\underline{\Delta}^{\sigma})^2, \underline{\Delta}^{\sigma} \rangle = \underbrace{\langle (\underline{\Delta}^{\sigma})^3 \rangle}_0 - \underbrace{\langle (\underline{\Delta}^{\sigma})^2 \rangle}_0 \underbrace{\langle \underline{\Delta}^{\sigma} \rangle}_0 = 0 . \quad (\text{C.337})$$

**QED**

---

<sup>11</sup>Do not confuse the sample index  $\sigma$  and the standard deviation  $\sigma$ .

**Claim 16**

$$\left\langle \widehat{\underline{\sigma}^2}, \widehat{\underline{\mu}} \right\rangle = 0 . \quad (\text{C.338})$$

**proof:**

$$\left\langle \widehat{\underline{\sigma}^2}, \widehat{\underline{\mu}} \right\rangle = \frac{1}{n(n-1)} \sum_{\sigma, \sigma'} \left\langle \left( \underline{x}^\sigma - \frac{1}{n} \sum_{\sigma''} \underline{x}^{\sigma''} \right)^2, \underline{x}^{\sigma'} \right\rangle \quad (\text{C.339})$$

$$= \frac{1}{n(n-1)} \sum_{\sigma, \sigma'} \left\langle \left( \underline{x}^\sigma - \frac{1}{n} \sum_{\sigma''} \underline{x}^{\sigma''} \right)^2, \underline{\Delta}^{\sigma'} \right\rangle \quad (\text{C.340})$$

$$= \frac{1}{n(n-1)} \sum_{\sigma, \sigma'} \left\langle \left( \underline{\Delta}^\sigma - \frac{1}{n} \sum_{\sigma''} \underline{\Delta}^{\sigma''} \right)^2, \underline{\Delta}^{\sigma'} \right\rangle \quad (\text{C.341})$$

$$= 0 \quad \text{by Claim 15 .} \quad (\text{C.342})$$

**QED**

## C.36 Chi-square distribution

This section is based on Ref.[100].

$$\underline{q} \longleftrightarrow \underline{z}.$$

Figure C.12: Bnet used to define the Chi-square distribution.

Let  $q \in \mathbb{R}$  and  $\underline{z} = \{z_i\}_{i=0,1,\dots,\nu-1}$  where  $z_i \in \mathbb{R}$ . Consider the bnet of Fig.C.12. The TPMs, printed in blue, for that bnet, are as follows:<sup>12</sup>

$$P(z_i) = \mathcal{N}(z_i; \mu = 0, \sigma^2 = 1) . \quad (\text{C.343})$$

We want

$$\underline{q} = \sum_{i=0}^{\nu-1} (z_i)^2 \quad (\text{C.344})$$

so  $P(q|z.)$  is a Dirac delta function:

$$P(q|z.) = \delta(q - \sum_{i=0}^{\nu-1} (z_i)^2) . \quad (\text{C.345})$$

---

<sup>12</sup>Don't confuse the  $q$  independent constant  $\mathcal{N}(!q)$  with the normal probability distribution  $\mathcal{N}(x; \mu, \sigma^2)$ .

Therefore

$$P(q) = \prod_{i=0}^{\nu-1} \left\{ \int dz_i P(z_i) \right\} P(q|z.) \quad (\text{C.346})$$

$$= \mathcal{N}(!q) q^{\frac{\nu}{2}-1} e^{-q/2} = \chi^2(q; \nu), \quad (\text{C.347})$$

where  $\mathcal{N}(!q)$  is a constant that does not depend on  $q$  and is adjusted so that  $\int_0^\infty dq P(q) = 1$ .

## C.37 Student's t-distribution

This section is based on Ref.[156].

Let  $x[\sigma] = x^\sigma$ . Consider i.i.d.real variables  $(x^\sigma)_{\sigma=0,1,\dots,n-1}$  such that<sup>13</sup>

$$E[\underline{x}^\sigma] = \mu \quad (\text{C.348})$$

$$\langle \underline{x}^\sigma, \underline{x}^{\sigma'} \rangle = \delta(\sigma, \sigma') \sigma^2. \quad (\text{C.349})$$

$$\widehat{\mu} = \bar{x} = \frac{1}{n} \sum_{\sigma} x^\sigma \quad (\text{C.350})$$

$$(\widehat{\sigma^2})_\infty = \frac{1}{n} \sum_{\sigma} (x^\sigma - \mu)^2 \quad (\text{C.351})$$

$$\widehat{\sigma^2} = \frac{1}{n-1} \sum_{\sigma} (x^\sigma - \widehat{\mu})^2. \quad (\text{C.352})$$

If we define

$$z = \frac{\widehat{\mu} - \mu}{\frac{\sigma}{\sqrt{n}}}, \quad (\text{C.353})$$

then  $\underline{z}$  has a Standard Normal Distribution (SND):

$$P(z) = \frac{1}{\sqrt{2\pi}} e^{-\frac{z^2}{2}} = \mathcal{N}(z; \mu = 0, \sigma^2 = 1) \quad (\text{C.354})$$

But what if we allow the standard deviation  $\sigma$  to fluctuate in the expression Eq.(C.353) for  $z$ ? Define

$$t = \frac{\widehat{\mu} - \mu}{\sqrt{\frac{\widehat{\sigma^2}}{n}}}. \quad (\text{C.355})$$

---

<sup>13</sup>Do not confuse the sample index  $\sigma$  and the standard deviation  $\sigma$ .

Then one can show that  $\underline{t}$  has the **Student's t-distribution**  $\text{Stud}(t; \nu = n - 1)$  given by:

$$P(t) = \mathcal{N}(!t)(1 + \frac{t^2}{\nu})^{-\frac{\nu+1}{2}} = \text{Stud}(t; \nu = n - 1) \quad (\text{C.356})$$

Note that if we use the approximation  $e^x \approx 1 + x + \mathcal{O}(x^2)$ , we can show that  $\text{Stud}(t)$  tends to the SND when  $n \gg 1$ :

$$P(t) = \mathcal{N}(!t)(1 + \frac{t^2}{\nu})^{-\frac{\nu+1}{2}} \quad (\text{C.357})$$

$$\approx \mathcal{N}(!t)e^{-\frac{t^2}{2}\frac{\nu+1}{\nu}} \quad (\text{C.358})$$

$$\approx \mathcal{N}(t; \mu = 0, \sigma^2 = 1). \quad (\text{C.359})$$

---

#### Partial derivation of the explicit form of $\text{Stud}(t)$ .

Note that the  $z$  definition Eq.(C.353) and the  $t$  definition Eq.(C.355), imply that

$$t = z \underbrace{\sqrt{\frac{\sigma^2}{\hat{\sigma}^2}}}_{\varrho}, \quad (\text{C.360})$$

In the expression  $\underline{t} = \underline{z}\varrho$ , the random variables  $\underline{z}$  and  $\varrho$  are independent because, as shown in Section C.35,  $\hat{\mu}$  and  $\hat{\sigma}^2$  are independent. Therefore, the random variable  $\underline{t}$  can be defined using the bnet of Fig.C.13.

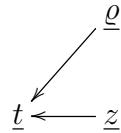


Figure C.13: Bnet used to define the Student's t-distribution.

The TPMs, printed in blue, for the bnet Fig.C.13, are as follows:

$$P(t|z, \varrho) = \delta(t - z\varrho) \quad (\text{Dirac delta function}) \quad (\text{C.361})$$

$$P(z) = \mathcal{N}(z; \mu = 0, \sigma^2 = 1) \quad (\text{C.362})$$

$$P(\varrho) = \text{given by Eq.(C.375) below.} \quad (\text{C.363})$$

Note that

$$P(\underline{t} = t) = P(\underline{z}\underline{\varrho} = t) \quad (\text{C.364})$$

$$= \int d\varrho P(\underline{z} = \frac{t}{\varrho} | \varrho) P(\varrho) \quad (\text{C.365})$$

$$= \int d\varrho \mathcal{N}(\frac{t}{\varrho}; 0, 1) P(\varrho) \quad (\text{C.366})$$

$$= \int d\varrho \frac{1}{\sqrt{2\pi}} e^{-\frac{1}{2}(\frac{t}{\varrho})^2} P(\varrho) . \quad (\text{C.367})$$

If we define  $q$  by

$$q = \frac{n-1}{\varrho^2} , \quad (\text{C.368})$$

then

$$q = \frac{(n-1)\widehat{\sigma}^2}{\sigma^2} = \frac{1}{\sigma^2} \sum_{\sigma=0}^{n-1} (x^\sigma - \widehat{\mu})^2 . \quad (\text{C.369})$$

As a consequence of "Cochran's Theorem" (see Ref.[102]),  $\underline{q}$  given by Eq.(C.369) must have a Chi-square probability distribution with  $\nu = n - 1$  degrees of freedom:<sup>14</sup>

$$P(q) = \chi^2(q; \nu = n - 1) \quad (\text{C.370})$$

Henceforth, let  $\nu = n - 1$ . From the definition Eq.(C.368) of  $q$ , we get

$$dq = \frac{-2\nu}{\varrho^3} d\varrho . \quad (\text{C.371})$$

Therefore,

$$P(\varrho)d\varrho = P(q)dq \quad (\text{C.372})$$

$$= \chi^2\left(\frac{\nu}{\varrho^2}; \nu\right) \frac{(-2\nu)}{\varrho^3} d\varrho \quad (\text{C.373})$$

$$= \mathcal{N}(!\varrho) \left(\frac{\nu}{\varrho^2}\right)^{\frac{\nu}{2}-1} e^{-\frac{\nu}{2\varrho^2}} \frac{d\varrho}{\varrho^3} \quad (\text{C.374})$$

$$= \mathcal{N}(!\varrho) \frac{d\varrho}{\varrho^{\nu+1}} e^{-\frac{\nu}{2\varrho^2}} . \quad (\text{C.375})$$

---

<sup>14</sup>Note that this  $q$  is a quadratic form  $q = \vec{x}^T M \vec{x}$ , where  $\vec{x}$  is an  $n$  dimensional column vector with components  $x^\sigma$ , and  $M$  is an  $n \times n$  matrix. Cochran's Theorem diagonalizes  $M$  and replaces the vectors  $\vec{x}$  by equivalent ones in a new basis. Then the number of *DOFs* (degrees of freedom) of the chi-square distribution is the number of non-zero diagonal elements in the diagonalized  $M$  (this number is called the rank of  $M$ ). In the particular case of Eq.(C.369), *DOF* =  $n - 1$ .

Hence,

$$P(t) = \mathcal{N}(!t) \int_0^\infty \frac{d\varrho}{\varrho^{\nu+1}} e^{-\frac{\nu}{2\varrho^2}} e^{-\frac{1}{2}(\frac{t}{\varrho})^2} \quad (\text{C.376})$$

$$= \mathcal{N}(!t) \int_0^\infty \frac{d\varrho}{\varrho^{\nu+1}} e^{-\frac{1}{2}\frac{t^2+\nu}{\varrho^2}}. \quad (\text{C.377})$$

## C.38 Hypothesis testing and 3 classic test statistics (Likelihood, Score, Wald)

Suppose we have data  $\vec{x} = [x^\sigma]_{\sigma=0,1,\dots,n_{\text{sam}}-1}$  which is distributed according to a probability distribution  $P(\vec{x}; \theta)$  which depends on some parameters  $\theta = (\theta_i)_{i=0,1,\dots,n-1} \in \mathbb{R}^n$ . We define the

- **Likelihood of  $\theta$**  by

$$L(\theta) = P(\vec{x}|\theta), \quad (\text{C.378})$$

- the **Maximum Likelihood estimate of  $\theta$**  by

$$\hat{\theta} = \underset{\theta}{\operatorname{argmax}} L(\theta), \quad (\text{C.379})$$

- the **log likelihood of  $\theta$**  by

$$LL(\theta) = \ln L(\theta), \quad (\text{C.380})$$

- the **Score or Lagrange Multiplier vector<sup>15</sup>** of  $\theta$  by

$$sc(\theta) = [sc_i(\theta)] \in \mathbb{R}^n, \quad (\text{C.381})$$

where

$$sc_i(\theta) = \partial_{\theta_i} LL(\theta), \quad (\text{C.382})$$

---

<sup>15</sup> $sc_i(\theta) = \partial_{\theta_i} LL(\theta)$  is called a Lagrange multiplier because to maximize  $LL(\theta)$  over  $\theta$  subject to the constraint  $\theta = \theta^*$ , we maximize the Lagrangian  $\mathcal{L} = LL(\theta) - \sum_i \alpha_i [\theta_i - \theta_i^*]$  over  $(\theta_i, \alpha_i)$  for all  $i$ . The latter gives  $\alpha_i = \partial_{\theta_i} LL(\theta^*)$  and  $\theta = \theta^*$ . For a general constrained optimization problem,  $\mathcal{L} = LL(\theta) - \sum_i \alpha_i c_i(\theta)$  for some constraint functions  $c_i(\theta)$ . Hence,  $\alpha_i = \partial_{\theta_i} LL / \partial_{\theta_i} c_i$  and  $c_i(\theta) = 0$  for all  $i$ . So, in general, a Lagrange multiplier is a ratio of two partial derivatives.

- and the **Fisher Information Matrix** of  $\theta$  by

$$FI(\theta) = [FI_{i,j}(\theta)] \in \mathbb{R}^{n \times n} \quad (\text{C.383})$$

where

$$FI_{i,j}(\theta) = -E_{\vec{x}|\theta}[\partial_{\theta_i} \partial_{\theta_j} \overbrace{\ln P(\vec{x}|\theta)}^{LL(\theta)}] . \quad (\text{C.384})$$

Note that if

$$LL(\theta) = \ln P(x|\theta) = \frac{-(\theta - \hat{\theta})^2}{2\sigma^2} + \mathcal{N}(!\theta) , \quad (\text{C.385})$$

then

$$sc(\theta) = \frac{-(\theta - \hat{\theta})}{\sigma^2} \quad (\text{C.386})$$

and

$$FI(\theta) = \frac{1}{\sigma^2} \quad (\text{C.387})$$

In hypothesis testing, one has a **null hypothesis**  $H_0: \theta = \theta^*$ , and an **alternative hypothesis**  $H_1: \theta \neq \theta^*$ . We use a **test statistic**  $\lambda(\theta^*, \hat{\theta}) \geq 0$  which measures a kind of distance or separation between the estimate  $\hat{\theta}$  and the value  $\theta^*$  for the null Hypothesis  $H_0$ . For some **confidence level**  $C > 0$ , if  $\lambda(\theta^*, \hat{\theta}) > C$ ,  $H_0$  is **rejected**, whereas if  $\lambda(\theta^*, \hat{\theta}) \leq C$ ,  $H_0$  is **accepted**.

$\alpha = 1 - C$  is called the **significance level**. Usually  $\alpha \ll 1$  represents the area under both tails of a Normal distribution, and  $C \approx 1$  represents all the area except the tails of a Normal distribution.

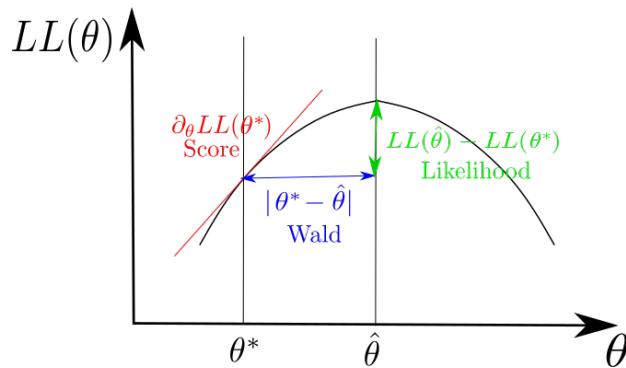


Figure C.14: For  $n = 1$  and  $\theta \in \mathbb{R}$ , this figure shows the geometrical significance of certain quantities that characterize the 3 classic test statistics (Likelihood, Score, Wald) for hypothesis testing.

Henceforth in this section, we will occasionally use the Einstein summation convention; i.e., implicit sum over repeated indices.

Three classic test statistics are (See Fig.C.14):

1. **Likelihood Ratio test statistic** (Ref.[133].)

$$\lambda_{Li} = 2 \ln \left[ \frac{L(\hat{\theta})}{L(\theta^*)} \right] = 2[LL(\hat{\theta}) - LL(\theta^*)] \quad (\text{C.388})$$

2. **Score (a.k.a. Lagrange multiplier) test statistic** (Ref.[151].)

$$\lambda_{Sc} = \partial_{\theta_i} LL(\theta^*) [FI(\theta^*)^{-1}]_{i,j} \partial_{\theta_j} LL(\theta^*) \quad (\text{C.389})$$

$$= \frac{[\partial_{\theta} LL(\theta^*)]^2}{FI(\theta^*)} \quad \text{if } n = 1 \quad (\text{C.390})$$

Doesn't depend on  $\hat{\theta}$ .

3. **Wald test statistic** (Ref.[166].)

$$\lambda_{Wa} = (\hat{\theta} - \theta^*)_i \left[ \langle \underline{\hat{\theta}}, \underline{\hat{\theta}}^T \rangle^{-1} \right]_{i,j} (\hat{\theta} - \theta^*)_j \quad (\text{C.391})$$

$$= \frac{(\theta^* - \hat{\theta})^2}{\langle \hat{\theta}, \hat{\theta} \rangle} \quad \text{if } n = 1 \quad (\text{C.392})$$

More generally, one can replace  $\theta^* \rightarrow R\theta^*$  and  $\hat{\theta} \rightarrow R\hat{\theta}$  in Eq.(C.391), where  $\theta^*$  and  $\hat{\theta}$  are  $n$  dimensional column vectors, and  $R \in \mathbb{R}^{\nu \times n}$ . The null and alternative hypotheses become:  $H_0 : R\theta = R\theta^*$  and  $H_1 : R\theta \neq R\theta^*$ . Note that  $\nu$  is the number of constraints imposed by the null hypothesis.  $R$  is called a reparametrization of  $\theta$ . The Wald test is not reparametrization invariant (i.e.,  $R$  invariant), but the Likelihood Ratio test is.

Note that if  $LL(\theta)$  is given by Eq.(C.385), then  $\langle \hat{\theta}, \hat{\theta} \rangle = \sigma^2 = \frac{1}{FI(\theta)}$ . Hence,

$$\lambda_{Li} = \lambda_{Sc} = \lambda_{Wa} = \frac{(\hat{\theta} - \theta^*)^2}{\sigma^2} \quad (\text{C.393})$$

Many other commonly used test statistics (or their squares) are special cases of one of the 3 classic test statistics. For example, the z-statistic used with normal distributions, the t-statistic used with the Student t-distribution, the F-statistic used in linear regression, the chi-squared statistic used to do Pearson's chi-squared test.

### Asymptotic Behavior

If the data  $\vec{x}$  is i.i.d.,

$$P(\vec{x}|\theta) = \prod_{\sigma=0}^{nsam-1} P(x^\sigma|\theta) \quad (\text{C.394})$$

Hence, as  $nsam \rightarrow \infty$ ,

$$LL(\theta) = \ln P(\vec{x}|\theta) \quad (\text{C.395})$$

$$= \sum_{\sigma} \ln P(x^\sigma|\theta) \quad (\text{C.396})$$

$$\rightarrow nsam \sum_x P(x|\theta) \ln P(x|\theta) \quad (\text{C.397})$$

$$= -nsam H(\underline{x}|\theta) \quad (\text{C.398})$$

Thus, *maximizing* the log likelihood  $LL(\theta)$  and *minimizing* the entropy  $H(\underline{x}|\theta)$  give the same estimate  $\hat{\theta}$ .

When the data is i.i.d. and  $nsam \rightarrow \infty$ , it is also possible to prove that the 3 test statistics defined above all tend to the same probability distribution, namely  $\mathcal{X}^2(\theta^*; \nu)$ , the chi-square distribution with  $\nu$  degrees of freedom, where  $\theta \in \mathbb{R}^n$ ,  $R \in \mathbb{R}^{\nu \times n}$ , and  $\nu = n$  if  $R = 1$ .

## C.39 Error Bars

Never report measurements without error bars!!

Assume a distribution with mean  $\mu$  and standard deviation  $\sigma$  for a subpopulation with  $n$  samples.

$SE = \frac{\sigma}{\sqrt{n}}$  is called the **standard error**.

Some popular types of error bars:

- **Box and Whiskers plot (a.k.a. Boxplot)**

See Fig.C.15.  $IQR$  stands for **Intermediate Quantile Range**. Sometimes, the endpoints of the error bars are taken to be the minimum and maximum samples instead of  $Q_1 - 1.5 * IQR$  and  $Q_3 + 1.5 * IQR$ . The points that fall in the intervals  $[\min, Q_1 - 1.5 * IQR]$  and  $[Q_3 + 1.5 * IQR, \max]$  are called **outliers**.

- **Standard Deviation**

Error bar endpoints are located one standard deviation away from the mean.

$$\mu - \sigma < \mu < \mu + \sigma \quad (\text{C.399})$$

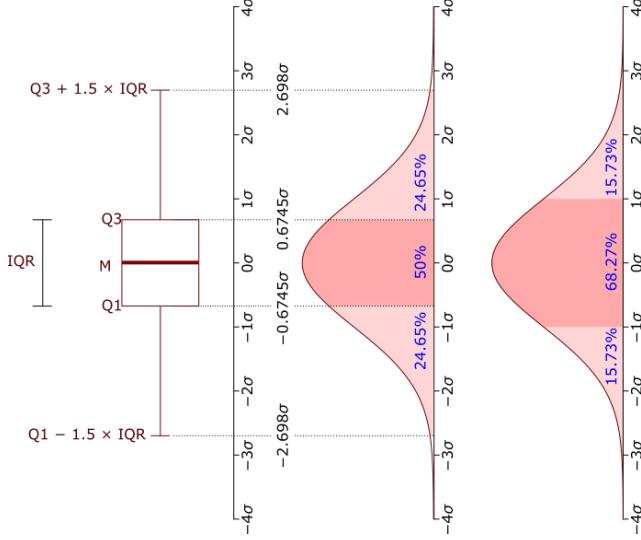


Figure C.15: Boxplot plot for Normal distribution  $\mathcal{N}(\mu = 0, \sigma)$ .  $Q_1$  and  $Q_3$  are the first and third quantiles, and  $M$  is the median (i.e., half-way point). For a non-normal skewed distribution,  $Q_1$  and  $Q_3$  are not equidistant from the median, and the median is not exactly equal to the mean.

- **Confidence Interval**

$$\mu - |z^*|SE < \mu < \mu + |z^*|SE \quad (\text{C.400})$$

$|z^*| = 1.96$  for a confidence level of 95%.

The origin of Eq.(C.400) is explained in the next section entitled “Confidence Intervals”. Confidence intervals are derived from the Gaussian in Fig.C.16, which should not be confused with the Gaussian of Fig.C.15. They are different!

## C.40 Confidence Interval

Normal distribution with mean  $\mu$  and standard deviation  $\sigma$ :

$$\mathcal{N}(x; \mu, \sigma^2) = \frac{1}{\sigma\sqrt{2\pi}} e^{-\frac{(x-\mu)^2}{2\sigma^2}}. \quad (\text{C.401})$$

Standard Normal Distribution (SND):

$$P(z) = \mathcal{N}(z; 0, 1) \quad (\text{C.402})$$

Cumulative distribution for  $P(z)$ :

$$\Phi(z) = \int_{-\infty}^z dz' P(z') . \quad (\text{C.403})$$

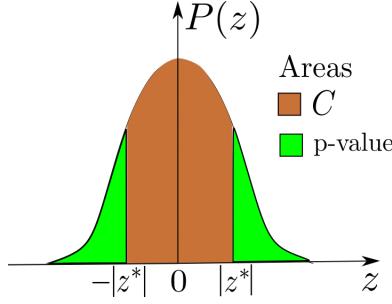


Figure C.16: Interpretation of confidence level  $C$  and p-value as areas under curve of the Standard Normal Distribution (SND).

**Confidence Level  $C$**  and corresponding  $|z^*|$  **value** (see Fig.C.16):

$$C = \int_{-|z^*|}^{|z^*|} dz P(z) = \Phi(|z^*|) - \Phi(-|z^*|) = 2 \left( \Phi(|z^*|) - \frac{1}{2} \right) \quad (\text{C.404})$$

Equivalent definition:

$$C = P \left( \underbrace{\frac{|\underline{x} - \mu|}{\frac{\sigma}{\sqrt{n}}}}_{|z|} < |z^*| \right) \quad (\text{C.405})$$

For  $C = 95\%$ ,  $|z^*| = 1.960 \approx 2$ . For  $C = 99\%$ ,  $|z^*| = 2.576$ .

Area of each tail in Fig.C.16 is usually called  $\alpha$ , and the area of both tails is called the **p-value**:

$$C + \underbrace{2\alpha}_{p\text{-value}} = 1. \quad (\text{C.406})$$

Estimators<sup>16</sup> of mean  $\mu$  and standard deviation  $\sigma$  from measurements  $x^\sigma$  of a sub-population  $\Sigma_1$  of size  $n = |\Sigma_1|$ :

$$\hat{\mu} = \bar{x} = \frac{1}{n} \sum_{\sigma \in \Sigma_1} x^\sigma \quad (\text{C.407})$$

$$\hat{\sigma}^2 = \frac{1}{n-1} \sum_{\sigma \in \Sigma_1} (x^\sigma - \bar{x})^2 \quad (\text{C.408})$$

We get from Eq.(C.405), the **Error bars (a.k.a. confidence intervals)** and **Error  $E$  (a.k.a. margin of error)**:

---

<sup>16</sup>Don't confuse the sample index  $\sigma$  with the standard deviation  $\sigma$ .

$$\text{estimate of } x \text{ with error bars} = \bar{x} \pm |z^*| \underbrace{\frac{\hat{\sigma}}{\sqrt{n}}}_{E} \quad (\text{C.409})$$

$$n = \left( \frac{|z^*| \hat{\sigma}}{E} \right)^2 \quad (\text{C.410})$$

So far, we have assumed that the sub-population (a.k.a. sample population) is normally distributed. This might be false for several reasons. Some red flags: (1)  $n$  is too small (according to a rule of thumb derived from Central Limit Theorem,  $n$  should be larger than 30 to insure a Normal Distribution). (2) Sub-population not truly random (i.i.d.) because was taken without replacement. In many cases, especially when  $n < 30$ , the Student's t-distribution models the sub-population statistics much better than the Normal distribution.

The Student's t-distribution  $\text{Stud}(t; \nu = n - 1)$ , depends on a parameter  $\nu$  called the number of degrees of freedom. In the case being considered here,  $\nu$  equals the sub-population size  $n$  minus one. When fitting the data with  $\text{Stud}()$ , variable  $t$  replaces variable  $z$ , and  $\text{Stud}(t; \nu = n - 1)$  replaces the Standard Normal distribution (SND)  $\mathcal{N}(z; \mu = 0, \sigma = 1)$ .  $\text{Stud}()$  is symmetric about the origin like SND, but its tails are fatter. When fitting the data with  $\text{Stud}()$ , the  $|z^*|$  value is replaced by a  $|t^*|$  value. Eq.(C.404) is replaced by

$$C = \int_{-|t^*|}^{|t^*|} dt \text{Stud}(t) = \Phi_S(|t^*|) - \Phi_S(-|t^*|) = 2 \left( \Phi_S(|t^*|) - \frac{1}{2} \right), \quad (\text{C.411})$$

where  $\Phi_S()$  is the cumulative distribution for  $\text{Stud}()$ . Also, Eq.(C.409) is replaced by

$$\text{estimate of } x \text{ with error bars} = \bar{x} \pm |t^*| \underbrace{\frac{\hat{\sigma}}{\sqrt{n}}}_{E}. \quad (\text{C.412})$$

Tables of  $|t^*|(C, \nu = n - 1)$  are available. Note that  $|t^*|$  depends on both  $C$  and  $\nu$ , whereas  $|z^*|(C)$  depends only on  $C$ .

## C.41 Score p-value

When defining error bars and confidence intervals in Fig.C.16, we defined a triplet of values  $(z, C, p)$  where  $C + p = 1$ . In this section, we will consider a different triplet of those values. We will refer to the triplet  $(z_{th}, C_{th}, p_{th})$  used in error bars as the **threshold triplet**, and to the triplet  $(z_{sc}, C_{sc}, p_{sc})$  introduced in this section as the **score triplet**. When we do hypothesis testing, if  $|z_{sc}| > |z_{th}|$  (i.e., if  $z_{sc}$  falls outside the error bars), we say that the null hypothesis is violated. Equivalently, we say the null hypothesis is violated if  $p_{sc} < p_{th} = 1 - C_{th} = 0.05$  typically. Most statistics

books do a poor job at distinguishing between the threshold and score triplets, and seldom use distinguishing subscripts like  $th$  and  $sc$ . In this book, we will often drop the  $sc$  subscripts, but we will try not to drop the  $th$  subscripts. Often, instead of a  $th$  subscript, we will use an asterisk superscript. For instance, instead of  $z_{th}$ , we might use  $z^*$ . When statisticians use the term “p-value”, they are usually referring to the score p-value, although not always.

Given a parameter  $\theta$ , call  $\theta = \theta_0$  (or  $\theta < \theta_0$  or  $\theta > \theta_0$ ) the **null hypothesis**  $h_0$ , and call the negation of  $h_0$  (i.e.,  $\theta \neq \theta_0$  (or  $\theta \geq \theta_0$  or  $\theta \leq \theta_0$ )) the **alternative or opposite hypothesis**  $h_1$ . Assume we are given data  $\vec{x} = \{x^\sigma | \sigma \in \Sigma\}$ . Assume also that we are given distributions  $P(\underline{x} = x|h)$  for  $h \in \{h_0, h_1\}$ , and  $P(\underline{x} = x)$ . Now let

$$P(\vec{x}|h) = \prod_{\sigma} P(\underline{x} = x^\sigma|h) \quad (\text{C.413})$$

$$P(\vec{x}) = \prod_{\sigma} P(\underline{x} = x^\sigma) \quad (\text{C.414})$$

(so the  $x^\sigma$  are i.i.d.).

A Bayesian would assume that there is a prior  $P(h)$ , and use it to calculate  $P(h|\vec{x}) = \frac{P(\vec{x}|h)P(h)}{P(\vec{x})}$ .  $P(\underline{h} = h_0|\vec{x})$  is the probability that the null hypothesis is true. A p-value is a monotonically increasing function of  $P(\underline{h} = h_0|\vec{x})$ , so Bayesians have no trouble saying that **a p-value is a measure of  $P(\underline{h} = h_0|\vec{x})$ , i.e., a measure of the probability that the null-hypothesis is true**.

Frequentists, on the other hand, believe that  $h$  is a “parameter” which has an priori value; therefore, it’s not a random variable, so  $P(\underline{h} = h_0|\vec{x})$  is undefined. To circumvent this objection, a frequentist would conduct a bunch of experiments to decide whether  $h$  equals  $h_0$  or  $h_1$ . Then he/she would say the p-value is the fraction of those experiments that claim  $h = h_0$ .

Next, we explain in more detail the correct way of thinking about p-values, according to Frequentists. p-values were invented by Frequentists, so it’s worth hearing what they have to say about them. The Frequentist definition is not against Bayesianism, and Bayesians, unlike Frequentists, don’t accuse Frequentists of having a sinfully incorrect definition of p-values. A Bayesian would just say: our definition of p-values (shown in red above) is not incorrect, but the Frequentist definition is more precise than ours, and doesn’t assume a particular form for a prior. We welcome it.

Call the random variable  $\underline{t}$  the **test or score statistic** and let  $t^*$  be a user defined parameter.  $\underline{t}$  and  $t^*$  are defined so that when  $\underline{t} = t^*$ , the  $h_0$  hypothesis is on the threshold between being and not being satisfied. Frequentists define the **p-value**  $p$  as

$$p = \begin{cases} P(\underline{t} \geq t^*|h_0) & \text{right-sided-tail, if } h_0 \text{ is } \theta < \theta_0 \\ P(\underline{t} \leq t^*|h_0) & \text{left-sided-tail, if } h_0 \text{ is } \theta > \theta_0 \\ P(|\underline{t}| > |t^*| |h_0) & \text{double-sided-tail, if } h_0 \text{ is } \theta = \theta_0 \end{cases} \quad (\text{C.415})$$

Thus, for a Frequentist, a p-value is a probabilistic weight of the region where the  $h_0$  hypothesis is defined (by the user) to be violated. If that weight is large, then the region where the  $h_0$  hypothesis is defined to be satisfied is small, which means the  $h_0$  hypothesis is expected to be close to the truth. The larger the p-value, the closer  $h_0$  is expected to be near the truth, just like the Bayesian definition says. Note that the p-value is a probability so it ranges in value from 0 to 1.

Suppose we are given a sub-population with  $n$  samples, mean  $\bar{x}$  and variance  $\hat{\sigma}^2$ . Let  $\theta_0 = \mu_0$ . Define

$$\underline{t} = \underline{z} = \frac{\underline{x} - \mu_0}{\frac{\hat{\sigma}}{\sqrt{n}}} . \quad (\text{C.416})$$

For  $n > 30$ ,

$$P(\underline{z} \geq z^* | h_0) = 1 - \Phi(z^*) = \Phi(-z^*) \quad \text{if } h_0 \text{ is } \mu < \mu_0 \quad (\text{C.417a})$$

$$P(\underline{z} \leq z^* | h_0) = \Phi(z^*) \quad \text{if } h_0 \text{ is } \mu > \mu_0 \quad (\text{C.417b})$$

$$P(|\underline{z}| \geq |z^*| | h_0) = 2\Phi(-|z^*|) \quad \text{if } h_0 \text{ is } \mu = \mu_0 \quad (\text{C.417c})$$

where  $\Phi(x)$  is the cumulative distribution for the Standard Normal Distribution  $\mathcal{N}(x; \mu = 0, \sigma = 1)$ . For  $n < 30$ ,  $\Phi()$  is replaced by  $\Phi_S()$ , where  $\Phi_S()$  is the cumulative distribution for the Student t-distribution  $\text{Stud}(x; \nu = n - 1)$ . Note that Eq.(C.417c) agrees with Eq.(C.405).

The quantity

$$\hat{z}_{sc} = \frac{\bar{x} - \mu_0}{\frac{\hat{\sigma}}{\sqrt{n}}} \quad (\text{C.418})$$

is called the **z score estimator**. If  $|\hat{z}_{sc}| > |z^*|$ , then the  $h_0$  hypothesis is defined to be violated (for the double sided case).

## C.42 Convex/Concave functions, Jensen's Inequality

Suppose  $f : \mathbb{R} \rightarrow \mathbb{R}$ .  $f(x)$  is a **concave function** if looks like a cave ( $\cap$ ) (i.e.,  $f''(x) > 0$  if differentiable) and it's a **convex function** if it looks like a valley ( $\cup$ ) (i.e.,  $f''(x) < 0$  if differentiable). More generally, if  $f : \mathbb{R}^a \rightarrow \mathbb{R}$ ,  $f(x)$  is said to be concave if  $f(\alpha x + \beta y) \geq \alpha f(x) + \beta f(y)$  and convex if  $f(\alpha x + \beta y) \leq \alpha f(x) + \beta f(y)$  for  $\alpha, \beta \in \mathbb{R}$  and  $x, y \in \mathbb{R}^a$ .

Suppose  $f : \mathbb{R}^a \rightarrow \mathbb{R}$  is a convex function. Let  $\alpha, \beta$  be non-negative numbers that sum to 1, and  $x, y \in \mathbb{R}^a$ . From the definition of convexity, it follows that (see Fig.C.17 for a geometrical representation of this when  $a = 1$ )

$$f(\alpha x + \beta y) \leq \alpha f(x) + \beta f(y) \quad (\text{C.419})$$

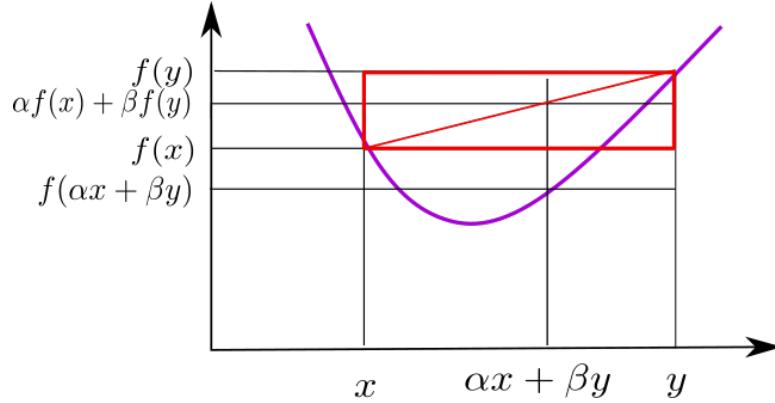


Figure C.17: Jensen's inequality for sum of 2 terms, when  $f : \mathbb{R} \rightarrow \mathbb{R}$  is convex.

**Jensen's inequality** is a simple generalization of this inequality to sums of more than 2 terms. Let  $\{p_i\}_{i=0}^n$  be non-negative numbers that sum to one. Also assume that  $\{x_i\}_{i=0}^n$  are elements of  $\mathbb{R}^a$ . Then

$$f\left(\sum_{i=1}^n p_i x_i\right) \leq \sum_{i=1}^n p_i f(x_i) \quad (\text{C.420})$$

or, written in terms of expected values,

$$f(E[\underline{x}]) \leq E[f(\underline{x})] \quad (\text{C.421})$$

The same result is true if  $f$  is concave instead of convex and we reverse the inequality signs.

## C.43 Chebyshev's inequality

Chebyshev's inequality (CI) gives an upper bound for the area under the 2 tails (left and right ones) of a probability distribution.

Below, we follow the common practice of proving CI as a corollary of Markov's Inequality (MI).

**Claim 17 (Markov's Inequality)** *Let  $\underline{x}$  be a non-negative random variable and let  $a > 0$ . Then*

$$P(\underline{x} \geq a) \leq \frac{E[\underline{x}]}{a} \quad (\text{C.422})$$

**proof:**

$$\frac{E[\underline{x}]}{a} = \frac{\int_0^\infty dx \ x P(x)}{a} \quad (\text{C.423})$$

$$\geq \frac{\int_a^\infty dx \ x P(x)}{a} \quad (\text{C.424})$$

$$\geq \frac{\int_a^\infty dx \ a P(x)}{a} \quad (\text{C.425})$$

$$= P(\underline{x} \geq a) \quad (\text{C.426})$$

**QED**

**Claim 18 (Chebyshev's inequality)** Let  $\underline{x}$  be a random variable with mean  $\mu$  and variance  $\sigma^2$ . Then for any real number  $k > 0$ ,

$$P(|\underline{x} - \mu| \geq k\sigma) \leq \frac{1}{k^2} \quad (\text{C.427})$$

**proof:**

$$P(|\underline{x} - \mu| \geq k\sigma) = P(|\underline{x} - \mu|^2 \geq k^2\sigma^2) \quad (\text{C.428})$$

$$\leq \frac{\sigma^2}{k^2\sigma^2} \quad (\text{by MI}) \quad (\text{C.429})$$

$$= \frac{1}{k^2} \quad (\text{C.430})$$

**QED**

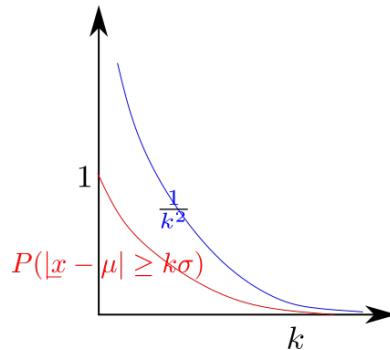


Figure C.18: Pictorial representation of Chebyshev's Inequality (CI). Markov's Inequality (MI) has a similar representation, but  $k$  is proportional to  $\sqrt{a}$ , so the upper bound for MI goes as  $1/a$  instead of  $1/k^2$ .

See Fig.C.18 for a pictorial representation of CI. Note that the CI approximation is always a bad approximation for small  $k$ , and might not become good

even for large  $k$ . For example, if the  $\underline{x}$  distribution is a box centered at  $\mu$ , then  $P(|\underline{x} - \mu| \geq k\sigma) = 0$  for  $k\sigma$  larger than the width of the box, so  $1/k^2$  is a terrible approximation for large  $k$  too.

---

A (1 dimensional) Center of Mass (CM) for a unit mass object is an expectation value where the probability distribution is a mass distribution. Hence, it's not too surprising that MI can be interpreted in terms of CMs.

### Physics Intuition for MI in terms of CMs:

$$\underbrace{\int_0^\infty dx xP(x)}_{E[\underline{x}] = CM} = \underbrace{\frac{\int_0^a dx xP(x)}{P(\underline{x} < a)}}_{E_{\underline{x} < a}[\underline{x}] = CM^-} \underbrace{P(\underline{x} < a)}_{f^-} + \underbrace{\frac{\int_a^\infty dx xP(x)}{P(\underline{x} > a)}}_{E_{\underline{x} > a}[\underline{x}] = CM^+} \underbrace{P(\underline{x} > a)}_{f^+} \quad (\text{C.431})$$

$$CM \underbrace{(f^+ + f^-)}_{=1} = CM^- f^- + CM^+ f^+ \quad (\text{C.432})$$

$$\geq CM^+ f^+ \quad (\text{C.433})$$

$$\geq af^+ \quad (\text{because } CM^+ \geq a) \quad (\text{C.434})$$

You can think of  $CM^+ f^+$  as a torque with moment arm=  $CM^+$  and force=  $f^+$ . In this picture, MI is the approximation of a torque with moment arm= CM and force= 1, by a smaller torque with moment arm= any real  $a > 0$  and force=  $f^+ \leq 1$ .

## C.44 Short Summary of Boolean Algebra

See Ref.[97] for more info about this topic.

Suppose  $x, y, z \in \{0, 1\}$ . Define

$$x \text{ or } y = x \vee y = x + y - xy , \quad (\text{C.435})$$

$$x \text{ and } y = x \wedge y = xy , \quad (\text{C.436})$$

and

$$\text{not } x = \bar{x} = 1 - x , \quad (\text{C.437})$$

where we are using normal addition and multiplication on the right hand sides.<sup>17</sup>

Actually, since  $x \wedge y = xy$ , we can omit writing the symbol  $\wedge$ . The symbol  $\wedge$  is useful to exhibit the symmetry of the identities, and to remark about the analogous identities for sets, where  $\wedge$  becomes intersection  $\cap$  and  $\vee$  becomes union  $\cup$ . However, for practical calculations,  $\wedge$  is an unnecessary nuisance.

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<sup>17</sup>Note the difference between  $\vee$  and modulus 2 addition  $\oplus$ . For  $\oplus$  (a.k.a. XOR):  $x \oplus y = x + y - 2xy$ .

Associativity	$x \vee (y \vee z) = (x \vee y) \vee z$ $x \wedge (y \wedge z) = (x \wedge y) \wedge z$
Commutativity	$x \vee y = y \vee x$ $x \wedge y = y \wedge x$
Distributivity	$x \wedge (y \vee z) = (x \wedge y) \vee (x \wedge z)$ $x \vee (y \wedge z) = (x \vee y) \wedge (x \vee z)$
Identity	$x \vee 0 = x$ $x \wedge 1 = x$
Annihilator	$x \wedge 0 = 0$ $x \vee 1 = 1$
Idempotence	$x \vee x = x$ $x \wedge x = x$
Absorption	$x \wedge (x \vee y) = x$ $x \vee (x \wedge y) = x$
Complementation	$x \wedge \bar{x} = 0$ $x \vee \bar{x} = 1$
Double negation	$\overline{(\bar{x})} = x$
De Morgan Laws	$\bar{x} \wedge \bar{y} = \overline{(x \vee y)}$ $\bar{x} \vee \bar{y} = \overline{(x \wedge y)}$

Table C.1: Boolean Algebra Identities

Since  $x \in \{0, 1\}$ ,

$$P(\bar{x}) = 1 - P(x). \quad (\text{C.438})$$

Clearly, from analyzing the simple event space  $(x, y) \in \{0, 1\}^2$ ,

$$P(x \vee y) = P(x) + P(y) - P(x \wedge y). \quad (\text{C.439})$$

## C.45 Laplace transform

This section is a watered down version of the Wikipedia entry for Laplace Transforms (Ref.[130]), which we highly recommend.

Let  $0^- = 0 - \epsilon$ ,  $0^+ = 0 + \epsilon$  for some  $\epsilon \in \mathbb{R}$  such that  $0 < \epsilon \ll 1$ .

Let  $s = \sigma + i\omega$  for  $\sigma, \omega \in \mathbb{R}$ .  $\sigma$  is called the **decay constant** and  $\omega$  is called the **angular frequency**.

The **Laplace Transform (LT)** of  $f : [0, \infty] \rightarrow \mathbb{C}$  is defined as

$$\mathcal{L}[f](s) = \tilde{f}(s) = \int_{0^-}^{\infty} dt e^{-st} f(t) \quad (\text{C.440})$$

Note that the LT is a linear functional<sup>18</sup> because

---

<sup>18</sup>A functional  $\mathcal{F}[f]$  is a function of a function  $f$ , or, equivalently, a function of a vector with possibly infinitely many components given by  $[f(x)]_{\forall x}$ .

$$\mathcal{L}[af + bg](t) = a\mathcal{L}[f](t) + b\mathcal{L}[g](t) \quad (\text{C.441})$$

for  $f, g : [0, \infty] \rightarrow \mathbb{C}$  and  $a, b \in \mathbb{C}$ .

The **Inverse Laplace Transform** is defined so that

$$\mathcal{L}^{-1}[\underbrace{\mathcal{L}[f]}_{\tilde{f}}](t) = f(t) \quad (\text{C.442})$$

For LTs, we assume functions  $f(t)$  that vanish for  $t < 0^-$ . They can jump to a finite value (with a step function) or an infinite value (with a Dirac delta function) at  $t = 0$ , but must vanish for  $t < 0^-$ . LTs are ideally suited for solving ordinary differential equations with **initial conditions** such as  $x(0) = 5$ ,  $\partial_t x(0) = 10$ .

name	formula	comment
<b>Bilateral Laplace transform (BLT)</b>	$\mathcal{B}[f](s) = \int_{-\infty}^{\infty} dt e^{-st} f(t)$	same as LT but with $-\infty < t < \infty$ instead of $t > 0$
<b>Fourier transform (FT)</b>	$\mathcal{F}[f](\omega) = \int_{-\infty}^{\infty} dt e^{-i\omega t} f(t)$	Same as BLT but with $s = i\omega \in i\mathbb{R}$
<b>Star Transform (ST)</b>	$\mathcal{L}^*[f](s) = \sum_{n=0}^{\infty} e^{-snT} f(nT)$	Same as LT but it samples only discrete points at $t = nT$
<b>Moment Generating Function</b>	$E_{\underline{x}}[e^{-s\underline{x}}] = \int_0^{\infty} dx e^{-sx} P(x)$ $\langle \underline{x}^n \rangle = [(-\partial_s)^n E_{\underline{x}}[e^{-s\underline{x}}]]_{s=0}$	Same as LT but for probability distribution $P : [0, \infty] \rightarrow [0, 1]$

Table C.2: Transforms that are akin to the Laplace transform. Don't be intimidated by all these transforms. They are all just fancy dot products like  $\vec{a} \cdot \vec{b}$ .

Table C.2 is a table of transforms that are akin to the LT. If the function  $f(t)$  does not vanish for  $t < 0$ , we can use the **Bilateral Laplace Transform (BLT)**. The BLT becomes the **Fourier transform (FT)** when  $s = i\omega$ . In this section, we will only discuss the LT.

The following intuition about LTs might be helpful to the reader. A LT is like a dot product of two vectors,  $e^{-st}$  and  $f(t)$ , except that in this case the index  $t$  for their components is an uncountable set  $[0, \infty)$ . As with all dot products, its maximum is achieved if the two vectors point in the same direction (this is what the Cauchy Schwartz inequality  $\vec{a} \cdot \vec{b} = |\vec{a}| |\vec{b}| \cos \theta \leq |\vec{a}| |\vec{b}|$  says). In this case, if we substitute  $f(t) = \tilde{f}(s_0) e^{s_0 t}$  on the right hand side of Eq.(C.440), we get

$$\tilde{f}(s) = \tilde{f}(s_0) \int_{0^-}^{\infty} dt e^{-(s-s_0)t} \quad (\text{C.443})$$

$$= \tilde{f}(s_0) \delta_+(s - s_0) \quad (\text{C.444})$$

So our intuition is this: whenever you see an equation involving LTs, replace each  $f(t)$  by the special case  $f(t) = e^{s_0 t} \tilde{f}$  (this is called a **phasor** when  $s_0 = i\omega_0$ ), and convince yourself that that the equation is valid in the special case of phasors.

Define the **Dirac delta function** by

$$\delta(t) = \int_{-\infty}^{\infty} d\omega e^{i\omega t} = \begin{cases} \infty & \text{if } t = 0 \\ 0 & \text{otherwise} \end{cases} \quad (\text{C.445})$$

and the **Heaviside step function** by

$$\mathbf{H}_a(t) = \mathbb{1}(t - a > 0) \quad (\text{C.446})$$

Next, we will list some examples and properties of LTs. Henceforth, we will use the following notation:

$$a, b \in \mathbb{C}$$

$$f, g : [0, \infty] \rightarrow \mathbb{C}$$

$$f(t) \xrightarrow{\mathcal{L}} \tilde{f}(s) \text{ means } \mathcal{L}[f](s) = \tilde{f}(s)$$

### C.45.1 Examples

- Dirac delta function

$$\delta(t - a) \xrightarrow{\mathcal{L}} e^{-sa} \quad (\text{C.447})$$

- Heaviside step function

$$\mathbf{H}_a(t) \xrightarrow{\mathcal{L}} \frac{1}{s} e^{-sa} \quad (\text{for } \operatorname{Re}(s) > 0, a > 0) \quad (\text{C.448})$$

- box

$$\mathbf{H}_0(t) - \mathbf{H}_a(t) \xrightarrow{\mathcal{L}} \frac{1}{s} (1 - e^{-sa}) \quad (\text{for } \operatorname{Re}(s) > 0, a > 0) \quad (\text{C.449})$$

- ramp

$$t \mathbf{H}_0(t) \xrightarrow{\mathcal{L}} \frac{1}{s^2} \quad (\text{for } \operatorname{Re}(s) > 0) \quad (\text{C.450})$$

- curved ramp

$$\frac{t^n}{n!} \mathbf{H}_0(t) \xrightarrow{\mathcal{L}} \frac{1}{s^{n+1}} \quad (\text{for } Re(s) > 0 \text{ and } n \geq 0) \quad (\text{C.451})$$

- sine, cosine

$$\sin(at) \mathbf{H}_0(t) \xrightarrow{\mathcal{L}} \frac{a}{s^2 + a^2} \quad (\text{C.452})$$

$$\cos(at) \mathbf{H}_0(t) \xrightarrow{\mathcal{L}} \frac{s}{s^2 + a^2} \quad (\text{C.453})$$

- polynomial rise, exponential drop

$$\frac{t^n}{n!} e^{-at} \mathbf{H}_0(t) \xrightarrow{\mathcal{L}} \frac{1}{(s+a)^{n+1}} \quad (\text{for } Re(s) > -a) \quad (\text{C.454})$$

- Exponential approach to steady state

$$(1 - e^{-at}) \mathbf{H}_0(t) \xrightarrow{\mathcal{L}} \frac{a}{s(s+a)} \quad (\text{for } Re(s) > 0, Re(s) > -a) \quad (\text{C.455})$$

## C.45.2 Properties

- Taylor series of  $f(t)$

$$\int_0^\infty dx e^{-x} \frac{x^n}{n!} = 1 \quad (\text{C.456})$$

$$\int_0^\infty dt e^{-st} \frac{t^n}{n!} = \frac{1}{s^{n+1}} \quad (\text{C.457})$$

$$\frac{t^n}{n!} \mathbf{H}_0(t) \xrightarrow{\mathcal{L}} \frac{1}{s^{n+1}} \quad (\text{C.458})$$

$$f(t) \mathbf{H}_0(t) = \mathbf{H}_0(t) \sum_{n=0}^{\infty} \frac{t^n}{n!} \partial_t^n f(0) \quad (\text{C.459})$$

$$\xrightarrow{\mathcal{L}} \sum_{n=0}^{\infty} \frac{1}{s^{n+1}} \partial_t^n f(0) \quad (\text{C.460})$$

- derivatives of  $\tilde{f}(s)$

$$(-t)f(t) \xrightarrow{\mathcal{L}} \partial_s \tilde{f}(s) \quad (\text{C.461})$$

$$(-t)^k f(t) \xrightarrow{\mathcal{L}} (\partial_s)^k \tilde{f}(s) \quad (\text{C.462})$$

- derivatives of  $f(t)$

Define

$$f^{\geq 1}(t) = f(t) - f(0^+) \mathbf{H}_0(t) \quad (\text{C.463})$$

$$f^{\geq 2}(t) = f(t) - f(0^+) \mathbf{H}_0(t) - t f'(0^+) \mathbf{H}_0(t) \quad (\text{C.464})$$

$$\partial_t f(t) \xrightarrow{\mathcal{L}} s \widetilde{f}^{\geq 1}(s) \quad (\text{C.465})$$

$$= s \widetilde{f}(s) - f(0^+) \quad (\text{a.k.a. } f(t) \text{ \textbf{differentiator}}) \quad (\text{C.466})$$

For example, for  $f(t) = \frac{t^n}{n!} \mathbf{H}_0(t)$ , we have  $\tilde{f}(s) = \frac{1}{s^{n+1}}$ , so Eq.(C.466) becomes

$$\frac{t^{n-1}}{(n-1)!} \xrightarrow{\mathcal{L}} \frac{1}{s^n} \quad (\text{C.467})$$

$$(\partial_t)^2 f(t) \xrightarrow{\mathcal{L}} s^2 \widetilde{f}^{\geq 2}(s) \quad (\text{C.468})$$

$$= s^2 \widetilde{f}(s) - s f'(0^+) - f(0^+) \quad (\text{C.469})$$

- integral of  $f(t)$  (a.k.a.  $f(t)$  **integrator**)

$$\int_0^t d\tau f(\tau) \xrightarrow{\mathcal{L}} \frac{1}{s} \tilde{f}(s) \quad (\text{C.470})$$

For example, for  $f(t) = \frac{t^n}{n!} \mathbf{H}_0(t)$ , we have  $\tilde{f}(s) = \frac{1}{s^{n+1}}$ , so Eq.(C.470) becomes

$$\frac{t^{n+1}}{(n+1)!} \mathbf{H}_0(t) \xrightarrow{\mathcal{L}} \frac{1}{s^{n+2}} \quad (\text{C.471})$$

Note that

$$\int_0^t d\tau f(\tau) = \int_{-\infty}^{\infty} d\tau f(\tau) \mathbf{H}_0(\tau) \mathbf{H}_0(t - \tau) \quad (\text{C.472})$$

$$= ((f \mathbf{H}_0) \circledast \mathbf{H}_0)(t) \quad (\text{C.473})$$

- integral of  $\tilde{f}(s)$

$$\frac{1}{t} f(t) \xrightarrow{\mathcal{L}} \int_s^{\infty} d\sigma \tilde{f}(\sigma) \quad (\text{C.474})$$

- shifting  $\tilde{f}(s)$  (frequency shifting)

$$e^{at} f(t) \xrightarrow{\mathcal{L}} \tilde{f}(s - a) \quad (\text{for } a > 0) \quad (\text{C.475})$$

- shifting  $f(t)$  (time shifting).

$$f(t - a) \mathbf{H}_a(t) \xrightarrow{\mathcal{L}} e^{-as} \tilde{f}(s) \quad (\text{for } a > 0) \quad (\text{C.476})$$

- time scaling

$$f(at) \xrightarrow{\mathcal{L}} \frac{1}{a} \tilde{f}\left(\frac{s}{a}\right) \quad (\text{for } a > 0) \quad (\text{C.477})$$

- multiplication

$$f(t)g(t) \xrightarrow{\mathcal{L}} \frac{1}{2\pi i} \lim_{T \rightarrow \infty} \int_{c-iT}^{c+iT} ds' \tilde{f}(s') \tilde{g}(s - s') \quad (\text{C.478})$$

- convolution

The **convolution** of  $f : \mathbb{R} \rightarrow \mathbb{C}$  and  $g : \mathbb{R} \rightarrow \mathbb{C}$  is defined by

$$(f \circledast g)(t) = \int_{-\infty}^{\infty} d\tau f(\tau)g(t - \tau) \quad (\text{C.479})$$

If  $f(t) = g(t) = 0$  for  $t < 0$ ,

$$(f \circledast g)(t) = \int_0^t d\tau f(\tau)g(t - \tau) \quad (\text{see Fig.C.19.}) \quad (\text{C.480})$$

It's not hard to show that

$$f \circledast g = g \circledast f \quad (\text{C.481})$$

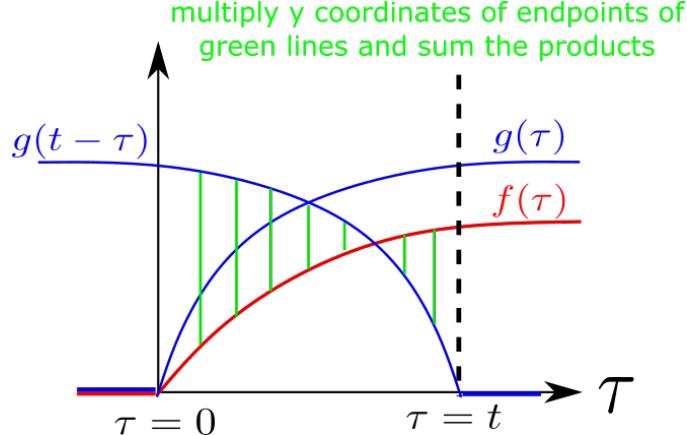


Figure C.19: Pictorial representation of the convolution  $(f * g)(t)$ .

and that

$$(f * g)(t) \xrightarrow{\mathcal{L}} \tilde{f}(s)\tilde{g}(s) \quad (\text{C.482})$$

Eq.(C.482) is easy to check with phasors. Indeed, if we substitute  $f(\tau) = e^{i\omega_0\tau}\tilde{f}$  and  $g(t - \tau) = e^{i\omega_0(t-\tau)}\tilde{g}$ , on the right hand side of Eq.(C.480), the right hand side becomes  $e^{i\omega_0 t}\tilde{f}\tilde{g}$ , and the LT of that is  $\tilde{f}\tilde{g}$ .

A common question is how does one evaluate convolutions in practice. If one can sample and remember the waveforms  $f(\tau)$  and  $g(\tau)$  for all  $\tau \in [0, t]$ , then it's just a matter of multiplication and addition of samples. Sometimes, even if we have no memory resources, it's possible to calculate a convolution. For example, if  $g(t) = e^{st}\mathbf{H}_0(t)$

$$(f * g)(t) = \int_0^t d\tau f(\tau)e^{s(t-\tau)} \quad (\text{C.483})$$

$$= \underbrace{e^{st}}_{g(t)} \tilde{f}(s) \quad (\text{C.484})$$

so convolving this  $g(\cdot)$  merely evaluates it at  $t$  and multiplies it by a constant  $\tilde{f}(s)$ .

- circular convolution

If  $f_T, g_T$  are periodic functions with period  $T$ , their **circular convolution** is defined as

$$(f_T * g_T)(t) = \int_0^T d\tau f_T(\tau)g_T(t - \tau) \quad (\text{C.485})$$

One can show that

$$(f_T \circledast_C g_T)(t) \xrightarrow{\mathcal{L}} \widetilde{f}_T(s)\widetilde{g}_T(s) \quad (\text{C.486})$$

- complex conjugation

$$f^*(t) \xrightarrow{\mathcal{L}} \widetilde{f}^*(s^*) \quad (\text{C.487})$$

- cross correlation

The **cross correlation** of functions  $f, g : [0, \infty] \rightarrow \mathbb{C}$  is defined as

$$(f, g)_{CC} = \int_0^\infty d\tau f^*(\tau)g(t + \tau) \quad (\text{C.488})$$

One can show that

$$(f, g)_{CC} \xrightarrow{\mathcal{L}} \widetilde{f}^*(-s^*)\widetilde{g}(s) \quad (\text{C.489})$$

- LT of periodic function

If  $f_T(t)$  is a periodic function with period  $T$ , then

$$f_T(t)\mathbf{H}_0(t) \xrightarrow{\mathcal{L}} \frac{1}{1 - e^{-sT}} \int_0^T dt e^{-st} f_T(t) \quad (\text{C.490})$$

To show this, define

$$\mathcal{I}_a^b = \int_a^b dt e^{-st} f_T(t) \quad (\text{C.491})$$

Then

$$\widetilde{f}_T(s) = \mathcal{I}_0^T + \mathcal{I}_T^{2T} + \mathcal{I}_{2T}^{3T} + \dots \quad (\text{C.492})$$

$$= \mathcal{I}_0^T(1 + e^{-sT} + e^{-s2T} + \dots) \quad (\text{C.493})$$

$$= \frac{1}{1 - e^{-sT}} \mathcal{I}_0^T \quad (\text{C.494})$$

- periodic summation

$$\sum_{n=0}^{\infty} f(t - nT)\mathbf{H}_0(t - nT) \xrightarrow{\mathcal{L}} \frac{1}{1 - e^{-Ts}} \widetilde{f}(s) \quad (\text{C.495})$$

$$\sum_{n=0}^{\infty} (-1)^n f(t - nT)\mathbf{H}_0(t - nT) \xrightarrow{\mathcal{L}} \frac{1}{1 + e^{-Ts}} \widetilde{f}(s) \quad (\text{C.496})$$

- limits of  $f(t)$

$$\lim_{s \rightarrow \infty} s\tilde{f}(s) = \lim_{s \rightarrow \infty} s \int_0^\infty dt e^{-st} f(t) \quad (\text{C.497})$$

$$\approx f(0^+) \underbrace{\lim_{s \rightarrow \infty} s \int_0^\infty dt e^{-st}}_{=1} \quad (\text{C.498})$$

$$= f(0^+) \quad (\text{C.499})$$

$$\lim_{s \rightarrow 0} s\tilde{f}(s) = f(\infty) \quad (\text{a.k.a. steady state}) \quad (\text{C.500})$$

- Inverse LT

The inverse LT of a function  $\tilde{f}(s)$  can be calculated by performing the following complex contour integral:

$$\underbrace{\mathcal{L}^{-1}[\tilde{f}(s)](t)}_{f(t)} = \frac{1}{2\pi i} \lim_{T \rightarrow \infty} \int_{\gamma-iT}^{\gamma+iT} ds e^{st} \tilde{f}(s) \quad (\text{C.501})$$

where  $\gamma, T \in \mathbb{R}$  and all singularities of  $\tilde{f}(s)$  must be located on the left side of the contour of integration. Another way of calculating the inverse LT of  $\tilde{f}(s)$ , is to express  $\tilde{f}(s)$  as a linear combination of functions for which the inverse LT is known from LT tables. For instance,

$$\mathcal{L}^{-1}\left[\frac{1}{s(s-1)}\right] = \mathcal{L}^{-1}\left[\frac{1}{s} - \frac{1}{s+1}\right] \quad (\text{partial fractions expansion}) \quad (\text{C.502})$$

$$= \mathcal{L}^{-1}\left[\frac{1}{s}\right] - \mathcal{L}^{-1}\left[\frac{1}{s+1}\right] \quad (\text{C.503})$$

$$= \mathbf{H}_0(t)[1 - e^{-t}] \quad (\text{C.504})$$

- Bode, Nyquist plots

Let  $s = \sigma + i\omega$ .

**Bode plot:** plot of

$$(\log_{10}(\omega), \log_{10}|\tilde{f}(i\omega)|)$$

and, right below it, plot of

$$(\log_{10}(\omega), \text{phase}\{\tilde{f}(i\omega)\})$$

**Nyquist plot:** plot of

$$(Re\tilde{f}(i\omega), Im\tilde{f}(i\omega))$$

or, equivalently, plot of

$$(|\tilde{f}(i\omega)|, phase(\tilde{f}(i\omega)))$$

on polar graph paper.

Usually,  $\tilde{f}(i\omega)$  is a gain (i.e., LT of output divided by LT of input).

- uncertainty principle

Here is some “Heisenberg uncertainty principle” type intuition about the relationship between a function  $f(t)$  and its LT  $\tilde{f}(s)$  for  $s = i\omega \in i\mathbb{R}$ .

$f(t)$	$\tilde{f}(i\omega)$	$ \tilde{f}(i\omega) $	$phase(\tilde{f}(i\omega))$	
$\delta(t)$	1	1	0	
$\mathbf{H}_0(t)$	$\frac{1}{i\omega}$	$\frac{1}{ \omega }$	$-\frac{\pi}{2}$	(C.505)
$t \mathbf{H}_0(t)$	$\frac{1}{(i\omega)^2}$	$\frac{1}{\omega^2}$	$-\pi$	
$\frac{t^2}{2} \mathbf{H}_0(t)$	$\frac{1}{(i\omega)^3}$	$\frac{1}{ \omega ^3}$	$\frac{\pi}{2}$	

Hence, the narrower  $f(t)$  is, the broader  $|\tilde{f}(i\omega)|$  is. Also, the more  $f(t)$  is a high pass filter, the more  $|\tilde{f}(i\omega)|$  is a low pass filter.

## C.46 Z-transform

This section is a watered down version of the Wikipedia entry for Z-transforms (Ref.[167]), which we highly recommend. Before reading this section, we recommend that the reader read Section C.45 on Laplace transforms, as those are the continuous in time version of Z-transforms.

Suppose  $x^{[n]} \in \mathbb{C}$  for all  $n \in \mathbb{Z}^{\geq 0}$  ( $\mathbb{Z}^{\geq 0}$  =non-negative integers), and  $z \in \mathbb{C}$ . Then we define the **Z-transform (ZT)** by

$$\mathcal{Z}[x](z) = \tilde{x}(z) = \sum_{n=0}^{\infty} x^{[n]} z^{-n} \quad (\text{C.506})$$

Note that the ZT is a linear functional because

$$\mathcal{Z}[ax^{[n]} + by^{[n]}] = a\mathcal{Z}[x^{[n]}] + b\mathcal{Z}[y^{[n]}] \quad (\text{C.507})$$

for  $x^{[n]}, y^{[n]} \in \mathbb{C}$  for all  $n \in \mathbb{Z}^{\geq 0}$ , and  $a, b \in \mathbb{C}$ .

The **Inverse Z-transform** is defined so that

$$\mathcal{Z}^{-1}[\underbrace{\mathcal{Z}[x^{[n]}]}_{\tilde{x}(z)}]^{[n]} = x^{[n]} \quad (\text{C.508})$$

name	formula	comment
<b>Bilateral ZT (BZT)</b>	$\tilde{x}(z) = \sum_{n=-\infty}^{\infty} x^{[n]} z^{-n}$	Same as ZT but with $n \in \mathbb{Z}$ instead of $n \in \mathbb{Z}^{>0}$
<b>Discrete time Fourier transform (DTFT)</b>	$\tilde{x}_{2\pi}(\omega) = \sum_{n=-\infty}^{\infty} x^{[n]} e^{-i\omega n}$	same as BZT but with $z = e^{i\omega}$
<b>Discrete Fourier transform (DFT)</b>	$\tilde{x}^{[k]} = \sum_{n=0}^{N-1} x^{[n]} e^{-i\frac{2\pi k n}{N}}$	Same as ZT but a finite ( $N$ ) number of $x^{[n]}$ components, and with $z = e^{i\frac{2\pi k}{N}}$ for $k = 0, 1, \dots, N-1$ ( $N$ roots of unity on unit circle)
<b>Probability Generating Function</b>	$\tilde{P}(z) = \sum_{n=0}^{\infty} P^{[n]} z^n$	same as ZT but with $n \rightarrow -n$ and $P^{[n]} : \mathbb{Z}^{>0} \rightarrow [0, 1]$ is a discrete prob. distribution. If $z = e^{-T}$ , get moment generating function.

Table C.3: Transforms that are akin to the Z-transform. Don't be intimidated by all these transforms. They are all just fancy dot products like  $\vec{a} \cdot \vec{b}$ .

Table C.3 is a table of transforms that are akin to the ZT.

For models that are continuous in time (i.e., analog) we use Laplace transforms (LTs), and for models that are discrete in time (i.e., digital), we use Z-transforms (ZTs). Digital models are often obtained by sampling analog models at discrete times separated by a time interval  $T$ . Hence, it is useful to know how LTs and ZTs are related. To find out, let

$$e^{-st} = z^{-n} \quad (\text{C.509})$$

and

$$t = nT \quad (\text{C.510})$$

Hence, we arrive at the very useful formula

$$z = e^{sT}$$

(C.511)

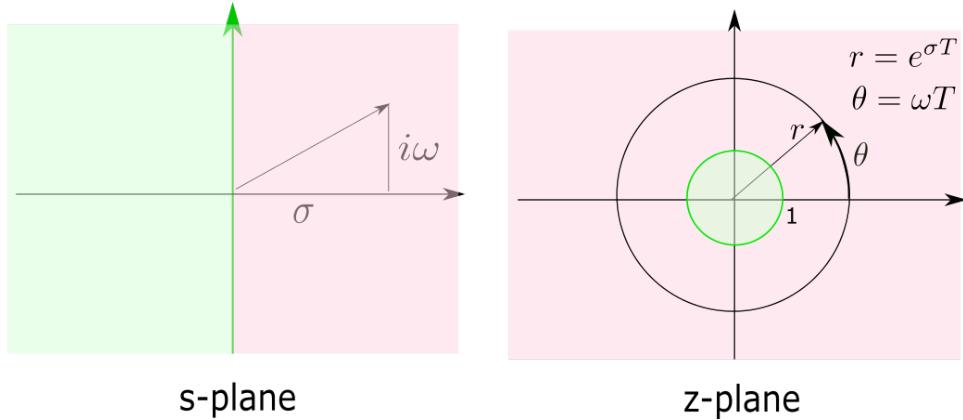


Figure C.20: Relationship between the s-plane (for Laplace transform) and z-plane (for Z-transform.).

If

$$s = \sigma + i\omega, \quad z = re^{i\theta} \quad (\text{C.512})$$

then

$$r = e^{\sigma T}, \quad \theta = \omega T \quad (\text{C.513})$$

The map given by Eqs.(C.513) is illustrated by Fig.C.20. As shown in Fig.C.20, the map from the s-plane (for LTs) to the z-plane (for ZTs) maps:

- left half plane (LHP)  $\rightarrow$  inside of the unit circle
- imaginary axis  $\rightarrow$  unit circle. In particular, the s-plane origin  $s = 0$  and points with  $\sigma = 0, \omega = \frac{2\pi k}{T}$ , where  $k \in \mathbb{Z}$ , are all mapped to  $z = 1$ .
- right half plane (RHP)  $\rightarrow$  outside of unit circle

Define the the **Kronecker delta function** by

$$\delta_j^{[n]} = \mathbb{1}(n = j) \quad (\text{C.514})$$

and the **discrete Heavyside step function** by

$$\mathbf{H}_j^{[n]} = \mathbb{1}(n \geq j) \quad (\text{C.515})$$

Note that

$$H_0^{[n]} = \sum_{k=0}^{\infty} \delta_k^{[n]} \quad (\text{C.516})$$

Next, we will list some examples and properties of ZTs. Henceforth, we will use the following notation:

$$\begin{aligned} x^{[n]}, x_1^{[n]}, x_2^{[n]} &\in \mathbb{C} \text{ are defined only for } n \in \mathbb{Z}^{\geq 0} \\ x^{[n]} &\xrightarrow{\mathcal{Z}} \tilde{x}(z) \text{ means } \mathcal{Z}[x^{[n]}] = \tilde{x}(z) \end{aligned}$$

The **Region Of Convergence (ROC)** for a ZTs is very important (Without knowing the ROC, you can't invert a ZT  $\tilde{x}(z)$ ). We won't list ROCs here, but they can be found in ZT tables like those in Ref.[167].

Note that ZT formulae can be "sanity checked" by replacing  $z = e^{sT}$  and checking that for  $0 < T \ll 1$ ,

$$\mathcal{Z}[x](e^{sT}) \approx \frac{1}{T} \mathcal{L}[f](s) \quad (\text{C.517})$$

Note also that for  $T \ll 1$ :

$$z \approx 1, \quad z\partial_z = \partial_{\ln z} = \partial_{sT}, \quad (z-1)^n \approx (sT)^n \quad (\text{C.518})$$

$$\begin{aligned} \int_{0-}^{\infty} dt \delta(t) &= 1 = \sum_{n=0}^{\infty} \delta_0^{[n]} \text{ so by dimensional analysis, } \delta_0^{[n]} \approx T\delta(t). \\ \mathbf{H}_0^{[n]} &\approx \mathbf{H}_0(t) \end{aligned}$$

### C.46.1 Examples

- Kronecker delta function

$$\delta_{n_0}^{[n]} \xrightarrow{\mathcal{Z}} z^{-n_0} \quad (\text{C.519})$$

Compare this with

$$\delta(t - t_0) \xrightarrow{\mathcal{L}} e^{-st_0} \quad (\text{C.520})$$

with  $t_0 = n_0 T$  and  $z = e^{sT}$ .

Note that

$$\mathcal{Z}[\mathbf{H}_0^{[n]}] = \sum_{k=0}^{\infty} \mathcal{Z}[\delta_k^{[n]}] \quad (\text{C.521})$$

$$= \sum_{k=0}^{\infty} z^{-k} \quad (\text{C.522})$$

$$= \frac{1}{1 - 1/z} \quad (\text{C.523})$$

- unit step

For  $a \in \mathbb{C}$ ,

$$a^n \mathbf{H}_0^{[n]} \xrightarrow{\mathcal{Z}} \frac{1}{1 - az^{-1}} \quad \text{for } |z| > |a| \quad (\text{C.524})$$

$$-a^n \mathbf{H}_0^{[-n-1]} \xrightarrow{\mathcal{Z}} \frac{1}{1 - az^{-1}} \quad \text{for } |z| < |a| \quad (\text{C.525})$$

Compare this with

$$\mathbf{H}_0(t) \xrightarrow{\mathcal{L}} \frac{1}{s} \quad (\text{for } \operatorname{Re}(s) > 0) \quad (\text{C.526})$$

for  $a = 1$ ,  $z = e^{sT} \approx 1 + sT$ .

- ramp

For  $a \in \mathbb{C}$ ,

$$na^n \mathbf{H}_0^{[n]} \xrightarrow{\mathcal{Z}} \frac{az^{-1}}{(1 - az^{-1})^2} \quad \text{for } |z| > |a| \quad (\text{C.527})$$

$$-na^n \mathbf{H}_0^{[-n-1]} \xrightarrow{\mathcal{Z}} \frac{az^{-1}}{(1 - az^{-1})^2} \quad \text{for } |z| < |a| \quad (\text{C.528})$$

- sine, cosine

For  $a \in \mathbb{C}$ ,

$$a^n \sin(\omega_0 n) \mathbf{H}_0^{[n]} \xrightarrow{\mathcal{Z}} \frac{az^{-1} \sin \omega_0}{1 - 2az^{-1} \cos \omega_0 + a^2 z^{-2}} \quad (\text{C.529})$$

$$a^n \cos(\omega_0 n) \mathbf{H}_0^{[n]} \xrightarrow{\mathcal{Z}} \frac{1 - az^{-1} \cos \omega_0}{1 - 2az^{-1} \cos \omega_0 + a^2 z^{-2}} \quad (\text{C.530})$$

## C.46.2 Properties

- time expansion

$$x^{[n/K]} \mathbb{1}(n/K \in \mathbb{Z}) \xrightarrow{\mathcal{Z}} \tilde{x}(z^K) \quad (\text{C.531})$$

- decimation

$$x^{[Kn]} \xrightarrow{\mathcal{Z}} \frac{1}{K} \sum_{p=0}^{K-1} \tilde{x}\left(z^{\frac{1}{K}} e^{-i2\pi \frac{p}{K}}\right) \quad (\text{C.532})$$

- time delay

$$x^{[n-k]} \xrightarrow{\mathcal{Z}} z^{-k} \tilde{x}(z) \quad (\text{for } k > 0) \quad (\text{C.533})$$

- time advance

$$x^{[n+k]} \xrightarrow{\mathcal{Z}} z^k \left( \tilde{x}(z) - z^k \sum_{n=0}^{k-1} x^{[n]} z^{-n} \right) \quad (\text{for } k > 0) \quad (\text{C.534})$$

- first difference backwards

$$x^{[n]} - x^{[n-1]} \xrightarrow{\mathcal{Z}} (1 - z^{-1}) \tilde{x}(z) \quad (\text{C.535})$$

- first difference forward

$$x^{[n+1]} - x^{[n]} \xrightarrow{\mathcal{Z}} z ((1 - z^{-1}) \tilde{x} - x^{[0]}) \quad (\text{C.536})$$

- time reversal

$$x^{[-n]} \xrightarrow{\mathcal{Z}} \tilde{x}(z^{-1}) \quad (\text{C.537})$$

- scaling in z-domain

For  $a \in \mathbb{C}$ ,

$$a^n x^{[n]} \xrightarrow{\mathcal{Z}} \tilde{x}(a^{-1}z) \quad (\text{C.538})$$

- complex conjugation

$$(x^{[n]})^* \xrightarrow{\mathcal{Z}} \tilde{x}^*(z^*) \quad (\text{C.539})$$

$$Re(x^{[n]}) \xrightarrow{\mathcal{Z}} \frac{1}{2}(\tilde{x}(z) + \tilde{x}^*(z^*)) \quad (\text{C.540})$$

$$Im(x^{[n]}) \xrightarrow{\mathcal{Z}} \frac{1}{2i}(\tilde{x}(z) - \tilde{x}^*(z^*)) \quad (\text{C.541})$$

- $\tilde{x}(z)$  differentiation

$$nx^{[n]} \xrightarrow{\mathcal{Z}} -z\partial_z \tilde{x}(z) \quad (\text{C.542})$$

- convolution

Define the **(discrete) convolution** of  $x_1^{[n]}$  and  $x_2^{[n]}$  by

$$x_1^{[n]} \circledast x_2^{[n]} = \sum_{k=0}^n x_1^{[k]} x_2^{[n-k]} \quad (\text{C.543})$$

One can show that

$$x_1^{[n]} \circledast x_2^{[n]} \xrightarrow{\mathcal{Z}} \tilde{x}_1(z) \tilde{x}_2(z) \quad (\text{C.544})$$

- cross-correlation

$$(x_1^{[-n]})^* \circledast x_2^{[n]} \xrightarrow{\mathcal{Z}} \tilde{x}_1^*(\frac{1}{z^*}) \tilde{x}_2(z) \quad (\text{C.545})$$

- accumulation

$$\sum_{k=-\infty}^{\infty} x^{[k]} \xrightarrow{\mathcal{Z}} \frac{1}{1-z^{-1}} \tilde{x}(z) \quad (\text{C.546})$$

- multiplication

$$x_1^{[n]} x_2^{[n]} \xrightarrow{\mathcal{Z}} \frac{1}{2\pi i} \oint_C \frac{dw}{w} \tilde{x}_1(w) \tilde{x}_2(\frac{z}{w}) \quad (\text{C.547})$$

- Parseval's theorem

$$\sum_{k=-\infty}^{\infty} x_1^{[n]} (x_2^{[n]})^* = \frac{1}{2\pi i} \oint_C \frac{dw}{w} \tilde{x}_1(w) \tilde{x}_2^*(\frac{1}{w^*}) \quad (\text{C.548})$$

- limits of  $x^{[n]}$

initial value theorem

$$x^{[0]} = \lim_{z \rightarrow \infty} \tilde{x}(z) \quad (\text{C.549})$$

final value theorem

$$x^{[\infty]} = \lim_{z \rightarrow 1} (z-1) \tilde{x}(z) \quad (\text{C.550})$$

- Inverse ZT

$$\underbrace{\mathcal{Z}^{-1}[\tilde{x}(z)]}_{x^{[n]}} = \frac{1}{2\pi i} \oint_C dz \tilde{x}(z) z^{n-1} \quad (\text{C.551})$$

where  $C$  is a counterclockwise closed path containing the origin and all singularities of  $\tilde{x}(z)$ .

## C.47 Legendre Transformation (dual functions)

This section is a watered down version of the Wikipedia article Ref.[132], which we highly recommend.

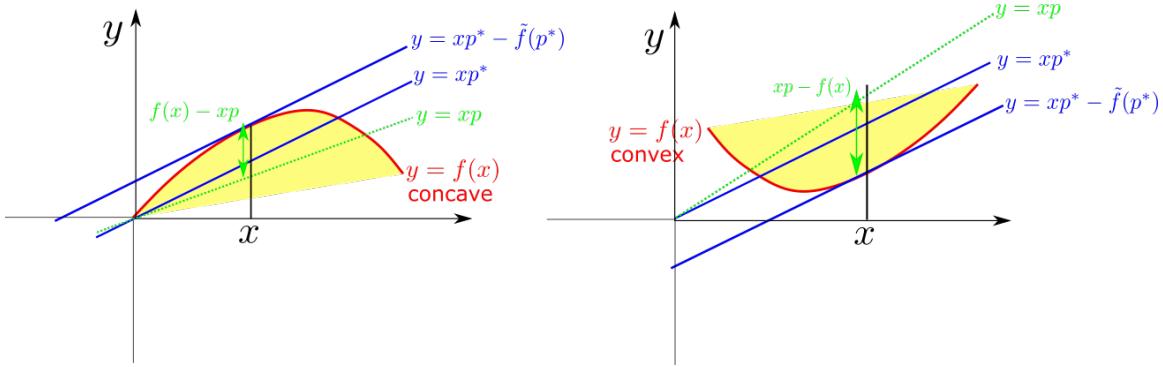


Figure C.21: The line  $y = xp$  goes through the origin and has arbitrary slope  $p$ .  $p^*$  is the special slope at  $x$  for which the line  $y = xp^*$ , if displaced parallelly, can be made tangential (kissing) to the curve  $y = f(x)$ .

Let  $x, p \in \mathbb{R}^n$ . If  $f : \mathbb{R}^n \rightarrow \mathbb{R}$  is a concave function, we define its **dual (a.k.a. conjugate) function**  $\tilde{f} : \mathbb{R}^n \rightarrow \mathbb{R}$  by

$$\tilde{f}(p) = \min_x(p^T x - f(x)) . \quad (\text{C.552})$$

This definition also applies if one replaces the words “concave” by “convex” and “min” by “max”.<sup>19</sup>  $\tilde{f}(p)$  is also called the **Legendre transformation (or Legendre transform)** (LT) of  $f(x)$ .

In Physics,  $x$  is the position vector and  $p$  is the momentum vector of a system.

See Figs. C.21 and C.22 for a pictorial representation of LT.

---

<sup>19</sup>This book does not try to be mathematically rigorous beyond the level of applied math. To be truly rigorous and general, replace “max” by “supremum” and “min” by “infimum”. Pure mathematicians use min and max only over finite sets, but physicists and engineers often discretize to obtain a max or min over a finite set with  $N$  points, and then, afterwards, take the limit  $N \rightarrow \infty$ . Not perfect, but good enough for most applied work.

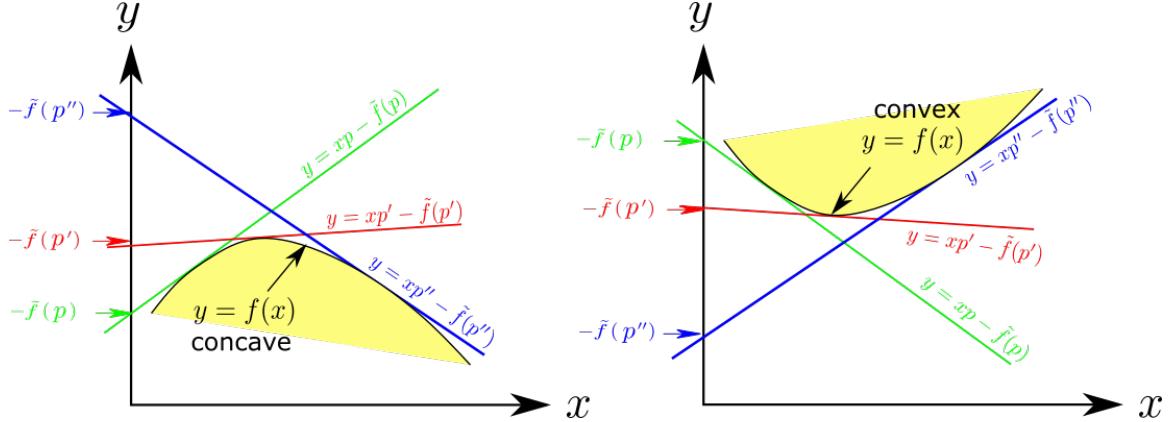


Figure C.22: The dual function  $\tilde{f}(p)$  of a concave or convex function  $f(x)$  is the osculating (kissing) locus of the family of lines  $y = px - \tilde{f}(p)$ , where  $p$  is the slope at  $x$  of the curve  $y = f(x)$ .

Note that the right hand side of Eq.(C.552) implies that

$$\sum_i (p_i - \partial_{x_i} f(x)) \delta x_i = 0 \quad (\text{C.553})$$

for all variations  $\delta x_i$ . If minimization is achieved when  $x = x^*$ , then

$$p = \nabla_{x^*} f(x^*), \quad x^* = (\nabla_{x^*} f)^{-1}(p) \quad (\text{C.554})$$

### C.47.1 Examples

- Find the dual function of

$$\boxed{f(x) = e^x}. \quad (\text{C.555})$$

$$p = \partial_{x^*} f \quad (\text{C.556})$$

$$= e^{x^*} \quad (\text{C.557})$$

$$x^* = \ln p \quad (\text{C.558})$$

$$f(x^*) = p \quad (\text{C.559})$$

$$\tilde{f}(p) = x^* p - f(x^*) \quad (\text{C.560})$$

$$= p \ln p - p \quad (\text{C.561})$$

2. Find the dual function of

$$\boxed{f(x) = f + f'x + \frac{1}{2}f''x^2}. \quad (\text{C.562})$$

$$p = \partial_{x^*} f \quad (\text{C.563})$$

$$= f' + f''x^* \quad (\text{C.564})$$

$$x^* = \frac{p - f'}{f''} \quad (\text{C.565})$$

$$f(x^*) = f + f' \left[ \frac{p - f'}{f''} \right] + \frac{1}{2}f'' \left[ \frac{p - f'}{f''} \right]^2 \quad (\text{C.566})$$

$$= \left[ f - \frac{(f')^2}{2f''} \right] + p^2 \left[ \frac{1}{2f''} \right] \quad (\text{C.567})$$

$$\tilde{f}(p) = px^* - f(x^*) \quad (\text{C.568})$$

$$= p \left[ \frac{p - f'}{f''} \right] - f(x^*) \quad (\text{C.569})$$

$$= \left[ -f + \frac{(f')^2}{2f''} \right] + p \left[ \frac{-f'}{f''} \right] + p^2 \left[ \frac{1}{2f''} \right] \quad (\text{C.570})$$

Note that when  $f = f' = 0$ , we get

$$f(x) = \frac{f''x^2}{2}, \quad \tilde{f}(p) = \frac{p^2}{2f''} \quad (\text{C.571})$$

---

Note that if  $f$  is convex (resp., concave),  $\tilde{f}$  is convex too (resp., concave too).

3. Find the dual function of

$$\boxed{f(x) = \ln(1 - e^{-x})}. \quad (\text{C.572})$$

$$p = \partial_{x^*} f(x^*) \quad (\text{C.573})$$

$$= \frac{e^{-x^*}}{1 - e^{-x^*}} \quad (\text{C.574})$$

$$p = (1 + p)e^{-x^*} \quad (\text{C.575})$$

$$x^* = \ln \frac{1 + p}{p} \quad (\text{C.576})$$

$$f(x^*) = \ln \left( 1 - \frac{p}{1 + p} \right) = -\ln(1 + p) \quad (\text{C.577})$$

$$\tilde{f}(p) = px^* - f(x^*) \quad (\text{C.578})$$

$$= p \ln \frac{1 + p}{p} + \ln(1 + p) \quad (\text{C.579})$$

$$= -p \ln p + (1 + p) \ln(1 + p) \quad (\text{C.580})$$

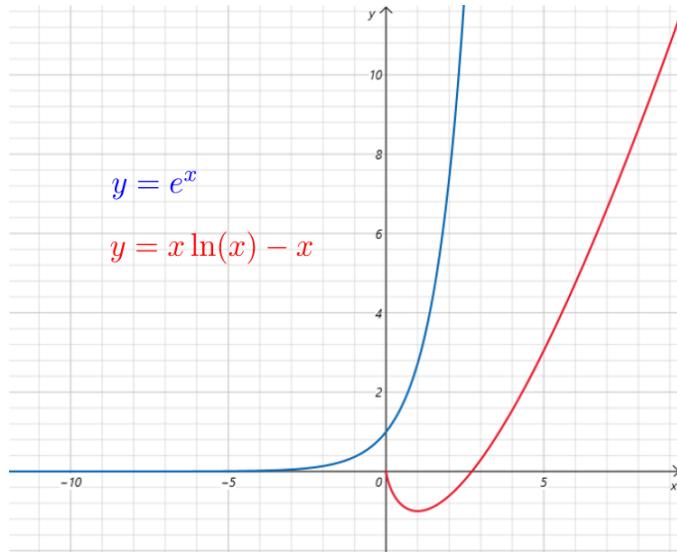


Figure C.23:  $f(x) = e^x$  and its dual.

## C.47.2 Properties

**Claim 19** If  $f(x)$  is a concave function with dual  $\tilde{f}(p)$ , then

$$f(x) = \min_p (p^T x - \tilde{f}(p)) \quad (\text{C.581})$$

$$\nabla_p \tilde{f}(p(x)) = (\nabla_x f)^{-1}(x) \quad (\text{C.582})$$

Eqs. (C.552) and (C.581) are also true if we replace the words "concave" with "convex" and "min" with "max".

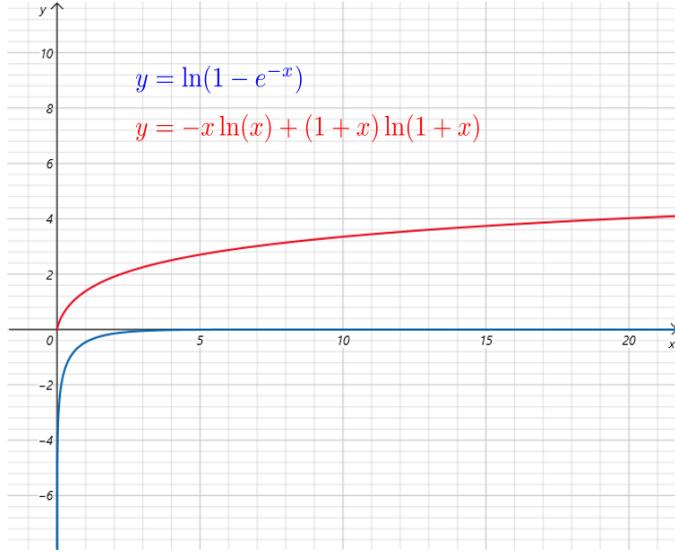


Figure C.24:  $f(x) = \ln(1 - e^{-x})$  and its dual.

**proof:**

Let  $x^*$  be the value of  $x$  which minimizes  $y = p^T x - f(x)$  with respect to  $x$ . Hence,

$$\tilde{f}(p) = p^T x^* - f(x^*) . \quad (\text{C.583})$$

Rearranging terms in Eq.(C.583), we get

$$f(x^*) = p^T x^* - \tilde{f}(p) \quad (\text{C.584})$$

Let  $p^*$  be the value of  $p$  which minimizes  $y = p^T x - \tilde{f}(p)$  with respect to  $p$ . Hence,

$$f(x) = (p^*)^T x - \tilde{f}(p^*) \quad (\text{C.585})$$

Replacing  $p^*$  by  $p$  and  $x$  by  $x^*$  in Eq.(C.585) yield Eq.(C.584).

Note that minimization with respect to  $x$  is achieved if

$$p_i = \partial_{x_i} f(x), \quad p = \nabla_x f(x) \quad (\text{C.586})$$

whereas minimization with respect to  $p$  is achieved if

$$x_i = \partial_{p_i} \tilde{f}(p), \quad x = \nabla_p \tilde{f}(p) \quad (\text{C.587})$$

Hence,

$$x = \nabla_p \tilde{f}(\nabla_x f(x)) \quad (\text{C.588})$$

**QED**

**Claim 20** If  $f(x)$  is concave (resp., convex), then  $\tilde{f}(p)$  is also concave (resp., convex)

**proof:**

$$\tilde{f}(p) = x^*p - f(x^*) \quad (\text{C.589})$$

$$\frac{d\tilde{f}}{dp} = x^* + \underbrace{(p - f'(x^*))}_{=0} \frac{dx^*}{dp} = x^* \quad (\text{C.590})$$

$$\frac{d^2\tilde{f}}{dp^2} = \frac{dx^*}{dp} \quad (\text{C.591})$$

$$p = f'(x^*), \quad x^* = (f')^{-1}(p) \quad (\text{C.592})$$

$$dp = f''(x^*)dx^*, \quad \frac{dx^*}{dp} = \frac{1}{f''(x^*)} \quad (\text{C.593})$$

$$\frac{d^2\tilde{f}}{dp^2} = \frac{1}{f''(x^*)} \quad (\text{C.594})$$

**QED**

**Claim 21** LT is its own inverse (i.e., LT is a self-inverse or involution transformation)

$$\tilde{\tilde{f}}(x) = f(x) \quad (\text{C.595})$$

**proof:**  $x = x_1, p = x_2$

$$\tilde{f}(x_2) = x_2x_1^* - f(x_1^*), \quad x_2 = f'(x_1^*) \quad (\text{C.596})$$

$$\tilde{\tilde{f}}(x_3) = x_3x_2^* - \tilde{f}(x_2^*), \quad x_3 = (\tilde{f})'(x_2^*) \quad (\text{C.597})$$

$$\tilde{\tilde{f}}(x_3) = x_3x_2^* - x_2^*x_1^* + f(x_1^*) \quad (\text{C.598})$$

$$= f(x_1^*) \quad (\text{for } x_1^* = x_3) \quad (\text{C.599})$$

$$x = x_3 = (\tilde{f})'(x_2^*) = (\tilde{f})'(f'(x_1^*)) = x_1^* \quad (\text{C.600})$$

**QED**

Additional properties

- Scaling

$$ag(bx) \xrightarrow{LT} a\tilde{g}\left(\frac{p}{ab}\right) \quad (\text{C.601})$$

for  $a, b > 0$

- Translation

$$g(x + y) + b \xrightarrow{LT} \tilde{g}(p) - p^T y - b \quad (\text{C.602})$$

- Frenchel's inequality

$$p^T x \leq f(x) + \tilde{f}(p) \quad (\text{C.603})$$

### C.47.3 Connection to Fourier transform and Quantum Mechanics

Recall how Fourier transforms (FTs) arise in Quantum Mechanics. Suppose  $x, p \in \mathbb{R}$  and

$$\psi(x) = \langle x|\psi\rangle, \quad \tilde{\psi}(p) = \langle p|\psi\rangle, \quad \langle p|x\rangle = \frac{e^{-ipx}}{\sqrt{2\pi}} \quad (\text{C.604})$$

Then

$$\tilde{\psi}(p) = \int_{-\infty}^{\infty} dx \langle p|x\rangle \langle x|\psi\rangle \quad (\text{C.605})$$

$$= \int_{-\infty}^{\infty} \frac{dx}{\sqrt{2\pi}} e^{-ipx} \psi(x) \quad (\text{C.606})$$

and

$$\psi(x) = \int_{-\infty}^{\infty} dp \langle x|p\rangle \langle p|\psi\rangle \quad (\text{C.607})$$

$$= \int_{-\infty}^{\infty} \frac{dp}{\sqrt{2\pi}} e^{ipx} \tilde{\psi}(p) \quad (\text{C.608})$$

Define a **convolution** of two wave functions  $\psi_1, \psi_2 : \mathbb{R} \rightarrow \mathbb{C}$  by

$$(\psi_1 \circledast \psi_2)(x) = \int_{-\infty}^{\infty} dy \psi_1(y) \psi_2(x - y) \quad (\text{C.609})$$

Then

$$(\psi_1 \circledast \psi_2)^\sim(p) = \widetilde{\psi_1}(p) \widetilde{\psi_2}(p) \quad (\text{C.610})$$

If, in the definition of LT, we replace the minimum over  $x$  of an arbitrary function  $\Gamma : \mathbb{R} \rightarrow \mathbb{R}$  by

$$\min_x \Gamma(x) \rightarrow i \ln \int_{-\infty}^{\infty} \frac{dx}{\sqrt{2\pi}} \exp\{-i\Gamma(x)\} \quad (\text{C.611})$$

then we get the definition of a FT:

$$\underbrace{e^{-i\tilde{f}(p)}}_{\tilde{\psi}(p)} = \int_{-\infty}^{\infty} \frac{dx}{\sqrt{2\pi}} e^{-ip^T x} \underbrace{e^{if(x)}}_{\psi(x)} \quad (\text{C.612})$$

Define the **infimal convolution** of two functions  $f, g : \mathbb{R}^n \rightarrow \mathbb{R}$  by

$$(f \circledast_{inf} g)(x) = \min_y \{f(y) + g(x - y)\} \quad (\text{C.613})$$

Then

$$(f \circledast_{inf} g)^\sim(p) = \tilde{f}(p) + \tilde{g}(p) \quad (\text{C.614})$$

Eq.(C.614) requires a proof that we leave to the reader, but note that it's just what would be expected from our "mapping" of LT to FT.

## C.48 Numpy tensor methods

Numpy contains excellent documentation which we highly recommend. So why this appendix? The purpose of this appendix is to compare the tensor operations used in Physics<sup>20</sup> to the tensor operations used in Machine Learning (ML) as exemplified by Numpy.

But first, some notation.

For integers  $m > n$ , let

$$[n : m] = [n, n + 1, \dots, m - 2, m - 1] \quad (\text{C.615})$$

and

$$[n] = [0 : n] \quad (\text{C.616})$$

$[n : m]$  acts the the same way as the function `range(n,m)` in Python.

We will use

$$A^{[n]} = \begin{bmatrix} A^0 \\ A^1 \\ \vdots \\ A^{n-1} \end{bmatrix} = A^{[n],[1]} \quad (\text{C.617})$$

---

<sup>20</sup>Elasticity, Fluid Mechanics, General Relativity and Quantum Mechanics all use tensors. Tensors in various guises are ubiquitous in Physics.

to denote column vector,

$$A^{[n]T} = [A^0, A^1, \dots, A^{n-1}] = A^{[1],[n]} \quad (\text{C.618})$$

to denote a row vector and

$$A = \begin{bmatrix} A^{0,0} & \dots & A^{0,m-1} \\ \vdots & \vdots & \vdots \\ A^{n-1,0} & \dots & A^{n-1,m-1} \end{bmatrix} = A^{[n],[m]} \quad (\text{C.619})$$

to denote an  $n \times m$  matrix.

Let

$$pow(a, r) = \underbrace{[a, a, \dots, a]}_{r \text{ repetitions}} \quad (\text{C.620})$$

For increased clarity, we will use Greek letters to denote tensor indices.

For **scalars**  $a, b \in \mathbb{R}$ , the **linear combination of tensors**  $T, S$  is defined by

$$[T^{\alpha,\beta,\gamma}, S^{\alpha,\beta,\gamma}] \rightarrow aT^{\alpha,\beta,\gamma} + bS^{\alpha,\beta,\gamma} \quad (\text{C.621})$$

The **Kronecker (K) delta function** is defined by

$$\delta_\alpha^\beta = \delta_{\alpha,\beta} = \mathbb{1}(\alpha = \beta) \quad (\text{C.622})$$

Upper indices can be lowered by means of the K delta function :

$$S_\beta = \sum_\alpha S^\alpha \delta_{\alpha,\beta} \quad (\text{C.623})$$

In this case, since the metric  $\delta_{\alpha,\beta}$  is the K delta function,  $S^\alpha = S_\alpha$ .

The **Einstein implicit summation convention** is the practice of omitting the summation sign and assuming that repeated indices are summed over if one index is covariant (upper) and the other is contravariant (lower).

$$S^\alpha T_\alpha = \sum_\alpha S^\alpha T_\alpha \quad (\text{C.624})$$

Sums between a lower and an upper index are called **contractions**.

$dim$  refers to the positions of indices in a tensor (e.g.,  $dim = 0$  for  $\alpha$ ,  $dim = 1$  for  $\beta$  and  $dim = 2$  for  $\gamma$  in  $T^{\alpha,\beta,\gamma}$ ).  $axis \in [n]$  refers to the values of an index along a particular dimension (e.g., we say  $axis = \alpha$  along  $dim = 0$  in  $T^{\alpha,\beta,\gamma}$ ). For a 2-dim array: (1) swapping axes along  $dim = 0$  (resp.,  $dim = 1$ ) refers to swapping rows (resp., columns). (2) swapping dimensions 0 and 1 means transposing the array.

Numpy contains a huge number of tensor methods. Among those, there are 3 broad types of methods that concern us here:

1. **tensor algebra methods.** These include element-wise (i.e., entry-wise) summation, subtraction, multiplication and division (+, -, \*, /) of 2 tensors of the same shape, or a tensor and a scalar.
2. **methods for permuting the entries of a tensor.** These entry permutation methods can be of 3 kinds (1) methods that permute entries by permuting the locations of indices of a tensor (2) methods that permute entries by permuting the axes of a tensor along a particular dimension (e.g., row permutation and column permutation for 2-dim arrays) (3) methods that are neither pure 1 or pure 2.
3. **methods for adding or removing tensor entries.**

Out of these three categories, ML uses all three frequently. Physics uses all three too, but it often favors (1). <sup>21</sup> This is probably due to the fact that Physicists always assume linearity first, because it's simpler to solve than the non-linear case, plus it often describes the weak interaction case well.

Next I will discuss in a visual manner<sup>22</sup>, a random assortment of Numpy methods that I find interesting, and difficult to understand to the beginner (like me). This discussion in no way pretends to be a substitute for the excellent Numpy documentation.

Besides the usual Physics notation discussed at the beginning of this appendix, I will use below my own way of visualizing Numpy tensor methods. Specifically, I will use a graphical box (what I call a "box of puzzle pieces") to indicate a box containing all the pieces of information from which a tensor is constructed. If you don't like my graphical box, just replace it by  $f(X)$ , where  $X$  is the contents of the box and  $f$  is some function.

Below, let  $\alpha \in [a]$ ,  $\beta \in [b]$ ,  $\gamma \in [c]$ ,  $\nu \in [n]$ ,  $\mu \in [m]$ ,  $\nu_i \in [n_i]$ .

### 1. broadcasting

$$T^{\alpha,0} + S^{0,\beta} \rightarrow Y^{\alpha,\beta} = T^{\alpha,0} + S^{0,\beta} \quad (\text{C.625})$$

### 2. concatenate() along $dim = 0$

$$[T_0^{[n_0],\beta,\gamma}, T_1^{[n_1],\beta,\gamma}, T_2^{[n_2],\beta,\gamma}] \rightarrow \boxed{T_0^{[n_0],\beta,\gamma} \\ T_1^{[n_1],\beta,\gamma} \\ T_2^{[n_2],\beta,\gamma}}^{[n],\beta,\gamma} \quad (\text{C.626})$$

---

<sup>21</sup>Category (1) echoes the Linear Algebra and category (2) the Group Representation Theory used in Quantum Mechanics to describe lossless, reversible physical phenomena. Category (3) echoes the Information Theory, Thermodynamics, Renormalization Group Theory, Noise Theory and Fluid Turbulence Theory used to describe lossy, irreversible phenomena.

<sup>22</sup>The Numpy methods in this list are discussed here visually and analytically only; that is, without numerical examples. For numerical examples, see the excellent Numpy docs.

where  $n = n_0 + n_1 + n_2$ .

3. **expand\_dims()** (same as **unsqueeze()**) along  $dim = 0$

$$T^{[b],[c]} \rightarrow Y^{0,[b],[c]} \quad (\text{C.627})$$

$$T^{\beta,\gamma} \rightarrow Y^{0,\beta,\gamma} = T^{\beta,\gamma} \quad (\text{C.628})$$

4. **flatten()**

$$T^{[n_0],[n_1],[n_2]} \rightarrow Y^{[n]} \quad (\text{C.629})$$

where  $n_0 n_1 n_2 = n$ . A more fine grained description is

$$T^{\alpha,\beta,\gamma} \rightarrow Y^{\nu(\alpha,\beta,\gamma)} \quad (\text{C.630})$$

where  $n_0 n_1 n_2 = n$  and  $\nu : [n_0] \times [n_1] \times [n_2] \rightarrow [n]$  is a 1-1 onto function.

5. **gather()**<sup>23</sup> along  $dim = 0$

$$S^{[a],[n_1],[n_2]} \rightarrow Y^{[b],[n_1],[n_2]} \quad (\text{C.631})$$

$$S^{\alpha,\nu_1,\nu_2} \rightarrow Y^{\beta,\nu_1,\nu_2} = S^{\beta(\alpha,\nu_1,\nu_2),\nu_1,\nu_2} \quad (\text{C.632})$$

$$I^{\alpha,\nu_1,\nu_2} = \beta(\alpha, \nu_1, \nu_2) \quad (\text{C.633})$$

**source**=  $S^{[a],[n_1],[n_2]}$ , **index**=  $I^{[a],[n_1],[n_2]}$

6. **max()** and **argmax()** along  $dim = 0$

$$\max : T^{[a],[b]} \rightarrow T^{\alpha_0,[b]} \quad (\text{C.634})$$

$$\operatorname{argmax} : T^{[a],[b]} \rightarrow \alpha_0 \quad (\text{C.635})$$

where  $T^{\alpha_0,\beta} = \max\{T^{\alpha,\beta} : \alpha \in [a]\}$

---

<sup>23</sup>This operation is available in PyTorch. So far Numpy doesn't have it in direct form.

7. **repeat()** with  $r = [r_0, r_1, \dots, r_{n-1}]$  along  $dim = 0$

$$T^{[n],\beta,\gamma} \rightarrow \boxed{pow(T^{0,\beta,\gamma}, r_0) \\ pow(T^{1,\beta,\gamma}, r_1) \\ \vdots \\ pow(T^{n-1,\beta,\gamma}, r_{n-1})}^{[R],\beta,\gamma} \quad (C.636)$$

where  $R = \sum_{i=0}^{n-1} r_i$ . note that concatenate() along  $dim = 0$  and repeat() with  $r = pow(1, n)$  along  $dim = 0$ , are the same thing. So repeat() is a souped up version of concatenate().

8. **reshape()** from shape  $(n_0, n_1, n_2)$  to shape  $(n, m)$

$$T^{[n_0],[n_1],[n_2]} \rightarrow Y^{[n],[m]} \quad (C.637)$$

where  $n_0 n_1 n_2 = nm$ . A more fine grained description is

$$T^{\alpha,\beta,\gamma} \rightarrow Y^{\mu(\alpha,\beta,\gamma),\nu(\alpha,\beta,\gamma)} \quad (C.638)$$

where  $n_0 n_1 n_2 = nm$  and  $\mu : [n_0] \times [n_1] \times [n_2] \rightarrow [n]$  and  $\nu : [n_0] \times [n_1] \times [n_2] \rightarrow [m]$  are 1-1 onto functions. flatten() is clearly a special case of reshape().

9. **split()** along  $dim = 0$

$$\boxed{T_0^{[n_0],\beta,\gamma} \\ T_1^{[n_1],\beta,\gamma} \\ T_2^{[n_2],\beta,\gamma}}^{[n],\beta,\gamma} \rightarrow [T_0^{[n_0],\beta,\gamma}, T_1^{[n_1],\beta,\gamma}, T_2^{[n_2],\beta,\gamma}] \quad (C.639)$$

where  $n = n_0 + n_1 + n_2$

10. **squeeze()**  $dim = 0$

$$T^{0,[b],[c]} \rightarrow Y^{[b],[c]} \quad (C.640)$$

$$T^{0,\beta,\gamma} \rightarrow Y^{\beta,\gamma} = T^{0,\beta,\gamma} \quad (C.641)$$

11. **stack()** along  $dim = 0$

$$[T_0^{\alpha,\beta,\gamma}, T_1^{\alpha,\beta,\gamma}, T_2^{\alpha,\beta,\gamma}] \rightarrow \boxed{T_0^{\alpha,\beta,\gamma} \\ T_1^{\alpha,\beta,\gamma} \\ T_2^{\alpha,\beta,\gamma}}^{[3],\alpha,\beta,\gamma} \quad (C.642)$$

Compare this to `concatenate()`. `stack()` creates a new dimension whereas `concatenate()` doesn't. `concatenate()` just increases the range of an existing dimension.

12. `sum()` along  $dim = 0$

$$T^{[a],[b]} \rightarrow \sum_{\alpha} T^{\alpha,[b]} \quad (\text{C.643})$$

13. `tensordot()` (i.e., contraction) along  $dim = 0$

$$[T^{[n],\beta}, S^{[n],\beta}] \rightarrow T^{\alpha,\beta} \delta_{\alpha,\alpha'} S^{\alpha',\beta} = \sum_{\alpha} T^{\alpha,\beta} S^{\alpha,\beta} \quad (\text{C.644})$$

14. `tile()`<sup>24</sup>

$$\texttt{reps} = [2, 3] \quad (\text{C.645})$$

$$T^{[a],[b]} \rightarrow \boxed{T^{[a],[b]} \quad T^{[a],[b]} \quad T^{[a],[b]} \\ T^{[a],[b]} \quad T^{[a],[b]} \quad T^{[a],[b]}}^{[2a],[3b]} \quad (\text{C.646})$$

$$T^{\alpha,\beta} \rightarrow \boxed{T^{[a],[b]} \quad T^{[a],[b]} \quad T^{[a],[b]} \\ T^{[a],[b]} \quad T^{[a],[b]} \quad T^{[a],[b]}}^{A(\alpha,\beta),B(\alpha,\beta)} \quad (\text{C.647})$$

15. `transpose()` by a permutation  $\sigma : [3] \rightarrow [3]$ . <sup>25</sup>

$$T^{\alpha,\beta,\gamma} \rightarrow T^{\alpha_1,\beta_1,\gamma_1} \delta_{\alpha_1,\beta_1,\gamma_1}^{\sigma(\alpha,\beta,\gamma)} \quad (\text{C.648})$$

For example,

$$T^{\alpha,\beta,\gamma} \rightarrow T^{\alpha_1,\beta_1,\gamma_1} \delta_{\alpha_1,\beta_1,\gamma_1}^{\gamma,\beta,\alpha} \quad (\text{C.649})$$

---

<sup>24</sup>`tile()` in Numpy corresponds to `repeat()` in PyTorch.

<sup>25</sup>a permutation  $\sigma : [n] \rightarrow [n]$  is a bijection, i.e., a 1-1 onto map.

# Appendix D

## Definition of a Bayesian Network

A **directed graph**  $G = (V, E)$  consists of two sets,  $V$  and  $E$ .  $V$  contains the **vertices (nodes)** and  $E$  contains the **edges (arrows)**. An arrow  $\underline{a} \rightarrow \underline{b}$  is an ordered pair  $(\underline{a}, \underline{b})$  where  $\underline{a}, \underline{b} \in V$ .

The **parents** of a node  $\underline{x}$  are those nodes  $\underline{a}$  such that there are arrows  $\underline{a} \rightarrow \underline{x}$ . The **children** of a node  $\underline{x}$  are those nodes  $\underline{b}$  such that there are arrows  $\underline{x} \rightarrow \underline{b}$ . A **root node** is a node with no parents. A **leaf node** is a node with no children. The **neighbors** of a node  $\underline{x}$  is the set of parents and children of  $\underline{x}$ .

A **path** is a set of nodes that are connected by arrows, so that all nodes have 1 or 2 neighbors, but only two nodes (**open path**) or zero nodes (**closed path**) have only one neighbor. A **directed path** is a path in which all the arrows point in the same direction. A **loop** is a closed path; i.e., a path in which all nodes have exactly 2 neighbors. A **cycle** is a directed loop. A **Directed Acyclic Graph (DAG)** is a directed graph that has no cycles.

A **fully connected directed graph** is a directed graph in which every node has all other nodes as neighbors. Figs.D.1 and D.2 show 2 different ways of drawing the same directed graph, a fully connected graph with 4 nodes. Note that a convenient way to label the nodes of a fully connected directed graph with  $N$  nodes is to point arrows from  $\underline{x}_k$  to  $\underline{x}_j$  where  $j = 0, 1, 2, \dots, N - 1$  and  $k = j - 1, j - 2, \dots, 0$ .



Figure D.1: Fully connected directed graph with 4 nodes, drawn as a line.

A **connected graph** is a graph for which there is no way of separating the nodes into two sets so that there is no arrow from one set to the other. A **tree** is a directed graph in which all nodes have a single parent except for a single node called the “root” node which has no parents. A **polytree** is a DAG with no loops.

A **Bayesian network (bnet)** consists of a DAG and a **Transition Probability Matrix (TPM)** associated with each node of the graph. A TPM is often

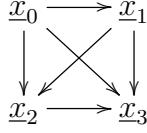


Figure D.2: Fully connected directed graph with 4 nodes, drawn as a square.

called a **Conditional Probability Table (CPT)**. The **structure** of a bnet is its DAG alone, sans the TPMs. The **skeleton** of a bnet is the undirected graph beneath the bnet's DAG.

In this book, random variables are indicated by underlined letters and their values by non-underlined letters. We use  $S_{\underline{x}}$  to denote the set of states (i.e., values) that a random variable  $\underline{x}$  can assume. Each node of a bnet is labelled by a random variable. Thus,  $\underline{x} = x$  means that node  $\underline{x}$  is in state  $x$ .

---

#### Some sets of nodes associated with each node $\underline{a}$ of a bnet

- $ch(\underline{a})$  = children of  $\underline{a}$ .
- $pa(\underline{a})$  = parents of  $\underline{a}$ .
- $nb(\underline{a}) = pa(\underline{a}) \cup ch(\underline{a})$  = neighbors of  $\underline{a}$ .
- $de(\underline{a}) = \cup_{n=1}^{\infty} ch^n(\underline{a}) = ch(\underline{a}) \cup ch \circ ch(\underline{a}) \cup \dots$ , descendants of  $\underline{a}$ .
- $an(\underline{a}) = \cup_{n=1}^{\infty} pa^n(\underline{a}) = pa(\underline{a}) \cup pa \circ pa(\underline{a}) \cup \dots$ , ancestors of  $\underline{a}$ .

In this book, we will use  $\underline{a}.$  to indicate a **multi-node (node set, node array)**  $\underline{a}. = (\underline{a}_j)_{j=0,1,\dots,na-1}$ . We will often treat multinodes as if they were sets, and combine them with the usual set operators. For instance, for two multinodes  $\underline{a}.$  and  $\underline{b}.$ , we define  $\underline{a}. \cup \underline{b}.$ ,  $\underline{a}. \cap \underline{b}.$ ,  $\underline{a}. - \underline{b}.$  and  $\underline{a}. \subset \underline{b}.$  in the obvious way. We will indicate a singleton set (single node multi-node)  $\underline{a}. = \{\underline{a}\}$  simply by  $\underline{a}. = \underline{a}.$  For instance,  $\underline{a}. - \underline{b} = \underline{a}. - \{\underline{b}\}.$

The TPM of a node  $\underline{x}$  of a bnet is a matrix of probabilities  $P(\underline{x} = x | pa(\underline{x}) = a.)$ , where  $x \in S_{\underline{x}}$  and  $a. \in S_{pa(\underline{x})}$ .

A **deterministic node** is a node such that its TPM is of the form

$$P(\underline{x} = x | pa(\underline{x}) = a.) = \delta(x, f(a.)) \quad (\text{D.1})$$

for some function  $f : S_{pa(\underline{x})} \rightarrow S_{\underline{x}}$ , where  $\delta(x, y)$  is the Kronecker delta function.

A bnet with nodes  $\underline{x}.$  represents a probability distribution

$$P(x.) = \prod_j P(\underline{x}_j = x_j | (\underline{x}_k = x_k)_{k: \underline{x}_k \in pa(\underline{x}_j)}). \quad (\text{D.2})$$

Note that for a fully connected bnet with  $N$  nodes, Eq.(D.2) becomes

$$P(x.) = \prod_{j=0}^{N-1} P(x_j | (x_k)_{k=j-1, j-2, \dots, 0}) . \quad (\text{D.3})$$

For example, if  $N = 4$ , Eq.(D.3) becomes

$$P(x_0, x_1, x_2, x_3) = P(x_3 | x_2, x_1, x_0)P(x_2 | x_1, x_0)P(x_1 | x_0)P(x_0) . \quad (\text{D.4})$$

We see that Eq.(D.3) is just the chain rule for conditional probabilities.

Of course, not all bnets are fully connected. So what determines whether in a bnet with nodes  $\underline{x}$  and  $\underline{y}$ , we draw or not draw, an arrow connecting the two nodes?

Recall that two random variables  $\underline{x}, \underline{y}$  are **(probabilistically) independent** (denoted by  $\underline{x} \perp \underline{y}$ ) if  $P(y|x) = P(y)$ . Let us denote the correlation between  $\underline{x}$  and  $\underline{y}$  by  $\langle \underline{x}, \underline{y} \rangle = \langle \underline{xy} \rangle - \langle \underline{x} \rangle \langle \underline{y} \rangle$ . It's easy to show that  $\underline{x} \perp \underline{y}$  implies  $\langle \underline{x}, \underline{y} \rangle = 0$ . However, the converse is not true: it's possible for  $\underline{x}$  and  $\underline{y}$  to be uncorrelated but dependent. For example, if  $\underline{y} = \underline{x} - \langle \underline{x}, \underline{x} \rangle$ , we get  $\langle \underline{x}, \underline{y} \rangle = 0$ , but  $P(y|x) \neq P(y)$ . However,  $\underline{x} \perp \underline{y}$  if and only if  $\langle f(\underline{x}), g(\underline{y}) \rangle$  for all functions  $f, g$ .

Consider the bnet  $\underline{x} \rightarrow \underline{m} \rightarrow \underline{y}$ . In this case,  $\underline{x}$  and  $\underline{y}$  are dependent, but there is no arrow connecting them. Henceforth, we will say that there is a **direct dependence** between nodes  $\underline{x}$  and  $\underline{y}$  if there is an arrow connecting them. Note that  $\underline{x}$  and  $\underline{y}$  are not directly dependent iff<sup>1</sup>  $P(y|do(x)) = P(y)$  (i.e., no  $\underline{x} \rightarrow \underline{y}$ ) and  $P(x|do(y)) = P(x)$  (i.e., no  $\underline{y} \rightarrow \underline{x}$ ).  $\underline{x}$  and  $\underline{y}$  can be dependent but not directly dependent.

---

In this book, we use the following conventions for bnet diagrams:

Random variables are underlined and their values are not. For example,  $\underline{a} = a$  means the random variable  $\underline{a}$  takes the value  $a$ . A diagram with all its nodes underlined represents a Bayesian Network (bnet), whereas the same diagram with the letters not underlined represents a specific **instantiation** of that bnet. For example  $\underline{a} \rightarrow \underline{b} \rightarrow \underline{c}$  represents the bnet with full probability distribution  $P(c|b)P(b|a)P(a)$ , whereas  $a \rightarrow b \rightarrow c$  represents  $P(c|b)P(b|a)$ . Note that, for convenience, we define  $a \rightarrow b \rightarrow c$  to exclude the priors of root nodes such as  $P(a)$ .

If  $\underline{a}$  is a root node, then  $\sum a$  signifies a weighted sum  $\sum_a P(a)$ . For example,

$$\sum a \rightarrow b \rightarrow c = \sum_a P(c|b)P(b|a)P(a) \quad (\text{D.5})$$

If  $\underline{a}$  is not a root node, then  $\sum a$  signifies a simple unweighted sum  $\sum_a$ . For example,

$$x \rightarrow \sum a \rightarrow y = \sum_a P(y|a)P(a|x) \quad (\text{D.6})$$

---

<sup>1</sup>As will be defined in Chapter 12,  $P(y|do(x))$  equals  $P(y|x)$  for the bnet in which all arrows entering node  $\underline{x}$  have been amputated and node  $\underline{x}$  has been set to state  $x$ .

Two bnets are equated if their full probability distributions (i.e., their full instantiations) are equal numerically. For example,

$$\underline{a} \rightarrow \underline{b} \rightarrow \underline{c} = P(c|b)P(b|a)P(a) = \underline{a} \leftarrow \underline{b} \leftarrow \underline{c} \quad (\text{D.7})$$

---

Unobserved (a.k.a. hidden, latent) nodes are indicated in a bnet by enclosing their label in a dashed circle. For example,  $\langle \underline{u} \rangle$ . Alternatively, they are indicated by using dashed arrows for all arrows emanating from the unobserved node.

In Chapter 34, we define a measure of goodness (G) of causal fit (CF) for each bnet of a finite set of bnets  $\mathcal{G}$ .

Given a dataset of samples for the random variables  $(\underline{x}_i)_{i=0,1,\dots,N-1}$ , and a finite set of possible bnets  $\mathcal{G}$ , set  $\mathcal{G}$  may contain several bnets (differing in the direction of some arrows) that fit the data well causally. However, the one with the highest GCF is most likely to be used by Nature. In this book, we will refer to that single one as the **best CF bnet**. We will also refer to a bnet in  $\mathcal{G}$  that has a high (resp., low) value of GCF, though not necessarily the highest (resp., lowest), as a **good (resp., bad) CF bnet**.<sup>2</sup>

It's important to realize that bnets that are not a good CF are far from useless; they are frequently used as intermediate calculational tools. They are incorrect causally, but they aren't incorrect numerically. For instance, in Bayes rule, we switch from a good CF bnet  $P(x|\theta)P(\theta) = \underline{x} \leftarrow \underline{\theta}$  to a bad CF bnet  $P(\theta|x)P(x) = \underline{x} \rightarrow \underline{\theta}$ , where  $x$  is the data and  $\theta$  are the parameters.

---

<sup>2</sup>In this book, the term "causal bnet" will mean a good CF bnet. Pearl is fond of using the term "causal bnet", but he uses it in a different sense that does not allude to a measure of goodness of causal fit.

# Appendix E

## Bayesian Networks, Causality and the Passage of Time

This chapter is based on a blog post (see Ref.[70]) from my blog “Quantum Bayesian Networks”.

### E.1 Unifying Principle of this book

The unifying principle of this book is Bayesian Networks (bnets). The main goal of this book is to explain as much of Artificial Intelligence (AI) and Machine Learning (ML) as possible using bnets.

Bayesian Networks are a graphical representation of the chain rule for conditional probabilities. They are not a “heuristic algorithm” like XGBoost or Neural Nets. They are a very simple, intuitive, basic and general definition. I would say that the definition of a Bayesian Network is as important to Probability Theory as the definition of a Group is to Abstract Algebra. Algebraic groups are never going to go out of fashion and neither are B nets.

An Artificial Neural Net can be defined as a Bayesian Network with a layered structure, and such that all its nodes are deterministic<sup>1</sup>. A decision tree is not exactly a Bayesian Network, but it can be trivially replaced by an equivalent B net that has the same tree structure (for more details about this equivalence, see the Chapter 16 on decision trees). The SCM diagrams favored by Pearl are just bnets whose internal nodes are deterministic and external ones are probabilistic. In fact, as I show in this book, most methods in AI can be understood in terms of B nets—just like many theorems in Abstract Algebra can be understood in terms of groups.

---

<sup>1</sup>Neural Nets (NNs) are DAGs, but they contain a lot of spurious arrows whose direction or very existence has no causal motivation, and they could be missing other arrows which would have a causal motivation. So I like to say that NNs are acausal DAGs.

## E.2 You say tomato, I say tomato

In this chapter, I will use the terms Bayesian Network (bnet), causal model and DAG as if they were synonymous. My justification for doing this is as follows.

A Bayesian Network is a DAG + probability tables. One can easily compute the probability tables from DAG + Dataset. Therefore,

You say DAG+Dataset, I say Bayesian Network.

The use of the terms “causal model” and “DAG”, as an alternative to the term “Bayesian Network”, has become popular in the last decade among economists, epidemiologists, AI researchers and even Judea Pearl himself. It seems some people think “causal models” and “DAGs” are revolutionary, whereas Bayesian Networks are a concept that was tried 25 years ago, and has been replaced since then by stuff that works better. But any time you have a Dataset, which is almost always true in practice in Economics, Epidemiology and AI, a DAG implies a Bayesian Network and vice versa.

## E.3 A dataset is causal model free

Time and time again, Judea Pearl makes the point on Twitter to neural net advocates that they are trying to do a provably impossible task, to derive a causal model from data. I could be wrong, but this is what I think he means.

When Pearl says “data”, he is referring to what is commonly called a dataset. A dataset is a table of data, where all the entries of each column have the same units, and measure a single feature, and each row refers to one particular sample or individual. Datasets are particularly useful for estimating probability distributions and for training neural nets. When Pearl says a “causal model”, he is referring to a DAG (directed acyclic graph) or a bnet (Bayesian Network= DAG + probability table for each node of DAG).

Sure, you can try to derive a causal model from a dataset, but you’ll soon find out that you can only go so far.

The process of finding a partial causal model from a dataset is called structure learning (SL). SL can be done quite nicely with Marco Scutari’s open source program bnlearn. There are 2 main types of SL algorithms: score-based and constraint based. The first and still very competitive constraint-based SL algorithm was the Inductive Causation (IC) algorithm proposed by Pearl and Verma in 1991. So Pearl is quite aware of SL. The problem is that SL often cannot narrow down the causal model to a single one. It finds an undirected graph (UG), and it can determine the direction of some of the arrows in the UG, but it is often incapable, for well understood fundamental—not just technical—reasons, of finding the direction of ALL the arrows of the UG. So it often fails to fully specify a DAG model.

Let’s call the ordered pair (dataset, causal model) a dataset++ . Then what I believe Pearl is saying is that a dataset is causal model-free or causal model-less

(although sometimes one can find a partial causal model hidden in there). A dataset is not a dataset++.

## E.4 What is causality?

What is Causality, really, and how do Bayesian Networks (a.k.a. Causal Models, DAGs) encode it? For me, Causality is a time-induced ordering between two events, the transmission of information (and its accompanying energy) from the earlier of the two events to the later one, and the physical response of the later event to the reception of that information.

Note that this definition of causality does not mention correlation. It is often assumed that even though correlation does not imply causation, causation implies correlation. But the latter statement is false; there are scenarios, albeit unusual, "fine tuned" ones, in which there is causation without correlation. For example, consider a bnet with arrows  $\underline{x} \rightarrow \underline{y}$  and  $\underline{x} \rightarrow \underline{c} \rightarrow \underline{y}$ . When we amputate the arrows entering  $\underline{x}$ , a dependence between  $\underline{x}$  and  $\underline{y}$  persists, so we say  $\underline{x}$  causes  $\underline{y}$ . Even though  $\underline{x}$  causes  $\underline{y}$ , it's possible to tune the probabilities of the bnet so that the effect of the path  $\underline{x} - \underline{c} - \underline{y}$  and the effect of the direct path  $\underline{x} - \underline{y}$  cancel each other out and produce zero correlation between  $\underline{x}$  and  $\underline{y}$ . As a trivial example, suppose  $\underline{c} = 2\underline{x}$ ,  $\underline{y} = \underline{c} - 2\underline{x} = 0$ . Since  $\underline{y} = 0$ , it's uncorrelated with  $\underline{x}$ .

The nodes of a bnet represent random variables. Some of those random variables are clearly events (i.e., they occur at a definite time). For example, let  $D=0$  if a patient is not given a drug,  $D=1$  if he/she is given it.  $D$  occurs at a definite time. But other random variables represent qualities which do not occur at a definite time. For example,  $G=\text{gender}=\text{male, female}$ .  $G$  does not occur at a definite time. But even in the case of a quality like  $G$ , its value is first decided at birth, so one can ascribe to  $G$  a particular, albeit fuzzy time interval during which it is decided. If  $M=0(\text{single}), 1(\text{married})$ , then we can assign to  $M$  the day of the marriage. Both the time interval assigned to  $G$  and to  $M$  are somewhat ambiguous, but still, most people would say that  $G$  occurs before  $M$  (if a marriage occurs at all). Saying the opposite, that  $M$  occurs before  $G$ , seems pretty hard to understand. If two nodes  $A$  and  $B$  of a bnet have time intervals ascribed to them such that the time interval of  $A$  does not clearly occur before or after the time interval of  $B$ , and if also there is a large causal correlation between  $A$  and  $B$ , then it probably does not matter much whether one draws an arrow from  $A$  to  $B$ , or the opposite.

Now that we understand that the arrows in a bnet really do encode the direction of time, it becomes clear why a dataset does not fully specify a bnet. By a dataset (think of a dataframe in Pandas or R), I mean an array of numbers where the columns refer to features and the rows refer to individuals in a population. The column labels of the dataset become the node names of the bnet. Nowhere in a dataset is there any indication of the time ordering of the features. Hence, it's impossible to create, from a dataset alone, a bnet, because bnets do carry such time-ordering

information.

Chapter 36 discusses Granger Causality (GC). The critics of GC point out that it assumes, somewhat erroneously, that if event A precedes B and the two events are correlated, A must cause B. I agree. Most roosters crow in response to the stimulus of the sunrise light. A rooster could crow before sunrise if, for example, he had an alarm clock that woke him up 30 minutes before sunrise, but such cases are uncommon, and seem to involve other intermediate events. The moral is that time ordering and correlation are not sufficient conditions for causality. To establish causality with more certainty, one also needs a pinch of prior expert knowledge, or one must gain that expert knowledge through “do” operator experimentation.

## E.5 Bayesian Networks and the passage of time

Now that we understand that a bnet’s arrows are encoding roughly the passage of time, it becomes possible to glean from this insight a simple method, which, although not very rigorous, is really helpful to me. I will illustrate said method with the famous “Asia” bnet in Fig.E.1. In this bnet, all nodes have two possible values, 0 and 1.

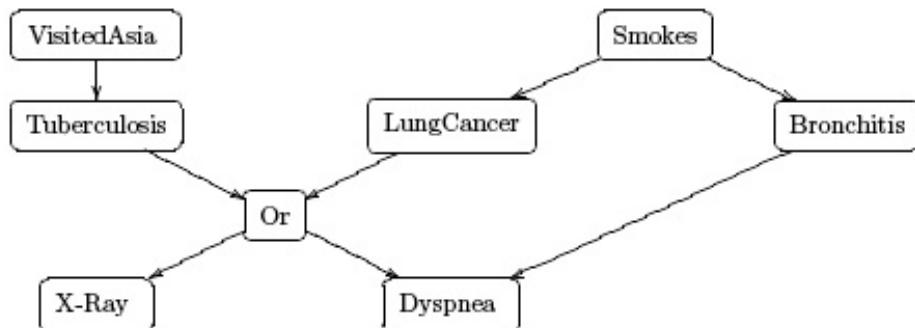


Figure E.1: Asia bnet. Dyspnea=trouble breathing

Given a dataset for this bnet, one can calculate the correlation between every 2 features of the dataset. The feature names become the node names, and links are drawn between any 2 nodes whose correlation is causal and greater in absolute value to some threshold value. This gives an undirected graph that can be obtained from bnet Fig.E.1 by erasing the directions of the arrows. So how can we guess the directions of the arrows? Well, one uses a little bit of “expert knowledge” to conclude that

$$\text{time(Visited Asia)} < \text{time(Tuberculosis)} < \text{time(Or)} < \text{time(X-Ray, Dyspnea)}$$

Also

$$\text{time(smokes)} < \text{time(LungCancer, Bronchitis)} < \text{time(Or)} < \text{time(Dyspnea)}$$

If  $\text{time}(A) < \text{time}(B)$ , then  $A \rightarrow B$ . Like I said before, the times we ascribe to these events are somewhat fuzzy and open to debate, so this algorithm is far from being rigorous. But often, saying that  $\text{time}(A) < \text{time}(B)$  makes much more sense than saying that  $\text{time}(B) < \text{time}(A)$ . When in doubt about the best direction to give to an arrow of an undirected graph, I recommend calculating a Goodness of Causal Fit metric (see Chapter 34) which makes use of “do” operator experimentation.

A dataset cannot fully specify a bnet because it lacks time ordering info. A dataset also cannot do the harder task of specifying a bnet that is a good causal fit to the problem, because it lacks time ordering info AND prior expert knowledge AND expert knowledge gained from posterior “do” operator experimentation.

## E.6 Advice for the DAG-phobic

DAGs are your friends. DAGs should be easy and fun to dream up. After all, I am convinced that DAGs are an integral part of how humans think, so they should come naturally to us. Nevertheless, many people are scared of, or detest, DAGs. I think it’s because they fail to grasp the following 3 things:

1. DAGs are not unique. Stop thinking that you have to find the unique DAG for the situation being considered. You just have to find a DAG that is a good causal fit for the situation. If a DAG is too complicated, you can always simplify it by merging several nodes into a single more abstract one, or by summing over unwanted nodes.
2. The nodes of a DAG are roughly ordered from past to present. The arrows of a DAG roughly reflect the passage of time.
3. DAGs represent scientific hypotheses that can and should be tested with do experiments. Causal Inference is an application of the scientific method, which consists of the following steps: formulate hypothesis (DAG), devise experiment to test it, test it.

# Chapter 1

## AdaBoost

This chapter is based on Ref.[87].

Adaptive Boosting (AdaBoost) is a method of constructing a strong classifier function as a linear combination of an ensemble of weak classifier functions.

Below, we will abbreviate “ensemble classifiers” by “e-classifiers” and “weak classifiers” by “w-classifiers”.

Chapter 16 defines decision trees (dtrees) and explains how to construct them. A **tree stump** is a dtree with only one parent and 2 children nodes. Usually the w-classifier functions for AdaBoost come from tree stumps (because tree stumps are w-classifiers and simple to compute), but the core AdaBoost algorithm is oblivious to where the w-classifier functions came from.

Boosting (see this chapter on AdaBoost and Chapter 101 on XGBoost) and bagging (see Chapter 74 on Random Forest) are two methods of building a classifier function from an ensemble of classifier functions. These two methods are most commonly applied to dtrees: Boosting for an ensemble of small dtrees, and Bagging for a random forest (which is an ensemble of dtrees that are usually much more complicated than small dtrees).

### 1.1 AdaBoost for general ensemble of w-classifiers

In this section we discuss the core AdaBoost algorithm, valid for a generic ensemble of w-classifiers.

Let  $L = [0, 1, 2, \dots, nsam - 1]$  be a list of individuals (samples) in a population. In this chapter, we will use the notation  $A^\sigma = A[\sigma]$  and  $\vec{A} = [A^\sigma : \sigma \in L]$  for a list (vector, 1-D array) indexed by  $L$ . We will refer to  $DS = (\vec{x}, \vec{y})$  where  $x^\sigma \in S_{\underline{x}}$ ,  $y^\sigma \in S_y$ , as a dataset. Let  $T = \{0, 1, \dots, nt - 1\}$ . Let  $x^\sigma = (x_0^\sigma, x_1^\sigma, \dots, x_{nt-1}^\sigma) \in S_{\underline{x}_0} \times S_{\underline{x}_1} \times \dots \times S_{\underline{x}_{nt-1}} = S_{\underline{x}}$ .

AdaBoost assumes that the classifier class set  $S_y$  and all the feature sets  $S_{\underline{x}_t}$  are binary:  $S_y = S_{\underline{x}_t} = \{-1, 1\}$  for all  $t \in T$ .

Suppose that we are given an ensemble of  $nt$  **w-classifiers**  $Y_t : S_{\underline{x}} \rightarrow \{-1, 1\}$ , where  $t \in T$ . Suppose we want to find **intermediate e-classifiers**  $\mathcal{Y}_t : S_{\underline{x}} \rightarrow \mathbb{R}$  given

by

$$\mathcal{Y}_t(x^\sigma) = \sum_{t'=0}^t \alpha_{t'} Y_{t'}(x^\sigma) \in \mathbb{R} \quad (1.1)$$

for  $t \in T$  and a **final e-classifier** given by

$$\mathcal{Y}_{fin}(x^\sigma) = \text{sign}(\mathcal{Y}_{nt-1}(x^\sigma)) \in \{-1, 1\}. \quad (1.2)$$

The AdaBoost algorithm yields a set of coefficients  $\alpha_t$  for which the final e-classifier is much stronger (i.e., less error prone) than any of the w-classifiers of the ensemble.

Note that

$$\mathcal{Y}_t(x^\sigma) = \mathcal{Y}_{t-1}(x^\sigma) + \alpha_t Y_t(x^\sigma) \quad (1.3)$$

for  $t \in T$  if we define  $\mathcal{Y}_{-1} = 0$ . Hence

$$\underbrace{e^{-y^\sigma \mathcal{Y}_t(x^\sigma)}}_{Z_t w_{t+1}^\sigma} = \underbrace{e^{-y^\sigma \mathcal{Y}_{t-1}(x^\sigma)}}_{Z_{t-1} w_t^\sigma} e^{-\alpha_t y^\sigma Y_t(x^\sigma)} \quad (1.4)$$

where the **weights**  $w_t^\sigma$  and the **partition function**  $Z_t$  are defined by

$$w_{t+1}^\sigma = \begin{cases} 1/nsam & \text{for } t = -1 \\ \frac{\exp(-y^\sigma \mathcal{Y}_t(x^\sigma))}{Z_t} & \text{for } t \geq 0 \end{cases} \quad (1.5)$$

and

$$Z_t = \sum_\sigma e^{-y^\sigma \mathcal{Y}_t(x^\sigma)}. \quad (1.6)$$

Note that the probability distribution  $P(\sigma|t+1) = w_{t+1}^\sigma$  of weights at time  $t+1$  emphasizes (i.e., gives higher probability to) the errors (i.e., occurrences of  $y^\sigma \mathcal{Y}_t(x^\sigma) = -1$  for some population individual  $\sigma$ ) of the previous (i.e., at time  $t$ ) intermediate e-classifier  $\mathcal{Y}_t$ . In other words, every new intermediate e-classifier  $\mathcal{Y}_{t+1}$  concentrates on those individuals  $\sigma$  on which the previous e-classifier  $\mathcal{Y}_t$  performed poorly.

Note also that the partition function  $Z_t$  is a good measure of the **classification error** (i.e., occurrences of  $y^\sigma \mathcal{Y}_t(x^\sigma) = -1$ ) of  $\mathcal{Y}_t$ . We will therefore use  $Z_t$  for that purpose, as an error measure.

For  $t > 1$ , we have

$$Z_t = \sum_\sigma e^{-y^\sigma \mathcal{Y}_t(x^\sigma)} \quad (1.7)$$

$$= \sum_\sigma \underbrace{e^{-y^\sigma \mathcal{Y}_{t-1}(x^\sigma)}}_{Z_{t-1} w_t^\sigma} e^{-\alpha_t y^\sigma Y_t(x^\sigma)} \quad (1.8)$$

$$= Z_{t-1} E_\sigma [e^{-\alpha_t y^\sigma Y_t(x^\sigma)}] \quad (1.9)$$

Define the **success rate** by

$$S_t = \sum_{\sigma} w_t^{\sigma} \mathbb{1}(y^{\sigma} Y_t(x^{\sigma}) = 1) \quad (1.10)$$

$$= E_{\sigma} [\underbrace{\mathbb{1}(y^{\sigma} Y_t(x^{\sigma}) = 1)}_{\text{iff } y^{\sigma} = Y_t(x^{\sigma})}] \quad (1.11)$$

and the **failure rate** by

$$F_t = \sum_{\sigma} w_t^{\sigma} \mathbb{1}(y^{\sigma} Y_t(x^{\sigma}) = -1) \quad (1.12)$$

$$= E_{\sigma} [\underbrace{\mathbb{1}(y^{\sigma} Y_t(x^{\sigma}) = -1)}_{\text{iff } y^{\sigma} \neq Y_t(x^{\sigma})}] . \quad (1.13)$$

Note that

$$S_t + F_t = 1 , \quad (1.14)$$

and

$$Z_t = Z_{t-1} (e^{-\alpha_t} S_t + e^{+\alpha_t} F_t) . \quad (1.15)$$

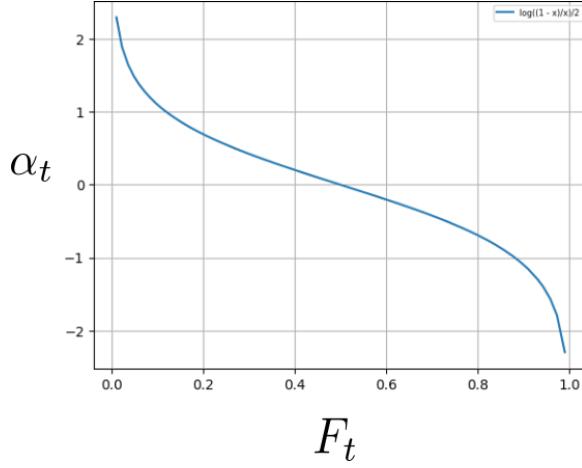


Figure 1.1: Plot of function  $\alpha_t = \frac{1}{2} \ln \frac{1-F_t}{F_t}$ .

We can find the  $\alpha_t$  values that minimize the classification error  $Z_t$ , and then evaluate  $Z_t$  at those optimum  $\alpha_t$  values:

$$\frac{dZ_t}{d\alpha_t} = Z_{t-1} (-e^{-\alpha_t} S_t + e^{\alpha_t} F_t) = 0 \quad (1.16)$$

$$e^{2\alpha_t} = \frac{S_t}{F_t} \quad (1.17)$$

$$\alpha_t = \frac{1}{2} \ln \frac{S_t}{F_t} = \frac{1}{2} \ln \frac{1 - F_t}{F_t} \quad (1.18)$$

$$\frac{Z_t}{Z_{t-1}} = 2\sqrt{S_t F_t} = 2\sqrt{(1 - F_t) F_t} \leq 1 \quad (1.19)$$

$f(x) = 2\sqrt{(1 - x)x}$  for  $x \in [0, 1]$  is dome shaped and its maximum is 1, which is achieved iff  $x = \frac{1}{2}$

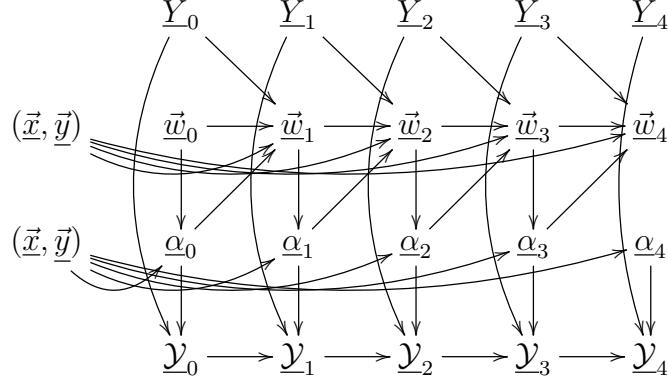


Figure 1.2: Bnet for AdaBoost with 5 w-classifiers,  $nt = 5$ . All nodes labelled  $(\vec{x}, \vec{y})$  are the same node.

The AdaBoost algo described in this chapter is summarized by the bnet of Fig.1.2. The TPMs, printed in blue, for that bnet, are as follows:

$$P(w_0^\sigma) = \frac{1}{nsam} \quad (1.20)$$

for all  $\sigma$ .

$$P(\vec{w}_{t+1} | \vec{w}_t, \alpha_t, Y_t, \vec{x}, \vec{y}) = \prod_\sigma \mathbb{1}( w_{t+1}^\sigma = \frac{w_t^\sigma e^{-\alpha_t y^\sigma Y_t(x^\sigma)}}{\sum_\sigma \text{numerator}} ) \quad (1.21)$$

for  $t \geq 0$ .

$$P(\alpha_t | \vec{w}_t, \vec{x}, \vec{y}) = \mathbb{1}( \alpha_t = \frac{1}{2} \ln \frac{1 - F_t}{F_t} \text{ where } F_t = F_t(\vec{w}_t, \vec{x}, \vec{y}) ) \quad (1.22)$$

for  $t \in T$ .

$$P(\mathcal{Y}_t | \mathcal{Y}_{t-1}, \alpha_t, Y_t) = \mathbb{1}( \mathcal{Y}_t = \mathcal{Y}_{t-1} + \alpha_t Y_t ) \quad (1.23)$$

for  $t \in T$ , where  $\mathcal{Y}_{-1} = 0$ .

## 1.2 AdaBoost for ensemble of tree stumps

Keep in mind that AdaBoost assumes  $S_y = S_{x_t} = \{-1, 1\}$  for all  $t \in T = \{0, 1, \dots, nt - 1\}$ . In order to implement AdaBoost, we need to specify  $nt$  w-classifiers  $Y_t : \{-1, 1\}^{nt} \rightarrow \{-1, 1\}$  for  $t \in T$ . One can either specify the  $nt$  w-classifiers a priori or build them on-the-fly.

- **w-classifiers specified a priori**

Define a classifier for each feature  $x_t$  where  $t \in T$  by:

$$Y_t(x^\sigma) = x_t^\sigma \in \{-1, 1\} \quad (1.24)$$

Hence, for this classifier,  $y^\sigma Y_t(x^\sigma) = y^\sigma x_t^\sigma$ .

- **w-classifiers built on-the-fly**

Recall dataset  $(\vec{x}, \vec{y}) = [(x^\sigma, y^\sigma) : \sigma \in L]$  is indexed by the list  $L = [0, 1, \dots, nsam - 1]$ . If  $L_j$  is a list (possibly with duplicate items) such that  $set(L_j) \subset set(L)$ , then define  $DS_j = (\vec{x}, \vec{y})_{L_j} = ((x^\sigma)_{\sigma \in L_j}, (y^\sigma)_{\sigma \in L_j})$ . We will refer to  $DS_j$  as the **restriction of  $(\vec{x}, \vec{y})$  to  $L_j$** .

The idea behind on-the-fly w-classifiers is to choose  $Y_t(x^\sigma) = x_t^\sigma$ , where  $x_t$  is the feature with the lowest Gini in the current dataset  $(\vec{x}, \vec{y})_{L_t}$ . To build  $(\vec{x}, \vec{y})_{L_t}$ , we select at random from  $L = [0, 1, \dots, nsam - 1]$ , a list  $L_t$  of the same length as  $L$ , using the probability distribution  $\vec{w}_{t-1}$ . By choosing  $L_t$  with probabilities  $\vec{w}_{t-1}$ , we emphasize individuals  $\sigma$  that are failing. Then we define  $(\vec{x}, \vec{y})_{L_t}$  as the restriction of  $(\vec{x}, \vec{y})$  to  $L_t$ .

Perhaps a causal diagram will make all these new steps clearer to the reader. The bnet Fig.1.3 is a modification of the bnet Fig.1.2 to include these new steps. The TPMs, printed in blue, for new or changed nodes, are as follows:

$$P(Y_t | (\vec{x}, \vec{y})_{L_t}) = \mathbb{1}(\text{ } Y_t(x^\sigma) = x_t^\sigma \text{ where } x_t \text{ is feature in } (\vec{x}, \vec{y})_{L_t} \text{ the with lowest Gini. }) \quad (1.25)$$

$$P(L_{t+1}^\sigma = \sigma' | \vec{w}_t) = w_t^{\sigma'} \quad (1.26)$$

$$P((\vec{x}, \vec{y})_{L_t} | L_t, (\vec{x}, \vec{y})) = \mathbb{1}(\text{ } (\vec{x}, \vec{y})_{L_t} = \text{ restriction of } (\vec{x}, \vec{y}) \text{ to } L_t \text{ }) \quad (1.27)$$

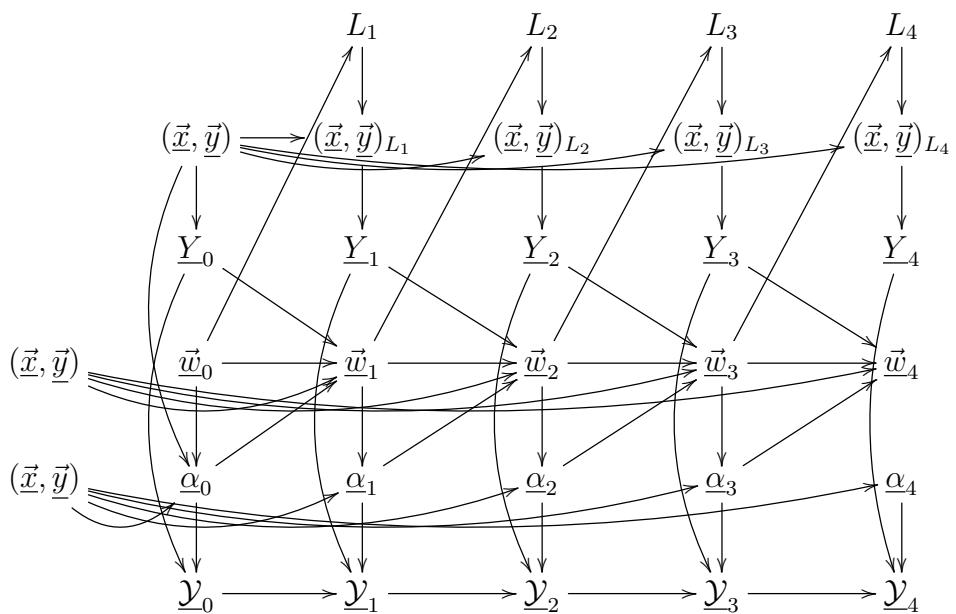


Figure 1.3: Modification of the bnet of Fig.1.2 to include on-the-fly generation of the w-classifiers.

# Chapter 2

## ANOVA

ANOVA stands for “Analysis of Variance”.

### 2.1 Law of Total Variance

**Claim 22** (*Law of Total Variance*) Suppose  $P : S_{\underline{x}} \times S_{\underline{y}} \rightarrow [0, 1]$  is a probability distribution. Suppose  $f : S_{\underline{x}} \times S_{\underline{y}} \rightarrow \mathbb{R}$  and  $f = f(x, y)$ . Then

$$Var_{\underline{x}, \underline{y}}(f) = E_{\underline{y}}[Var_{\underline{x}|\underline{y}}(f)] + Var_{\underline{y}}(E_{\underline{x}|\underline{y}}[f]). \quad (2.1)$$

In particular,

$$Var_{\underline{x}}(x) = E_{\underline{y}}[Var_{\underline{x}|\underline{y}}(x)] + Var_{\underline{y}}(E_{\underline{x}|\underline{y}}[x]). \quad (2.2)$$

**proof:**

Let

$$A = \sum_y P(y) \left( \sum_x P(x|y) f \right)^2. \quad (2.3)$$

Then

$$Var_{\underline{x}, \underline{y}}(f) = \sum_{x,y} P(x, y) f^2 - \left( \sum_{x,y} P(x, y) f \right)^2 \quad (2.4)$$

$$= \begin{cases} \sum_{x,y} P(x, y) f^2 - A \\ + \left( A - \left( \sum_{x,y} P(x, y) f \right)^2 \right) \end{cases} \quad (2.5)$$

$$E_{\underline{y}}[Var_{\underline{x}|\underline{y}}(f)] = \sum_y P(y) \left( \sum_x P(x|y) f^2 - \left( \sum_x P(x|y) f \right)^2 \right) \quad (2.6)$$

$$= \sum_{x,y} P(x, y) f^2 - A \quad (2.7)$$

$$Var_{\underline{y}}(E_{\underline{x}|\underline{y}}[f]) = \sum_y P(y) \left( \sum_x P(x|y)f \right)^2 - \left( \sum_y P(y) \sum_x P(x|y)f \right)^2 \quad (2.8)$$

$$= A - \left( \sum_{x,y} P(x,y)f \right)^2 \quad (2.9)$$

**QED**

## 2.2 Sum of Squares Estimates

Consider a population  $\Sigma$  partitioned into groups  $\Sigma_g$  such that  $\Sigma = \cup_{g=1}^{ng} \Sigma_g$ , where the  $\Sigma_g$  are mutually disjoint.

Let

*dof* stand for “degrees of freedom”

*SS* stand for “Sum of Squares”

*MS* stand for “Mean Square”

$x_{\Sigma_g} = \{x_{\sigma|g}\}_{\sigma \in \Sigma_g}$

Define the total and group mean values by

$$\bar{x} = \frac{1}{|\Sigma|} \sum_{g=1}^{ng} \sum_{\sigma \in \Sigma_g} x_{\sigma|g} \quad (2.10)$$

$$\bar{x}_g = \frac{1}{|\Sigma_g|} \sum_{\sigma \in \Sigma_g} x_{\sigma|g} \quad (2.11)$$

Define the **SS Total** by

$$SS_T = \sum_{g=1}^{ng} \sum_{\sigma \in \Sigma_g} (x_{\sigma|g} - \bar{x})^2 \quad (2.12)$$

$$= |\Sigma| Var_{\underline{x}}(x) \quad (2.13)$$

with *dof* and *MS* given by

$$dof_T = |\Sigma| - 1, \quad MS_T = \frac{SS_T}{dof_T} \quad (2.14)$$

Define the **SS Within** by

$$SS_W = \sum_{g=1}^{ng} \sum_{\sigma \in \Sigma_g} (x_{\sigma|g} - \bar{x}_g)^2 \quad (2.15)$$

$$= |\Sigma| \sum_{g=1}^{ng} \frac{|\Sigma_g|}{|\Sigma|} \left\{ \frac{1}{|\Sigma_g|} \sum_{\sigma \in \Sigma_g} (x_{\sigma|g} - \bar{x}_g)^2 \right\} \quad (2.16)$$

$$= |\Sigma| E_{\underline{g}}[Var_{\underline{x}|g}(x)] \quad (\text{note this is a mean value}) \quad (2.17)$$

with  $dof$  and  $MS$  given by

$$dof_W = |\Sigma| - ng, \quad MS_W = \frac{SS_W}{dof_W} \quad (2.18)$$

Define the **SS Between** by

$$SS_B = \sum_{g=1}^{ng} |\Sigma_g| (\bar{x}_g - \bar{x})^2 \quad (2.19)$$

$$= |\Sigma| \sum_{g=1}^{ng} \frac{|\Sigma_g|}{|\Sigma|} (\underbrace{\bar{x}_g}_{E_{\underline{x}|g}[x]} - \bar{x})^2 \quad (2.20)$$

$$= |\Sigma| Var_{\underline{g}}(E_{\underline{x}|g}[x]) \quad (\text{note this is a variance}) \quad (2.21)$$

with  $dof$  and  $MS$  given by

$$dof_B = ng - 1, \quad MS_B = \frac{SS_B}{dof_B} \quad (2.22)$$

### Claim 23

$$SS_T = SS_W + SS_B \quad (2.23)$$

$$dof_T = dof_W + dof_B \quad (2.24)$$

**proof:** By the just proven Law of Total Variance,

$$\underbrace{Var_{\underline{x}}(x)}_{SS_T/|\Sigma|} = \underbrace{E_{\underline{g}}[Var_{\underline{x}|g}(x)]}_{SS_W/|\Sigma|} + \underbrace{Var_{\underline{g}}(E_{\underline{x}|g}[x])}_{SS_B/|\Sigma|}. \quad (2.25)$$

**QED**

Fig.2.1 shows a bnet for calculating  $SS_T$ ,  $SS_W$  and  $SS_B$ , The TPMs, printed in blue, for the bnet Fig.2.1, are as follows.

$$P(\bar{x} | \{x_{\Sigma_g}\}_{g=1}^{ng}) = \mathbb{1} \left( \bar{x} = \frac{1}{|\Sigma|} \sum_{g=1}^{ng} \sum_{\sigma \in \Sigma_g} x_{\sigma|g} \right) \quad (2.26)$$

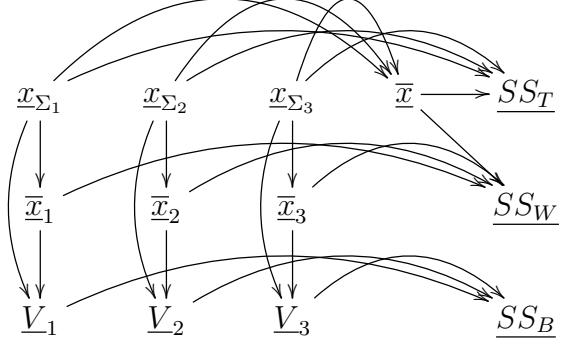


Figure 2.1: Bnet for calculating  $SS_T$ ,  $SS_W$  and  $SS_B$ .

$$P(\bar{x}_g | x_{\Sigma_g}) = \mathbb{1} \left( \bar{x}_g = \frac{1}{|\Sigma_g|} \sum_{\sigma \in \Sigma_g} x_{\sigma|g} \right) \quad (2.27)$$

$$P(V_g | x_{\Sigma_g}, \bar{x}_g) = \mathbb{1} \left( V_g = \frac{1}{|\Sigma_g|} \sum_{\sigma \in \Sigma_g} (x_{\sigma|g} - \bar{x}_g)^2 \right) \quad (2.28)$$

$$P(SS_T | \{x_{\Sigma_g}\}_{g=1}^{ng}, \bar{x}) = \mathbb{1}(SS_T = SS_T(\{x_{\Sigma_g}\}_{g=1}^{ng}, \bar{x})) \quad (2.29)$$

$$P(SS_B | \{\bar{x}_g\}_{g=1}^{ng}, \bar{x}) = \mathbb{1}(SS_B = SS_B(\{\bar{x}_g\}_{g=1}^{ng}, \bar{x})) \quad (2.30)$$

$$P(SS_W | \{V_g\}_{g=1}^{ng}) = \mathbb{1}(SS_W = SS_W(\{V_g\}_{g=1}^{ng})) \quad (2.31)$$

## 2.3 F-statistic and hypothesis testing

The **F-statistic** for ANOVA is defined by

$$F = \frac{MS_B}{MS_W} \quad \left( = \frac{\text{variance}}{\text{mean value}} \right) \quad (2.32)$$

(Note that  $F$  is the ratio of two chi-square distributions)

Consider  $ng = 3$  for definiteness. Let

$h_0$  = hypothesis that  $\mu_1 = \mu_2 = \mu_3$  (null hypothesis)

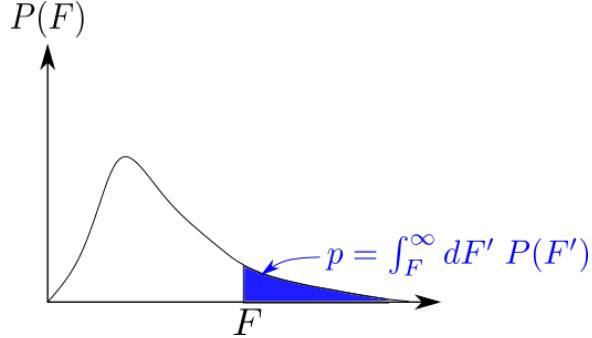


Figure 2.2: Probability distribution  $P(F)$  for the F-statistic, at fixed  $dof_B$  and  $dof_W$ . See Wikipedia article Ref.[111] for more info about  $P(F)$ .

$h_1$  = opposite of  $h_0$  (alternative, opposite hypothesis)

It's not hard to find on the Internet, tables and software calculators that give the score p-value<sup>1</sup>

$$p_{sc} = \int_F^\infty dF' P(F'; dof_B, dof_W) \quad (2.33)$$

of the  $F$  statistic, for a given  $dof_B$  and  $dof_W$ . See Fig.2.2 for a portrait of  $P(F)$  and  $p_{sc}$ . In Bayesian language,  $p_{sc}$  measures the probability that  $h_0$  is true. Assume  $p_{th} = 0.05$ .<sup>2</sup> To determine if the difference between group means is “statistically significant”, we compare  $p_{sc}$  with  $p_{th}$ . If  $p_{sc} < p_{th} = 0.05$ , we reject the null hypothesis. Otherwise, we fail to reject (accept) the null hypothesis.

If  $h_0$  is rejected, we can perform **post-hoc** tests to determine how much the groups differ from each other. There are several popular post-hoc tests, such as the Tukey test, Bonferroni test, and Scheffe test.

---

<sup>1</sup>Some tables give  $F = F(p_{sc}, dof_B, dof_W)$  instead of  $p_{sc} = p_{sc}(F, dof_B, dof_W)$ , but note that there is a 1-1/onto invertible map between  $F$  and  $p_{sc}$ . Some tables refer to  $p_{sc}$  as  $\alpha$ .

<sup>2</sup>The difference between threshold (th) and score (sc) p-values is discussed in Section C.41.

# Chapter 3

## ARACNE structure learning

This chapter is based on Ref.[36].

The ARACNE algo is an algo for learning the structure of a bnet from data. The algo considers data samples for  $n$  random variables  $(x_i)_{i=0,1,\dots,n-1}$ , and estimates the mutual information  $MI_{i,j} = H(\underline{x}_i : \underline{x}_j)$  between every pair of nodes. The set  $UG$  is initialized to contain all the edges of a fully connected undirected graph. Next the algo removes from  $UG$  every edge with  $MI_{i,j} < \epsilon$  for some threshold  $0 < \epsilon \ll 1$ . Then the algo examines every triplet of edges in  $UG$ , and marks for removal the edge of the triplet with the smallest MI. Finally, the algo removes from  $UG$  all edges marked for removal. Each triplet is analyzed irrespective of whether its edges have been marked for removal when considering a prior triplet. Thus the network constructed by the algorithm is independent of the order in which the triplets are examined. Some of the unoriented edges in  $UG$  can be given an orientation using the same techniques used to orient edges in constraint based structure learning (see Chapter 88).

Ref.[36] incorrectly claims that removing the smaller of 3 MI's is "an application" of the Data Processing Inequality (DPI) of Shannon Information Theory. See Chapter 52 for more info about DPI. Note that DPI is only valid for a Markov chain, and not all triplets of random variables are in a Markov chain. Removing the smaller of 3 numbers does not require DPI.

Fig.3.1 gives an example of the application of the ARACNE algo.

See Chapter 9 on Chow-Liu trees (CLT). A CLT is just a maximum spanning tree where the weights are mutual informations  $MI_{i,j}$  estimated from data.

Sometimes, the outcome of the ARACNE algo is a CLT. For example, Fig.3.1 (a) was considered in Chapter 9 on CLTs, and the CLT algo also gave Fig.3.1 (c) as the final structure.

According to Ref.[36], the ARACNE algo sometimes yields a polytree (i.e., a connected graph with no loops). It may even yield a structure with loops. Hence, it does not always yield a CLT.

By breaking all cliques (i.e., fully connected subgraphs) with 3 edges and 3 nodes, ARACNE breaks all cliques with 3 or more nodes. However, cliques are not uncommon in Nature, especially 3 node cliques. Cliques become less likely in Nature

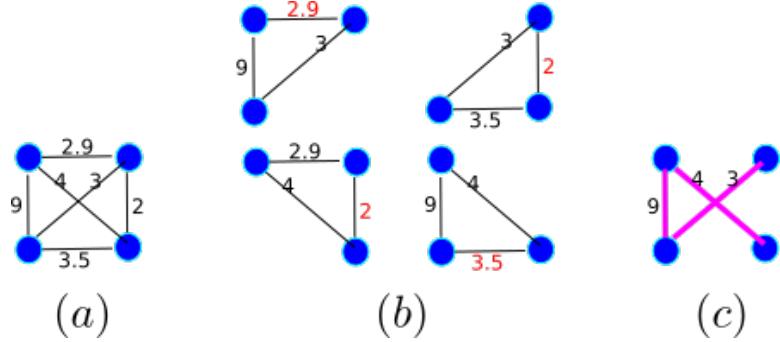


Figure 3.1: An example where the ARACNE algo gives a Chow-Liu tree. (a) Fully connected undirected graph with weights  $MI_{i,j}$  along the edges. (b) All 4 possible triplets of edges with nonzero weights. Edges marked for removal have their weights printed in red.(c) Final structure.

the bigger the number of nodes they have *after* 3. Therefore, a nice generalization of ARACNE would be to list all 4 node cliques, and break each of them by eliminating their edge with the smallest MI. This will have the effect of breaking all cliques with 4 or more nodes but keeping 3 node cliques. One could also break some, not all, of the 3 node cliques, by consecutively removing the clique-breaking-edge with the smallest MI of all edges of all 3 node cliques. Let  $\beta$  stand for banned clique number of nodes. Then the current ARACNE has  $\beta = 3$ . We are suggesting that a  $\beta$  of 4 might be more likely to occur in Nature.

# Chapter 4

## Backdoor Adjustment Formula

The backdoor (BD) adjustment formula is proven in Chapter 21 from the rules of Do Calculus. The goal of this chapter is to give examples of the use of that theorem. We will restate the theorem in this chapter, sans proof. There is no need to understand the theorem's proof in order to use it. However, you will need to skim Chapter 21 in order to familiarize yourself with the notation used to state the theorem. This chapter also assumes that you are comfortable with the rules for checking for d-separation. Those rules are covered in Chapter 23.

Suppose that we have access to data that allows us to estimate a probability distribution  $P(x., y., z.)$ . Hence, the variables  $\underline{x}.$ ,  $\underline{y}.$ ,  $\underline{z}.$  are ALL observed (i.e, not hidden). Then we say that the backdoor  $\underline{z}.$  satisfies the **backdoor adjustment criterion** relative to  $(\underline{x}., \underline{y}.)$  if

1. All backdoor paths from  $\underline{x}.$  to  $\underline{y}.$  are blocked by conditioning on  $\underline{z}..$
2.  $\underline{z}.. \cap de(\underline{x}.) = \emptyset$ .

### Claim 24 Backdoor Adjustment Formula

*If  $\underline{z}.$  satisfies the backdoor criterion relative to  $(\underline{x}., \underline{y}.)$ , then*

$$P(y.|D\underline{x}. = x.) = \sum_{z.} P(y.|x., z.)P(z.) \quad (4.1)$$

$$= \sum_{z.} \begin{array}{c} z. \\ \searrow \\ x. \longrightarrow y. \end{array} \quad (4.2)$$

where  $\sum z.$  means node  $\underline{z}.$  is summed over.

**proof:** See Chapter 21.

**QED**

## 4.1 Examples

1.



BD criterion satisfied if  $\underline{x}_\cdot = \underline{x}$ ,  $\underline{y}_\cdot = \underline{y}$ ,  $\underline{z}_\cdot = \emptyset$ . No adjustment necessary.

$$P(y|\mathcal{D}\underline{x} = x) = P(y|x) \quad (4.4)$$


---

2.



BD criterion satisfied if  $\underline{x}_\cdot = \underline{x}$ ,  $\underline{y}_\cdot = \underline{y}$ ,  $\underline{z}_\cdot = \emptyset$ . No adjustment necessary.

$$P(y|\mathcal{D}\underline{x} = x) = P(y|x) \quad (4.6)$$


---

3.



BD criterion satisfied if  $\underline{x}_\cdot = \underline{x}$ ,  $\underline{y}_\cdot = \underline{y}$ ,  $\underline{z}_\cdot = \underline{z}$ .

Note that here the backdoor formula adjusts the parents of  $x_\cdot$ .

---

4.



BD criterion satisfied if  $\underline{x}_\cdot = \underline{x}$ ,  $\underline{y}_\cdot = \underline{y}$ ,  $\underline{z}_\cdot = \underline{z}$ .

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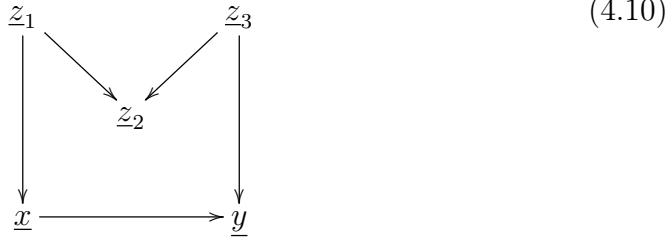
5.



BD criterion satisfied if  $\underline{x}_. = \underline{x}$ ,  $\underline{y}_. = \underline{y}$ ,  $\underline{z}_. = (\underline{z}_1, \underline{z}_2)$ .

---

6.



BD criterion satisfied if  $\underline{x}_. = \underline{x}$ ,  $\underline{y}_. = \underline{y}$  and  $\underline{z}_.$  = one of the following.

- $\emptyset$
  - $\underline{z}_3$
  - $\underline{z}_2, \underline{z}_3$
  - $\underline{z}_1, \underline{z}_3$
  - $\underline{z}_1$
  - $\underline{z}_1, \underline{z}_2$
  - $\underline{z}_1, \underline{z}_2, \underline{z}_3$
- 

7.



BD criterion is impossible to satisfy if  $\underline{x}_. = \underline{x}$ ,  $\underline{y}_. = \underline{y}$ . However, the frontdoor criterion can be satisfied. See Chapter 29.

---

8.



BD criterion satisfied if  $\underline{x}_. = \underline{x}$ ,  $\underline{y}_. = \underline{y}$ ,  $\underline{z}_. = \underline{z}$ . We are able to block the backdoor path by conditioning on  $\underline{z}$ .

---

9.



Conditioning on  $\underline{z}$  blocks backdoor path  $\underline{x}-\underline{z}-\underline{y}$ , but opens path  $\underline{x}-\underline{e}-\underline{z}-\underline{a}-\underline{y}$  because  $\underline{z}$  is a collider for that path. That path is blocked if we also condition on  $\underline{a}$ , which is possible because  $\underline{a}$  is observed. In conclusion, the BD criterion is satisfied if  $\underline{x}_. = \underline{x}$ ,  $\underline{y}_. = \underline{y}$  and  $\underline{z}_. = (\underline{z}, \underline{a})$ .

Conditioning on the parents of  $\underline{x}.$  is often enough to block all backdoor paths. However, sometimes some of the parents are unobserved and one must condition on other nodes that are not parents of  $\underline{x}.$  in order to satisfy the BD criterion.

---

10.



No need to control anything because only possible backdoor path is blocked by not conditioning on collider  $\underline{w}.$  Hence,

$$P(y|\mathcal{D}\underline{x} = x) = P(y|x) . \quad (4.15)$$

However, if for some reason we want to control  $\underline{t},$  we can do so. We can't control  $\underline{w}$  though, because  $\underline{w} \in de(\underline{x}).$  Thus, the BD criterion is satisfied if  $\underline{x} = \underline{x}, \underline{y} = \underline{y}$  and  $\underline{z} = \underline{t}.$  Therefore,

$$P(y|\mathcal{D}\underline{x} = x) = \sum_t P(y|x, t)P(t) . \quad (4.16)$$

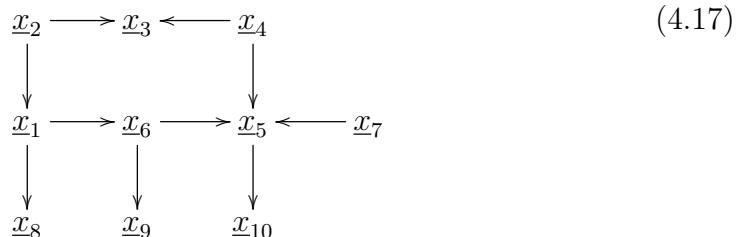

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11. Discuss what to do if several sets  $\underline{z}.$  satisfy the BD criterion.

- Can evaluate  $P(y|\mathcal{D}\underline{x} = x.)$  multiple ways and compare the results. This is a test that the causal bnet is correct.
  - It might be easier or less expensive to get data for some  $\underline{z}.$  more than for others.
- 

12. (Taken from online course notes Ref.[22])

Consider the bnet



If  $\underline{x} = \underline{x}_1$  and  $\underline{y} = \underline{x}_5,$  find all possible adjustment multinode  $\underline{z}.$  that satisfy the BD criterion. Ans:

- $\emptyset$
- $\underline{x}_4$
- $\underline{x}_2, \underline{x}_3$
- $\underline{x}_2, \underline{x}_3, \underline{x}_4$
- $\underline{x}_2$
- $\underline{x}_2, \underline{x}_4$
- $\underline{x}_3, \underline{x}_4$

Add  $\underline{x}_7$  to each of the previous 7 possible  $\underline{z}..$ . This gives a total of 14 possible adjustment multinodes  $\underline{z}..$ .

# Chapter 5

## Back Propagation (Automatic Differentiation)

### 5.1 Toy Example

This example comes from Ref.[45].

Consider the following system of 4 equations:

$$\begin{cases} b = w_1 a \\ c = w_2 a \\ d = w_3 b + w_4 c \\ L = 10 - d \end{cases} \quad (5.1)$$

To calculate  $\nabla_w L$  where  $w = (w_1, w_2, w_3, w_4)$ , we can use the chain rule for partial derivatives. This yields

$$\frac{\partial L}{\partial w_4} = \frac{\partial L}{\partial d} \frac{\partial d}{\partial w_4} = (-1)(c) \quad (5.2a)$$

$$\frac{\partial L}{\partial w_3} = \frac{\partial L}{\partial d} \frac{\partial d}{\partial w_3} = (-1)(b) \quad (5.2b)$$

$$\frac{\partial L}{\partial w_2} = \frac{\partial L}{\partial d} \frac{\partial d}{\partial c} \frac{\partial c}{\partial w_2} = (-1)(w_4)(a) \quad (5.2c)$$

$$\frac{\partial L}{\partial w_1} = \frac{\partial L}{\partial d} \frac{\partial d}{\partial b} \frac{\partial b}{\partial w_1} = (-1)(w_3)(a) \quad (5.2d)$$

Now note that the system of equations Eq.(5.1) can be represented graphically by the bnet (with deterministic nodes) of Fig.5.1. The calculation of  $\nabla_w L$  can also be represented graphically with the aid of the defining bnet Fig.5.1. This is done in Fig.5.2. As illustrated by that figure, the derivative  $\partial_{w_i} L$  for  $i = 1, 2, 3, 4$  is the product of the derivatives along the arrows from  $w_i$  to  $L$ .

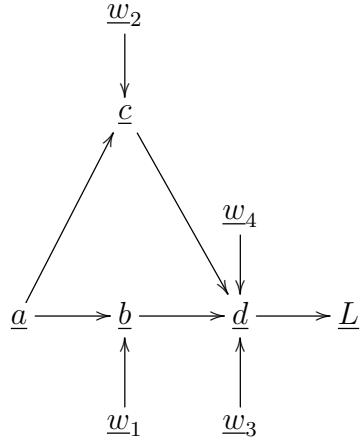


Figure 5.1: bnet for which we want to calculate  $\nabla_w L$  where  $w = (w_1, w_2, w_3, w_4)$

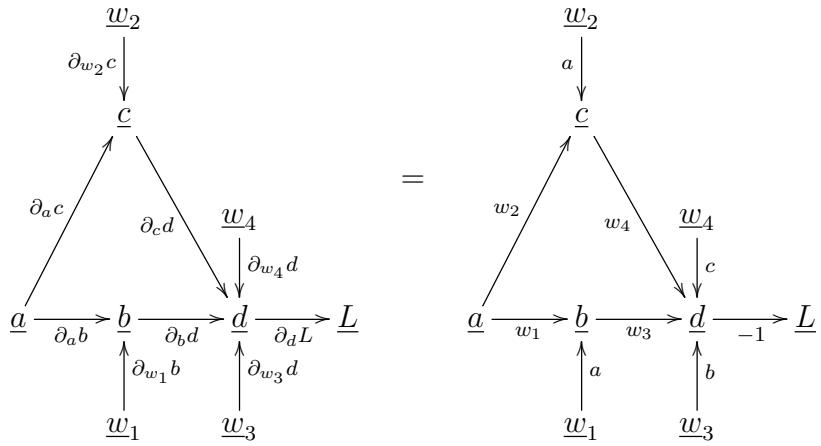


Figure 5.2: bnet of Fig. 5.1 with derivatives along each arrow.

## 5.2 General Theory

### 5.2.1 Jacobians

Suppose  $f : \mathbb{R}^{nx} \rightarrow \mathbb{R}^{nf}$  and

$$y = f(x) . \quad (5.3)$$

Then the Jacobian  $\frac{\partial y}{\partial x}$  is defined as the matrix with entries<sup>1</sup>

$$\left[ \frac{\partial y}{\partial x} \right]_{i,j} = \frac{\partial y_i}{\partial x_j}. \quad (5.4)$$

Jacobian of function composition. Suppose  $f : \mathbb{R}^{nx} \rightarrow \mathbb{R}^{nf}$ ,  $g : \mathbb{R}^{nf} \rightarrow \mathbb{R}^{ng}$ . If

$$y = g \circ f(x), \quad (5.5)$$

then

$$\frac{\partial y}{\partial x} = \frac{\partial g}{\partial f} \frac{\partial f}{\partial x}. \quad (5.6)$$

Right hand side of last equation is a product of two matrices so order of matrices is important.

### 5.2.2 Bnets for function composition, forward propagation and back propagation

Let

$$y = f^4 \circ f^3 \circ f^2 \circ f^1(x). \quad (5.7)$$

This function composition chain can be represented by the bnet Fig.5.3(a) with TPMs

$$P(f^\mu | f^{\mu-1}) = \mathbb{1}(f^\mu = f^\mu(f^{\mu-1})) \quad (5.8)$$

for  $\mu = 1, 2, 3, 4$ .

Note that

$$\frac{\partial y}{\partial x} = \frac{\partial y}{\partial f^3} \frac{\partial f^3}{\partial f^2} \left[ \frac{\partial f^2}{\partial f^1} \frac{\partial f^1}{\partial x} \right] \quad (5.9)$$

$$= \frac{\partial y}{\partial f^3} \left[ \frac{\partial f^3}{\partial f^2} \frac{\partial f^2}{\partial x} \right] \quad (5.10)$$

$$= \left[ \frac{\partial y}{\partial f^3} \frac{\partial f^3}{\partial x} \right] \quad (5.11)$$

$$= \frac{\partial y}{\partial x}. \quad (5.12)$$

This forward propagation can be represented by the bnet Fig.5.3(b) with node TPMs

$$P\left(\frac{\partial f^{\mu+1}}{\partial x} \mid \frac{\partial f^\mu}{\partial x}\right) = \mathbb{1}\left(\frac{\partial f^{\mu+1}}{\partial x} = \frac{\partial f^{\mu+1}}{\partial f^\mu} \frac{\partial f^\mu}{\partial x}\right) \quad (5.13)$$

---

<sup>1</sup>Mnemonic for remembering order of indices:  $i$  in numerator/ $j$  in denominator becomes index  $i/j$  of Jacobian matrix.

$$\underline{f}^4 \longleftarrow \underline{f}^3 \longleftarrow \underline{f}^2 \longleftarrow \underline{f}^1 \longleftarrow \underline{f}^0$$

(a) Composition

$$\frac{\partial f^4}{\partial x} \longleftarrow \frac{\partial f^3}{\partial x} \longleftarrow \frac{\partial f^2}{\partial x} \longleftarrow \frac{\partial f^1}{\partial x} \longleftarrow 1$$

(b) Forward-p

$$1 \longrightarrow \frac{\partial y}{\partial f^3} \longrightarrow \frac{\partial y}{\partial f^2} \longrightarrow \frac{\partial y}{\partial f^1} \longrightarrow \frac{\partial y}{\partial f^0}$$

(c) Back-p

Figure 5.3: bnets for function composition, forward propagation and back propagation for  $nf = 5$  nodes.

for  $\mu = 1, 2, 3$ .

Note that

$$\frac{\partial y}{\partial x} = \left[ \frac{\partial y}{\partial f^3} \frac{\partial f^3}{\partial f^2} \right] \frac{\partial f^2}{\partial f^1} \frac{\partial f^1}{\partial x} \quad (5.14)$$

$$= \left[ \frac{\partial y}{\partial f^2} \frac{\partial f^2}{\partial f^1} \right] \frac{\partial f^1}{\partial x} \quad (5.15)$$

$$= \left[ \frac{\partial y}{\partial f^1} \frac{\partial f^1}{\partial x} \right] \quad (5.16)$$

$$= \frac{\partial y}{\partial x}. \quad (5.17)$$

This back propagation can be represented by the bnet Fig.5.3(c) with node TPMs

$$P\left(\frac{\partial y}{\partial f^\mu} \mid \frac{\partial y}{\partial f^{\mu+1}}\right) = \mathbb{1}\left(\frac{\partial y}{\partial f^\mu} = \frac{\partial y}{\partial f^{\mu+1}} \frac{\partial f^{\mu+1}}{\partial f^\mu}\right) \quad (5.18)$$

for  $\mu = 2, 1, 0$ .

$\frac{\partial f^{\mu+1}}{\partial f^\mu}$  is a Jacobian matrix so the order of multiplication matters. In forward prop, it pre-multiplies, and in back prop it post-multiplies.

## 5.3 Application to Neural Networks

### 5.3.1 Absorbing $b_i^\lambda$ into $w_{i|j}$ .

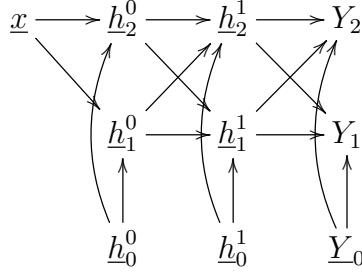


Figure 5.4: Nodes  $\underline{h}_0^0, \underline{h}_0^1, \underline{Y}_0$  are all set to 1. They allow us to absorb  $b_i^\lambda$  into the first column of  $w_{i|j}^\lambda$ .

The TPMs, printed in blue, for a NN bnet, as given in Chapter 64, are as follows.

For all hidden layers  $\lambda = 0, 1, \dots, \Lambda - 2$ ,

$$P(h_i^\lambda | h_{\cdot}^{\lambda-1}) = \delta \left( h_i^\lambda, \mathcal{A}_i^\lambda \left( \sum_j w_{i|j}^\lambda h_j^{\lambda-1} + b_i^\lambda \right) \right) \quad (5.19)$$

for  $i = 0, 1, \dots, nh(\lambda) - 1$ . For the output visible layer  $\lambda = \Lambda - 1$ :

$$P(Y_i | h_{\cdot}^{\Lambda-2}) = \delta \left( Y_i, \mathcal{A}_i^{\Lambda-1} \left( \sum_j w_{i|j}^{\Lambda-1} h_j^{\Lambda-2} + b_i^{\Lambda-1} \right) \right) \quad (5.20)$$

for  $i = 0, 1, \dots, ny - 1$ .

For each  $\lambda$ , replace the matrix  $w_{\cdot|}^\lambda$  by the augmented matrix  $[b_{\cdot|}^\lambda, w_{\cdot|}^\lambda]$  so that the new  $w_{\cdot|}^\lambda$  satisfies

$$w_{i|0}^\lambda = b_i^\lambda \quad (5.21)$$

Let the nodes  $\underline{h}_0^\lambda$  for all  $\lambda$  and  $\underline{Y}_0$  be root nodes (so no arrows pointing into them). For each  $\lambda$ , draw arrows from  $\underline{h}_0^\lambda$  to all other nodes in that same layer. Draw arrows from  $\underline{Y}_0$  to all other nodes in that same layer.

After performing the above steps, the TPMs, printed in blue, for the NN bnet, are as follows:

For all hidden layers  $\lambda = 0, 1, \dots, \Lambda - 2$ ,

$$P(h_0^\lambda) = \delta(h_0^\lambda, 1) , \quad (5.22)$$

and

$$P(h_i^\lambda \mid h_{\cdot}^{\lambda-1}, h_0^\lambda = 1) = \delta \left( h_i^\lambda, \mathcal{A}_i^\lambda \left( \sum_j w_{i|j}^\lambda h_j^{\lambda-1} \right) \right) \quad (5.23)$$

for  $i = 1, \dots, nh(\lambda) - 1$ . For the output visible layer  $\lambda = \Lambda - 1$ :

$$P(Y_0) = \delta(Y_0, 1) , \quad (5.24)$$

and

$$P(Y_i \mid h_{\cdot}^{\Lambda-2}, Y_0 = 1) = \delta \left( Y_i, \mathcal{A}_i^{\Lambda-1} \left( \sum_j w_{i|j}^{\Lambda-1} h_j^{\Lambda-2} \right) \right) \quad (5.25)$$

for  $i = 1, 2, \dots, ny - 1$ .

### 5.3.2 Bnets for function composition, forward propagation and back propagation for NN

$$\underline{\mathcal{A}}^3 \longleftarrow \underline{\mathcal{B}}^3 \longleftarrow \underline{\mathcal{A}}^2 \longleftarrow \underline{\mathcal{B}}^2 \longleftarrow \underline{\mathcal{A}}^1 \longleftarrow \underline{\mathcal{B}}^1 \longleftarrow \underline{\mathcal{A}}^0 \longleftarrow \underline{\mathcal{B}}^0 \longleftarrow \underline{x}$$

(a)

$$\frac{\partial \mathcal{A}^3}{\partial x} \longleftarrow \frac{\partial \mathcal{B}^3}{\partial x} \longleftarrow \frac{\partial \mathcal{A}^2}{\partial x} \longleftarrow \frac{\partial \mathcal{B}^2}{\partial x} \longleftarrow \frac{\partial \mathcal{A}^1}{\partial x} \longleftarrow \frac{\partial \mathcal{B}^1}{\partial x} \longleftarrow \frac{\partial \mathcal{A}^0}{\partial x} \longleftarrow \frac{\partial \mathcal{B}^0}{\partial x} \longleftarrow \underline{1}$$

(b)

$$\underline{1} \longrightarrow \frac{\partial Y}{\partial \mathcal{B}^3} \longrightarrow \frac{\partial Y}{\partial \mathcal{A}^2} \longrightarrow \frac{\partial Y}{\partial \mathcal{B}^2} \longrightarrow \frac{\partial Y}{\partial \mathcal{A}^1} \longrightarrow \frac{\partial Y}{\partial \mathcal{B}^1} \longrightarrow \frac{\partial Y}{\partial \mathcal{A}^0} \longrightarrow \frac{\partial Y}{\partial \mathcal{B}^0} \longrightarrow \frac{\partial Y}{\partial x}$$

(c)

Figure 5.5: bnets for (a) function composition, (b) forward propagation and (c) back propagation for a neural net with 4 layers (3 hidden and output visible).

From here on, we will rename  $y$  above by  $Y = \hat{y}$  and consider samples  $y[i]$  for  $i = 0, 1, \dots, nsam - 1$ . The Error (a.k.a. loss or cost function) is

$$\mathcal{E} = \frac{1}{nsam} \sum_{\sigma=0}^{nsam-1} \sum_{i=0}^{ny-1} |Y_i - y_i[\sigma]|^2 \quad (5.26)$$

To perform simple gradient descent, one uses:

$$(w_{i|j}^\lambda)' = w_{i|j}^\lambda - \eta \frac{\partial \mathcal{E}}{\partial w_{i|j}^\lambda}. \quad (5.27)$$

One has

$$\frac{\partial \mathcal{E}}{\partial w_{i|j}^\lambda} = \frac{1}{nsam} \sum_{\sigma=0}^{nsam-1} \sum_{i=0}^{ny-1} 2(Y_i - y_i[\sigma]) \frac{\partial Y}{\partial w_{i|j}^\lambda}. \quad (5.28)$$

Define  $\mathcal{B}_i^\lambda$  thus

$$\mathcal{B}_i^\lambda(h^{\lambda-1}) = \sum_j w_{i|j}^\lambda h_j^{\lambda-1}. \quad (5.29)$$

Then

$$\frac{\partial Y}{\partial w_{i|j}^\lambda} = \frac{\partial Y}{\partial \mathcal{B}_i^\lambda} \frac{\partial \mathcal{B}_i^\lambda}{\partial w_{i|j}^\lambda} \quad (5.30)$$

$$= \frac{\partial Y}{\partial \mathcal{B}_i^\lambda} h_j^{\lambda-1} \quad (5.31)$$

$$\frac{\partial \mathcal{E}}{\partial w_{i|j}^\lambda} = \frac{\partial \mathcal{E}}{\partial \mathcal{B}_j^\lambda} \frac{\partial \mathcal{B}_j^\lambda}{\partial w_{i|j}^\lambda} \quad (5.32)$$

$$= \frac{\partial \mathcal{E}}{\partial \mathcal{B}_j^\lambda} h_j^{\lambda-1}. \quad (5.33)$$

This suggest that we can calculate the derivatives of the error  $\mathcal{E}$  with respect to the weights  $w_{i|j}^\lambda$  in two stages, using an intermediate quantity  $\delta_j^\lambda$ :

$$\begin{cases} \delta_j^\lambda = \frac{\partial \mathcal{E}}{\partial \mathcal{B}_j^\lambda} \\ \frac{\partial \mathcal{E}}{\partial w_{i|j}^\lambda} = \delta_j^\lambda h_j^{\lambda-1} \end{cases} \quad (5.34)$$

To apply what we learned in the earlier General Theory section of this chapter, consider a NN with 4 layers (3 hidden, and the output visible one). Define the functions  $f_i$  as follows:

$$f_i^0 = x_i \quad (5.35)$$

$$\text{Layer 0: } f_i^1 = \mathcal{B}_i^0(x_i), \quad f_i^2 = \mathcal{A}_i^0(\mathcal{B}_i^0) \quad (5.36)$$

$$\text{Layer 1: } f_i^3 = \mathcal{B}_i^1(\mathcal{A}_i^0), \quad f_i^4 = \mathcal{A}_i^1(\mathcal{B}_i^1) \quad (5.37)$$

$$\text{Layer 2: } f_i^5 = \mathcal{B}_i^2(\mathcal{A}_i^1), \quad f_i^6 = \mathcal{A}_i^2(\mathcal{B}_i^2) \quad (5.38)$$

$$\text{Layer 3: } f_i^7 = \mathcal{B}_i^3(\mathcal{A}_i^2), \quad f_i^8 = \mathcal{A}_i^3(\mathcal{B}_i^3) \quad (5.39)$$

See Fig.5.5. The TPMs, printed in blue, for the bnet (c) for back propagation, are as follows:

$$P\left(\frac{\partial Y}{\partial \mathcal{B}^\lambda} \mid \frac{\partial Y}{\partial \mathcal{B}^{\lambda+1}}\right) = \mathbb{1}\left(\frac{\partial Y}{\partial \mathcal{B}^\lambda} = \frac{\partial Y}{\partial \mathcal{B}^{\lambda+1}} \frac{\partial \mathcal{B}^{\lambda+1}}{\partial \mathcal{A}^\lambda} \frac{\partial \mathcal{A}^\lambda}{\partial \mathcal{B}^\lambda}\right). \quad (5.40)$$

One has

$$\frac{\partial \mathcal{A}_i^\lambda}{\partial \mathcal{B}_j^\lambda} = D\mathcal{A}_i^\lambda(\mathcal{B}_i^\lambda)\delta(i,j) \quad (5.41)$$

where  $D\mathcal{A}_i^\lambda(z)$  is the derivative of  $\mathcal{A}_i^\lambda(z)$ .

From Eq.(5.29)

$$\mathcal{B}_i^{\lambda+1}(\mathcal{A}^\lambda) = \sum_j w_{i|j}^{\lambda+1} \mathcal{A}_j^\lambda \quad (5.42)$$

so

$$\frac{\partial \mathcal{B}_i^{\lambda+1}}{\partial \mathcal{A}_j^\lambda} = w_{i|j}^{\lambda+1}. \quad (5.43)$$

Therefore, Eq.(5.40) implies

$$P\left(\frac{\partial Y}{\partial \mathcal{B}_j^\lambda} \mid \frac{\partial Y}{\partial \mathcal{B}_j^{\lambda+1}}\right) = \mathbb{1}\left(\frac{\partial Y}{\partial \mathcal{B}_j^\lambda} = \sum_i \frac{\partial Y}{\partial \mathcal{B}_i^{\lambda+1}} D\mathcal{A}_j^\lambda(\mathcal{B}_j^\lambda) w_{i|j}^{\lambda+1}\right), \quad (5.44)$$

$$P\left(\frac{\partial \mathcal{E}}{\partial \mathcal{B}_j^\lambda} \mid \frac{\partial \mathcal{E}}{\partial \mathcal{B}_j^{\lambda+1}}\right) = \mathbb{1}\left(\frac{\partial \mathcal{E}}{\partial \mathcal{B}_j^\lambda} = \sum_i \frac{\partial \mathcal{E}}{\partial \mathcal{B}_i^{\lambda+1}} D\mathcal{A}_j^\lambda(\mathcal{B}_j^\lambda) w_{i|j}^{\lambda+1}\right), \quad (5.45)$$

$$P(\delta_j^\lambda \mid \delta_j^{\lambda+1}) = \mathbb{1}(\delta_j^\lambda = \sum_i \delta_i^{\lambda+1} D\mathcal{A}_j^\lambda(\mathcal{B}_j^\lambda) w_{i|j}^{\lambda+1}). \quad (5.46)$$

First delta of iteration, belonging to output layer  $\lambda = \Lambda - 1$ :

$$\delta_j^{\Lambda-1} = \frac{\partial \mathcal{E}}{\partial \mathcal{B}_j^{\Lambda-1}} \quad (5.47)$$

$$= \frac{1}{nsam} \sum_{\sigma=0}^{nsam-1} \sum_{i=0}^{ny-1} 2(Y_i - y_i[\sigma]) D\mathcal{A}_i^{\Lambda-1}(\mathcal{B}_i^{\Lambda-1}) \delta(i, j) \quad (5.48)$$

$$= \frac{1}{nsam} \sum_{\sigma=0}^{nsam-1} 2(Y_j - y_j[\sigma]) D\mathcal{A}_j^{\Lambda-1}(\mathcal{B}_j^{\Lambda-1}) \quad (5.49)$$

Cute expression for derivative of sigmoid function:

$$D\text{smoid}(x) = \text{smoid}(x)(1 - \text{smoid}(x)) \quad (5.50)$$

## 5.4 General bnets instead of Markov chains induced by layered structure of NNs

$$P(\delta_{\underline{x}} | (\delta_a)_{a \in ch(\underline{x})}) = \mathbb{1}(\delta_{\underline{x}} = \sum_{a \in ch(\underline{x})} \delta_a D\mathcal{A}_{\underline{x}}(\mathcal{B}_{\underline{x}})) w_{a|\underline{x}} \quad (5.51)$$

Reverse arrows of original bnet and define the TPM of nodes of “time reversed” bnet by

$$P(\delta_{\underline{x}} | (\delta_a)_{a \in pa(\underline{x})}) = \mathbb{1}(\delta_{\underline{x}} = \sum_{a \in pa(\underline{x})} \delta_a D\mathcal{A}_{\underline{x}}(\mathcal{B}_{\underline{x}})) w_{\underline{x}|a}^T \quad (5.52)$$

# Chapter 6

## Bell and Clauser-Horne Inequalities in Quantum Mechanics

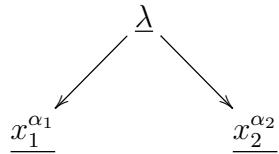


Figure 6.1: bnet used to discuss Bell and Clauser-Horne inequalities in Quantum Mechanics.

I wrote an article about this in 2008 for my blog “Quantum Bayesian Networks”. See Ref.[71].

# Chapter 7

## Berkson's Paradox

For more information about Berkson's Paradox (BP), see Ref.[92]

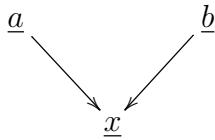


Figure 7.1: Bnet used to discuss Berkson's Paradox (BP).  $\underline{a}$  and  $\underline{b}$  are both causes of collider  $\underline{x}$ .

Consider the bnet of Fig.7.1. For that bnet, we have

$$P(a, b, x) = P(a)P(b)P(x|a, b) . \quad (7.1)$$

Summing Eq.(7.1) over  $x$ , we get

$$P(a, b) = P(a)P(b) \quad (7.2)$$

so  $\underline{a}$  and  $\underline{b}$  are independent. It follows that  $a$  can be ignored in calculating the probability of  $b$ ; i.e.,

$$\boxed{P(b|a) = P(b)} . \quad (7.3)$$

However,  $a$  cannot be ignored in calculating the probability of  $b$ , if  $x$  is being held fixed; i.e.,

$$\boxed{P(b|a, x) \neq P(b|x)} . \quad (7.4)$$

Indeed,

$$P(b|a, x) = \frac{P(b)P(x|a, b)}{\sum_b P(b)P(x|a, b)} \quad (7.5)$$

whereas

$$P(b|x) = \frac{\sum_a P(a)P(b)P(x|a,b)}{\sum_{a,b} P(a)P(b)P(x|a,b)} . \quad (7.6)$$

The two boxed equations are what is referred to as BP.

BP is also called **collider bias** because  $\underline{x}$  is a collider.

BP is also called **explaining away** in the special case that  $\underline{a}, \underline{b}, \underline{x} \in \{\text{false} = 0, \text{true} = 1\}$ . In that case, if  $\underline{x}$  is fixed to true, and the cause  $\underline{a}$  is known to be true, then the cause  $\underline{b}$  is less likely to be true. For example, suppose a car engine fails ( $\underline{x} = 1$ ) and the two most likely causes of the failure are alternator ( $\underline{a}$ ) and battery ( $\underline{b}$ ). Once we know that the alternator has failed ( $\underline{a} = 1$ ), it is less likely that the battery is failing ( $\underline{b} = 1$ ) than when the status of  $\underline{a}$  was not known; i.e.,  $P(\underline{b} = 1|\underline{x} = 1, \underline{a} = 1) < P(\underline{b} = 1|\underline{x} = 1)$ .

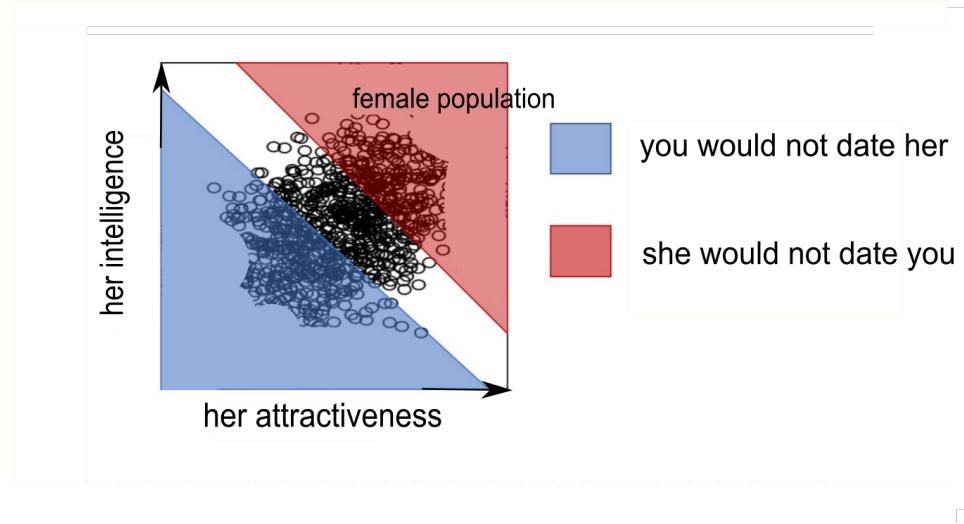


Figure 7.2: Example of Berkson's paradox (BP).

Fig.7.2 presents an example of BP. The figure consists of a scatter plot with axes  $a =$ her attractiveness,  $b =$ her intelligence, for a female population of possible dates for you, assuming you are a male person. Let  $x \in \{\text{false} = 0, \text{true} = 1\} =$  she goes out on a date with you. For the full population,

$$(a, b) \sim P(a, b) = P(a)P(b) \quad (7.7)$$

whereas for the population in the white swath,

$$(a, b) \sim P(a, b|x) = P(b|a, x)P(a|x) \neq P(b|x)P(a|x) . \quad (7.8)$$

As shown by Fig.7.2, BP is an example of **selection bias**. Selection bias happens when a non-representative subset of the total population is considered (i.e., selected).

# Chapter 8

## Binary Decision Diagrams

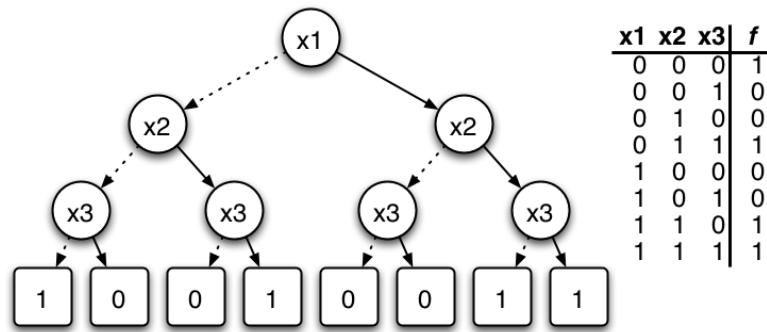


Figure 8.1: Binary decision tree and truth table for the function  $f(x_1, x_2, x_3) = \bar{x}_1(x_2 + \bar{x}_3) + x_1x_2$

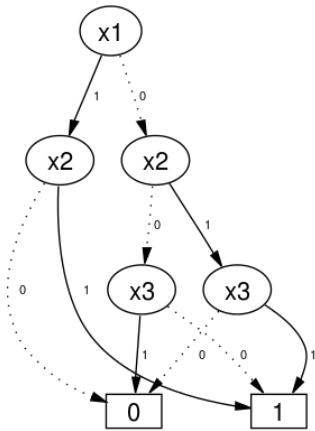


Figure 8.2: BDD for the function  $f$  of Fig.8.1.

This chapter is based on Wikipedia article Ref.[96].

Binary Decision Diagrams (BDDs) can be understood as a special case of Decision Trees (dtrees). We will assume that the reader has read Chapter 16 on dtrees before reading this chapter.

Both Figs.8.1 and 8.2 were taken from the aforementioned Wikipedia article. They give a simple example of a function  $f : \{0, 1\}^3 \rightarrow \{0, 1\}$  represented in Fig.8.1 as a **binary decision tree** and in Fig.8.2 as a **binary decision diagram (BDD)**. It is possible to find, for each of those two figures, a bnet with the same graph structure. We show how to do this next.

We begin by noting that the function  $f : \{0, 1\}^3 \rightarrow \{0, 1\}$  is a special case of a probability distribution  $P : \{0, 1\}^3 \rightarrow [0, 1]$ . In fact, if we restrict  $P$  to be deterministic, then  $P_{det} : \{0, 1\}^3 \rightarrow \{0, 1\}$  has the same domain and range as  $f$ . Henceforth, we will refer to  $f(x_1, x_2, x_3)$  as  $P(x_1, x_2, x_3)$ , keeping in mind that we are restricting our attention to deterministic probability distributions.

If we apply the chain rule for conditional probabilities to  $P(x_1, x_2, x_3)$ , we get

$$P(x_1, x_2, x_3) = P(x_3|x_1, x_2)P(x_2|x_1)P(x_1), \quad (8.1)$$

which can be represented by the bnet:

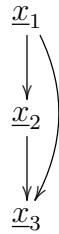


Figure 8.3: Most general 3 node bnet.

But in Chapter 16, we learned how to represent the dtree of Fig.8.1 as the image bnet Fig.8.4. The TPMs, printed in blue, for the image bnet Fig.8.4, are as follows. Note that the TPMs for Fig.8.4 can be constructed from the TPMs for the bnet Fig.8.3. If  $x_1, x_2, x_3, x_4 \in \{0, 1, null\}$  and  $a, b, c \in \{0, 1\}$ , then

$$P(\underline{x}_1 = x_1) = \begin{cases} P_{x_1}(x_1) & \text{if } x_1 \in \{0, 1\} \\ 0 & \text{if } x_1 = \text{null} \end{cases} \quad (8.2)$$

$$P(\underline{x}_2|a = x_2 | \underline{x}_1 = x_1) = \begin{cases} P_{x_2|x_1}(x_2|a) & \text{if } x_1 = a \\ \mathbb{1}(x_2 = \text{null}) & \text{otherwise} \end{cases} \quad (8.3)$$

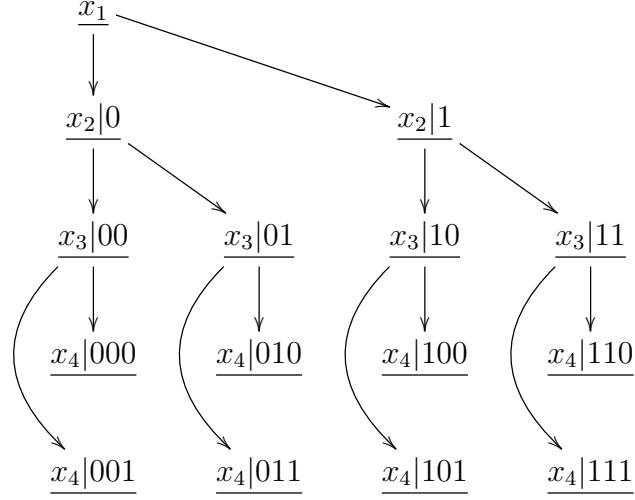


Figure 8.4: Image bnet for binary dtree of Fig.8.1.

$$P(\underline{x}_3|a, b = x_3 | \underline{x}_2|a = x_2) = \begin{cases} P_{\underline{x}_3|x_1, \underline{x}_2}(x_3|a, b) & \text{if } x_2 = b \\ \mathbb{1}(x_3 = \text{null}) & \text{otherwise} \end{cases} \quad (8.4)$$

$$P(\underline{x}_4|a, b, c = x_4 | \underline{x}_3|a, b = x_3) = \begin{cases} \delta(x_4, c) & \text{if } x_3 = c \\ \mathbb{1}(x_4 = \text{null}) & \text{otherwise} \end{cases} \quad (8.5)$$

Note that if  $P_{\underline{x}_3|x_1, \underline{x}_2} = P_{\underline{x}_3|x_2}$  in Eq.(8.4), then the bnet Fig.8.3 reduces to a Markov chain  $\underline{x}_1 \rightarrow \underline{x}_2 \rightarrow \underline{x}_3$ .

The BDD shown in Fig.8.2 emphasizes the fact that

$$P(x_1, x_2, x_3|x_1 = 1) = P(x_2|x_1 = 1) = x_2 . \quad (8.6)$$

The BDD of Fig.8.2 has as image bnet Fig.8.5. Define

$$pa(\underline{0}) = pa(\underline{1}) = (x_2|1, x_3|00, x_3|01) . \quad (8.7)$$

Let  $pa(\underline{0}) = abc$  mean the same as  $pa(\underline{0}) = (a, b, c)$ . The TPMs of the image bnet Fig.8.5 are the same as those for the image bnet Fig.8.4 except for the TPMs of the nodes  $\underline{0}$  and  $\underline{1}$ . For those two nodes, the TPMs, printed in blue, are as follows.

$$P(\underline{0} = x|pa(\underline{0})) = \begin{cases} \delta(x, 0) & \text{if } pa(\underline{0}) = 011 \\ \delta(x, \text{null}) & \text{otherwise} \end{cases} \quad (8.8)$$

$$P(\underline{1} = x|pa(\underline{1})) = \begin{cases} \delta(x, 1) & \text{if } pa(\underline{1}) = 101 \\ \delta(x, \text{null}) & \text{otherwise} \end{cases} \quad (8.9)$$

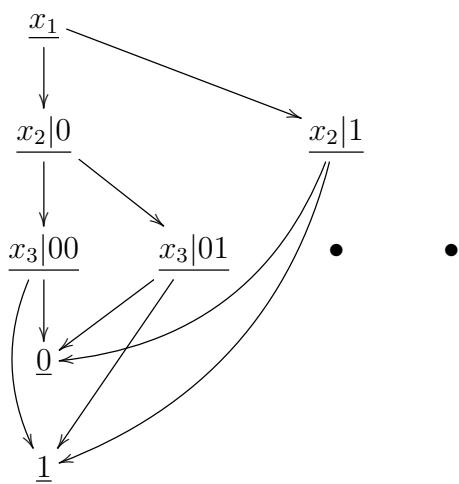


Figure 8.5: Image bnet for BDD of Fig.8.2.

# Chapter 9

## Chow-Liu Trees and Tree Augmented Naive Bayes (TAN)

This chapter is mostly based on chapter 8 of Pearl's 1988 book Ref.[50]. See also Ref.[101] and references therein.

This chapter uses various Shannon Information Theory entropies. Our notation for these entropies is described in Chapter C.

### 9.1 Chow-Liu Trees

Chow-Liu trees refers to an algorithm for finding a bnet tree that fits an a priori given probability distribution as closely as possible.

Consider a bnet with  $n$  nodes  $\underline{x}^n = (\underline{x}_0, \underline{x}_1, \dots, \underline{x}_{n-1})$  such that  $\underline{x}_i \in S_{\underline{x}_i}$  for all  $i$ . Let its total probability distribution be  $P_{\underline{x}^n}$ . For simplicity, we will abbreviate  $P_{\underline{x}^n}$  by  $P$ . Hence

$$P(x^n) = P_{\underline{x}^n}(x^n). \quad (9.1)$$

Suppose we want to fit  $P_{\underline{x}^n}$  by a tree bnet with nodes  $\underline{t}^n = (\underline{t}_0, \underline{t}_1, \dots, \underline{t}_{n-1})$  such that  $\underline{t}_i \in S_{\underline{t}_i} = S_{\underline{x}_i}$  for all  $i$ . For simplicity, we will abbreviate  $P_{\underline{t}^n}$  by  $P_T$ . Hence

$$P_T(x^n) = P_{\underline{t}^n}(x^n). \quad (9.2)$$

Throughout this chapter, let  $V = \{0, 1, \dots, n-1\}$ , the set of vertices. Suppose  $\mu$  is a function  $\mu : V \rightarrow V$  such that  $\mu(i) < i$ . Let  $T_\mu = \{\underline{t}_{\mu(i)} \rightarrow \underline{t}_i : i \in V - \{0\}\}$ . Then  $T_\mu$  is a tree that spans (i.e., it includes all nodes)  $\underline{t}^n$ . Its root node is  $\underline{t}_0$ , because  $\underline{t}_0$  has no parents. All other nodes  $\underline{t}_i$  have exactly one parent, namely  $\underline{t}_{\mu(i)}$ . Let  $P_T$ , the total probability distribution for the tree, be parameterized by the function  $\mu$  as follows:

$$P_T(x^n) = \prod_{i=0}^{n-1} P_T(x_i | x_{\mu(i)}), \quad (9.3)$$

where, for the root node 0,  $P_T(x_0|x_{\mu(0)}) = P_T(x_0)$ .

**Claim 25**  $D_{KL}(P \parallel P_T)$  is minimized over all probability distributions  $P_T$  that are expressible as Eq.(9.3) iff

$$P_T(x_i|x_{\mu(i)}) = P(x_i|x_{\mu(i)}) \quad (9.4)$$

for all  $i$ , and

$$\sum_i H(\underline{x}_i : \underline{x}_{\mu(i)}) \quad (9.5)$$

is maximized over all  $\mu$ .

**proof:**

$$D_{KL}(P \parallel P_T) = \sum_{x^n} P(x^n) \ln \frac{P(x^n)}{P_T(x^n)} \quad (9.6)$$

$$= - \sum_{x^n} \sum_i P(x^n) \ln P_T(x_i|x_{\mu(i)}) + \sum_i P(x^n) \ln P(x^n) \quad (9.7)$$

$$= - \sum_i \sum_{x_i, x_{\mu(i)}} P(x_i, x_{\mu(i)}) \ln P_T(x_i|x_{\mu(i)}) - H(\underline{x}^n) \quad (9.8)$$

$$= - \sum_i \underbrace{\sum_{x_{\mu(i)}} P(x_{\mu(i)}) \left[ \sum_{x_i} P(x_i|x_{\mu(i)}) \ln P_T(x_i|x_{\mu(i)}) \right]}_{=H(\underline{x}_i|\underline{x}_{\mu(i)})=H(\underline{x}_i:\underline{x}_{\mu(i)})-H(\underline{x}_i)} - H(\underline{x}^n) . \quad (9.9)$$

Now note that

$$\sum_{x_i} P(x_i|x_{\mu(i)}) \ln \frac{P(x_i|x_{\mu(i)})}{P_T(x_i|x_{\mu(i)})} \geq 0 \quad (9.10)$$

and this inequality becomes an equality iff

$$P(x_i|x_{\mu(i)}) = P_T(x_i|x_{\mu(i)}) . \quad (9.11)$$

Therefore

$$D_{KL}(P \parallel P_T) \geq - \underbrace{\sum_i \sum_{x_{\mu(i)}} P(x_{\mu(i)}) \left[ \sum_{x_i} P(x_i|x_{\mu(i)}) \ln P(x_i|x_{\mu(i)}) \right]}_{=H(\underline{x}_i|\underline{x}_{\mu(i)})=H(\underline{x}_i:\underline{x}_{\mu(i)})-H(\underline{x}_i)} - H(\underline{x}^n) , \quad (9.12)$$

and this inequality becomes an equality iff Eq.(9.11) is satisfied.

Note from the last equation that

$$\operatorname{argmin}_{\mu} D_{KL}(P \parallel P_T) = \operatorname{argmax}_{\mu} \sum_i H(\underline{x}_i : \underline{x}_{\mu(i)}) . \quad (9.13)$$

**QED**

**Claim 26**

$$\operatorname{argmin}_{\mu} H(\underline{x}^n) = \operatorname{argmax}_{\mu} \sum_i H(\underline{x}_i : \underline{x}_{\mu(i)}) \quad (9.14)$$

**proof:**

$$H(\underline{x}^n) = - \sum_{x^n} P(x^n) \sum_i \ln P(x_i | x_{\mu(i)}) \quad (9.15)$$

$$= - \sum_i \sum_{x_i, x_{\mu(i)}} P(x_i, x_{\mu(i)}) \ln P(x_i | x_{\mu(i)}) \quad (9.16)$$

$$= - \sum_i \sum_{x_i, x_{\mu(i)}} P(x_i, x_{\mu(i)}) \left[ \ln \frac{P(x_i | x_{\mu(i)})}{P(x_i)} + \ln P(x_i) \right] \quad (9.17)$$

$$= - \sum_i [H(\underline{x}_i : \underline{x}_{\mu(i)}) - H(\underline{x}_i)] \quad (9.18)$$

$$= \sum_i H(\underline{x}_i) - \sum_i H(\underline{x}_i : \underline{x}_{\mu(i)}) \quad (9.19)$$

**QED**

The meaning of Claims 25 and 26 is as follows. If  $D_{KL}(P \parallel P_T)$  is minimized over all  $P_T$ , then

1.  $P_T$  inherits its TPMs from  $P$ , and
2.  $P_T$  gets its structure, which is being parameterized by the function  $\mu$ , by maximizing the score given by

$$\text{score} = \sum_i H(\underline{x}_i : \underline{x}_{\mu(i)}) . \quad (9.20)$$

(mutual information  $H(\underline{a} : \underline{b})$  measures correlation between  $\underline{a}$  and  $\underline{b}$ ). Maximizing the score is the same as minimizing the entropy  $H(\underline{x}^n)$  over all the structures  $\mu$ . (i.e., finding least complex structure).

So far, we have studied the properties of those probability distributions  $P_T$  for a tree bnet that best approximates an a priori given probability distribution  $P$ , but we haven't yet described how to build a Chow-Liu tree based on empirical data. Next we give Chow-Liu's algorithm for doing so.

1. Find MST using Kruskal's algorithm<sup>1</sup>. (see Fig.9.1)

Calculate weights  $w_{i,j} = H(\underline{x}_i : \underline{x}_j)$  for all  $i, j \in V$  and store them in a dictionary  $D$  that maps edges to weights.

Order  $D$  by weight size.

Let  $T$  be a list of the edges in the tree. Initialize  $T$  to empty.

Repeat this until  $T$  has  $n - 1$  elements:

    Remove largest weight  $w$  from  $D$  and corresponding edge  $e$ .

    Add  $e$  to  $T$  if  $\{e\} \cup T$  has no loops. Otherwise discard  $e$  and  $w$ .

2. Give directions to edges in  $T$ . (see Fig.9.2)

Let  $DT$  be a list of directed edges. Initialize  $DT$  to empty.

Choose any node as root node.

Point arrows along edges in  $T$ , away from root node.

Add new arrows to  $DT$ .

Repeat this until  $DT$  has  $n - 1$  elements:

    Point arrows along edges in  $T$ , away from leaf nodes of current  $DT$ .

    Add new arrows to  $DT$ .

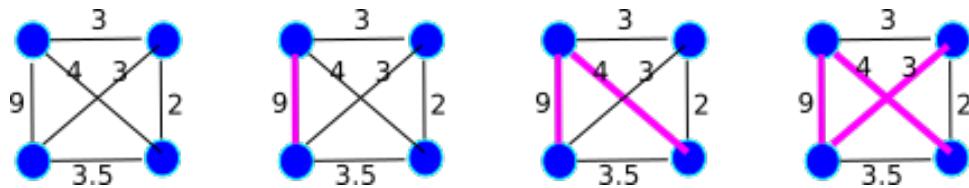


Figure 9.1: Example of finding MST (maximum spanning tree)

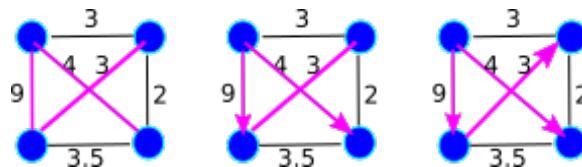


Figure 9.2: Example of giving directions to edges of spanning tree.

Nodes in a Chow-Liu tree can be rated in terms of their relative importance. Here are 2 possible metrics for measuring the importance of a node  $\underline{a}$ :

$$N_{nb}(\underline{a}) = \text{ number of neighbors of } \underline{a} \quad (9.21)$$

<sup>1</sup>Kruskal's algorithm is one several famous algorithms (Prim's algo is another one) for finding an MST (maximum or minimum spanning tree). An MST algorithm takes an undirected graph with weights along its edges as input. It then finds a tree subgraph (i.e., subset of the edges of the graph with no loops) that (1) spans the graph (i.e., includes every vertex of the graph) and (2) maximizes (or minimizes) the sum of weights among all possible tree subgraphs. For more information, see Ref[138] and references therein, or any other of numerous explanations of MST in the Internet.

$$\text{traffic}(\underline{a}) = \sum_{n \in nb(\underline{a})} H(\underline{a} : n) \quad (9.22)$$

For example, to get a tree with low depth, one can choose as the root node the node which has largest  $N_{nb}$ , and if there are several with the same largest  $N_{nb}$ , choose out of those the one with the largest traffic.

## 9.2 Tree Augmented Naive Bayes (TAN)

Recall from Chapter 63 that a Naive Bayes bnet consists of a class node  $\underline{c}$  with  $n$  children nodes  $\underline{x}^n$ , called the feature nodes. A Tree Augmented Naive Bayes (TAN) bnet is a Naive Bayes bnet with a tree grafted onto it like a chimera. More precisely, one starts with a Naive Bayes bnet and adds arrows between the feature nodes. The arrows are added in such a way that the TAN bnet sans node  $\underline{c}$  constitutes a tree. It's not the most well motivated bnet in human history, but at least it adds a bit of correlation between the feature nodes of the Naive Bayes bnet. Those nodes are independent at fixed  $\underline{c}$  in the Naive Bayes bnet, but are no longer so in the TAN bnet. See Figs.9.3 and 9.4 for an example of a TAN bnet.

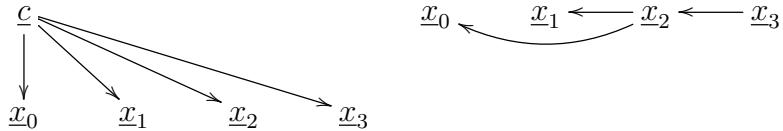


Figure 9.3: bnet for Naive Bayes with 4 feature nodes and another bnet for a tree made of the same feature nodes.

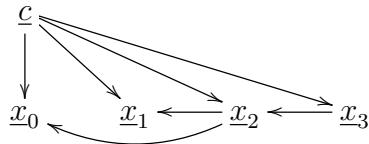


Figure 9.4: TAN bnet constructed by merging Naive Bayes bnet and tree bnet of Fig.9.3.

The total probability distribution  $P_{TAN}$  for a TAN bnet can be parameterized as follows.

$$P_{TAN}(x^n, c) = P_{TAN}(c) \prod_{i=0}^{n-1} P_{TAN}(x_i | x_{\mu(i)}, c). \quad (9.23)$$

As with Chow Liu trees, we can attempt to find a TAN bnet whose total probability  $P_{TAN} = P_{\underline{x}^n, \underline{c}}$  best approximates an a priori given probability distribution  $P = P_{\underline{x}^n, \underline{c}}$ .

Note that

**Claim 27**

$$\operatorname{argmin}_{\mu} H(\underline{x}^n, \underline{c}) = \operatorname{argmax}_{\mu} \sum_i H(\underline{x}_i : \underline{x}_{\mu(i)} | \underline{c}) \quad (9.24)$$

**proof:**

$$H(\underline{x}^n, \underline{c}) = - \sum_{x^n, c} P(x^n, c) \left[ \ln P(c) + \sum_i \ln P(x_i | x_{\mu(i)}, c) \right] \quad (9.25)$$

$$= - \sum_{x^n, c} P(x^n, c) \left[ \ln P(c) + \sum_i \ln \left( \frac{P(x_i, x_{\mu(i)} | c)}{P(x_i | c) P(x_{\mu(x_i)} | c)} P(x_i | c) \right) \right] \quad (9.26)$$

$$= \sum_i H(\underline{x}_i, \underline{c}) - \sum_i H(\underline{x}_i : \underline{x}_{\mu(i)} | \underline{c}) \quad (9.27)$$

**QED**

Following the same line of reasoning that we followed for Chow-Liu trees, we conclude that:

If  $D_{KL}(P \| P_{TAN})$  is minimized over all  $P_{TAN}$ , then

1.  $P_{TAN}$  inherits its TPMs from  $P$ , and
2.  $P_{TAN}$  gets its structure, which is being parameterized by the function  $\mu$ , by maximizing the score defined by

$$\text{score} = \sum_i H(\underline{x}_i : \underline{x}_{\mu(i)} | \underline{c}) \quad (9.28)$$

One can build a TAN bnet from empirical data as follows:

Calculate a Chow-Liu Tree for each  $c \in S_c$ . For each of those trees, create a TAN bnet, and calculate its score given by Eq.(9.28). Keep the TAN bnet with the largest score.

# Chapter 10

## Control Theory (linear, deterministic)

This chapter is based on Ref.[86] and [152].

We will assume that the reader has read Section C.45 on Laplace Transforms and Section C.46 on Z-transforms.

By **discrete time or discretizing time**, we mean sampling all signals at discrete times separated by a finite time interval  $T$  called the **sampling time**.

Control Theory (CT) studies the optimal control of systems with feedback. The systems studied can be

- linear or non-linear,
- deterministic or stochastic,
- continuous time (analog) or discrete time (digital).<sup>1</sup>

This chapter will deal with linear deterministic systems of either the analog or digital kind.

As explained in Chapter 25, dynamical bnets and feedback are two ways of viewing the same physical phenomenon. Also, there are numerous examples of dynamical bnets in this book: Kalman filters, Hidden Markov Models, Reinforcement Learning, Recursive Neural Nets, to name a few. Hence, a chapter on CT is very pertinent to this book.

Two acronyms commonly used in CT books are: **SISO** (single input single output) and **MIMO** (multiple input multiple output). We will consider both SISO and MIMO systems in this chapter.

Another distinction commonly made in CT books is between **time-variant** and **time-invariant** systems. We will explain what those terms mean later on in this chapter. This chapter will consider both types of systems.

---

<sup>1</sup>A signal  $x(t)$  is a function of time  $t$ . We can discretize  $t$  ( $\Delta t$ , sampling), or discretize  $x$  ( $\Delta x$ , quantization), or both. We will use the word “digital” or “sampled” to describe a theory with discretized  $t$ , but continuous  $x$ . Sometimes, the word “digital” is used instead to describe a theory with both  $x$  and  $t$  discretized.

## 10.1 Basic feedback model

CT uses feedback to control a **system or process**. Fig.10.1 shows a very basic feedback model, represented with 3 equivalent diagrams.

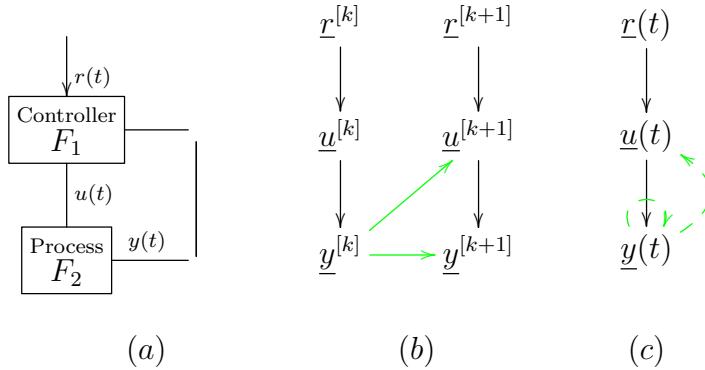


Figure 10.1: Basic feedback model represented as: (a) a wired time-dependent boxes diagram, (b) two time-slices of a dynamical bnet (see Chapter 25), and (c) a “rolled” dynamical bnet with feedback cycles.

The diagrams of Fig.10.1 represent graphically the following system of equations. Here  $t \in [0, \infty]$  is time and  $r, u, y : [0, \infty] \rightarrow \mathbb{C}$ .

$$\begin{cases} u(t) = F_1(y(t), r(t), t) \\ \partial_t y(t) = F_2(y(t), u(t), t) \end{cases} \quad (10.1)$$

If we approximate the time derivative of  $y(t)$  by

$$\partial_t y(t) \approx \frac{y(t + \Delta t) - y(t)}{\Delta t} \quad (10.2)$$

and we set

$$\begin{aligned} t_k &= t, t_{k+1} = t + \Delta t, 0 < \Delta t \ll 0, \\ f(t_k) &= f^{[k]} \text{ for } f = r, y, u, \end{aligned}$$

then we get Fig.10.1

The TPMs, printed in blue, of the bnet in Fig.10.1(b), are as follows:

$$P(r^{[k]}) = \text{given} \quad (10.3)$$

$$P(u^{[k]} | y^{[k]}, r^{[k]}) = \delta(u^{[k]} - F_1(y^{[k]}, r^{[k]}, t_k)) \quad (10.4)$$

$$P(y^{[k+1]}|y^{[k]}, u^{[k]}) = \delta(y^{[k+1]} - y^{[k]} - \Delta t F_2(y^{[k]}, u^{[k]}, t_k)) \quad (10.5)$$

## 10.2 Classical model (analog)

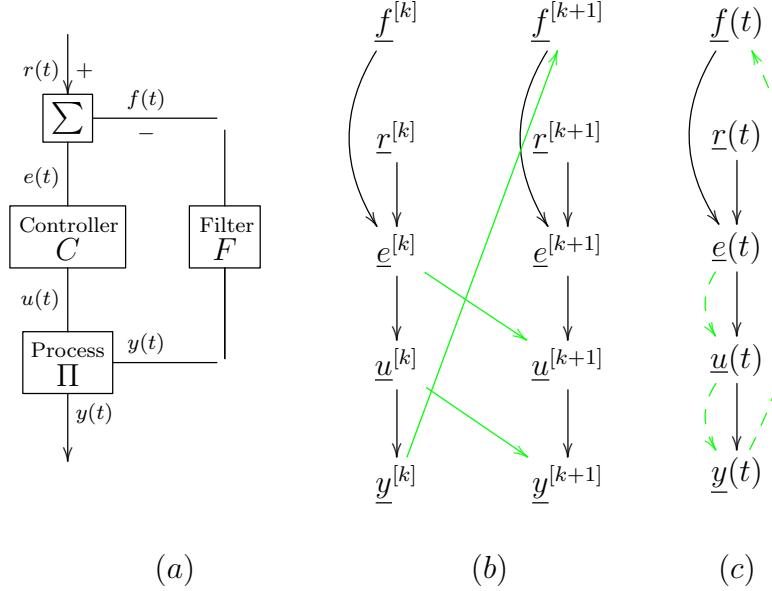


Figure 10.2: Classical Model represented with the same 3 types of diagrams as Fig.10.1. Bnet (b) doesn't show all the arrows. In reality, for any arrow  $a^{[k]} \rightarrow b^{[k+1]}$  that points from the time-slice  $t_k$  to the time-slice  $t_{k+1}$ , there should be arrows  $a^{[j]} \rightarrow b^{[k+1]}$  for  $j \in \{0, 1, 2, \dots, k\}$ . That's because the classical model is defined in terms of convolutions, and a convolution at time  $t$  requires memory for all times between 0 and  $t$ .

A **classical model** is a bunch of wired convolution boxes. See Fig.10.2 for 3 graphical representations of the classical model.

Let  $t \in [0, \infty]$  =time and  $f, e, r, u, y : [0, \infty] \rightarrow \mathbb{C}$ . The diagrams of Fig.10.2 represent graphically the following system of equations.

$$\begin{cases} f(t) = (F * y)(t) \\ e(t) = r(t) - f(t) \\ u(t) = (C * e)(t) \\ y(t) = (\Pi * u)(t) \end{cases} \quad (10.6)$$

where  $(f * g)(t)$  denotes a covolution, as defined in Section C.45 on Laplace transforms.

The TPMs, printed in blue, of the bnet in Fig.10.2, are as follows:

$$P(r(t)) = \text{given} \quad (10.7)$$

$$P(f(t)|y(\cdot)) = \delta(f(t) - \Pi[y](t)) \quad (10.8)$$

$$P(e(t)|r(t), f(t)) = \delta(e(t) - [r(t) - f(t)]) \quad (10.9)$$

$$P(u(t)|e(\cdot)) = \delta(u(t) - C[e](t)) \quad (10.10)$$

$$P(y(t)|u(\cdot)) = \delta(y(t) - \Pi[u](t)) \quad (10.11)$$

If we take the Laplace transform of Eqs.(10.6, we get

$$\begin{cases} \tilde{f}(s) = \tilde{F}(s)\tilde{y}(s) \\ \tilde{e}(s) = \tilde{r}(s) - \tilde{f}(s) \\ \tilde{u}(s) = \tilde{C}(s)\tilde{e}(s) \\ \tilde{y}(s) = \tilde{\Pi}(s)\tilde{u}(s) \end{cases} \quad (10.12)$$

Thus

$$\tilde{H}_{y|e} = \frac{\tilde{y}}{\tilde{e}} = \tilde{\Pi}\tilde{C} \quad (10.13)$$

$$\tilde{y} = \tilde{H}_{y|e}[\tilde{r} - \tilde{F}\tilde{y}] \quad (10.14)$$

$$[1 + \tilde{H}_{y|e}\tilde{F}]\tilde{y} = \tilde{H}_{y|e}\tilde{r} \quad (10.15)$$

$$\tilde{H}_{y|r}(s) = \frac{\tilde{y}(s)}{\tilde{r}(s)} \quad (\text{output/input}) \quad (10.16)$$

$$= \frac{\tilde{H}_{y|e}}{1 + \tilde{H}_{y|e}\tilde{F}} \quad (10.17)$$

$\tilde{H}_{y|e}$  and  $\tilde{H}_{y|r}(s)$  are both called **gain or transfer functions**.  $\tilde{H}_{y|e}$  is called the **open loop gain** and  $\tilde{H}_{y|r}(s)$  is called the **closed loop gain**. If  $|H_{y|r}|$  is less

than (resp., more than) 1, we say that there is **negative feedback** (resp., **positive feedback**) because the  $\tilde{r}$  signal is reduced (resp., magnified). If the open loop gain  $|\tilde{H}_{y|e}| \gg 1$ , then the closed loop gain  $|\tilde{H}_{y|r}| \approx \frac{1}{|\tilde{F}|}$ . So negative (resp., positive) feedback occurs if  $|\tilde{F}| > 1$  (resp.,  $|\tilde{F}| < 1$ )

A common type of controller box  $\tilde{C}(s)$  called the **Proportional-Integral-Derivative (PID) Controller** is defined as

$$u(t) = K_{\Pi}e(t) + K_I \int_0^t d\tau e(\tau) + K_D \partial_t e(t) \quad (10.18)$$

The Laplace transform of the PID controller is

$$\tilde{u}(s) = K_{\Pi}\tilde{e}(s) + K_I \frac{\tilde{e}(s)}{s} + K_D(s\tilde{e}(s) - e(0^+)) \quad (10.19)$$

$$= \underbrace{\left( \underbrace{K_{\Pi}}_{\text{proportional controller}} + \underbrace{\frac{K_I}{s}}_{\text{integrator controller}} + \underbrace{K_D s}_{\text{differentiator controller}} \right)}_{\tilde{C}(s), \text{ PID controller}} \tilde{e}(s) \quad (\text{assume } e(0^+) = 0) \quad (10.20)$$

**Claim 28** A PID controller has unit gain ( $\tilde{H}_{y|r}(s) = 1$ ) if:

$$K_{\Pi} = 2K, \quad K_D = KT, \quad K_I = \frac{K}{T} \quad (10.21)$$

$$\tilde{\Pi}(s) = \frac{1}{K(1+sT)} \quad (10.22)$$

and

$$\tilde{F}(s) = \frac{1}{1+sT} \quad (10.23)$$

**proof:**

$$\tilde{C} = \frac{K}{sT} (2sT + 1 + (sT)^2) \quad (10.24)$$

$$= \frac{K}{sT} (1 + sT)^2 \quad (10.25)$$

so

$$1 + \tilde{\Pi} \tilde{C} \tilde{F} = 1 + \frac{1}{sT} \quad (10.26)$$

$$= \frac{1}{sT} (1 + sT) \quad (10.27)$$

$$= \tilde{\Pi} \tilde{C} \quad (10.28)$$

Hence,

$$\tilde{H}_{y|r}(s) = 1 \quad (10.29)$$

**QED**

### 10.3 Modern model (analog)

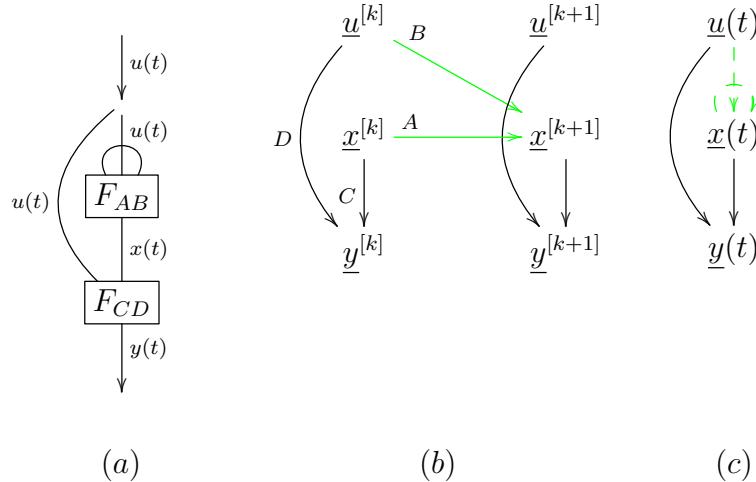


Figure 10.3: Modern Model represented with the same 3 types of diagrams as Fig.10.1.

A **modern model (a.k.a. state space model)** is a bunch of wired time-dependent boxes, some with first order time derivatives. See Fig.10.3 for 3 graphical representations of the modern model.

Let

$$t \in [0, \infty] = \text{time}$$

$$u : [0, \infty] \rightarrow \mathbb{C}^{nu}$$

$$x : [0, \infty] \rightarrow \mathbb{C}^{nx}$$

$$y : [0, \infty] \rightarrow \mathbb{C}^{ny}$$

for some integers  $nu, nx, ny$ . The diagrams of Fig.10.3 represent graphically the following system of equations.

$$\begin{cases} \partial_t x(t) = F_{AB}(x(t), u(t), t) \\ y(t) = F_{CD}(x(t), u(t), t) \end{cases} \quad (10.30)$$

These equations are called the **state space equations** and  $x(t)$  is called the **state** of the system. The equation for  $\partial_t x(t)$  is called the **state equation** and the one for  $y(t)$  is called the **output equation**.

The TPMs, printed in blue, of the bnet in Fig.10.3(b), are as follows:

$$P(u^{[k]}) = \text{given} \quad (10.31)$$

$$P(x^{[k+1]} | x^{[k]}, u^{[k]}) = \delta(-x^{[k+1]} - x^{[k]} - \Delta t F_{AB}(x^{[k]}, u^{[k]}, t_k)) \quad (10.32)$$

$$P(y^{[k]} | x^{[k]}, u^{[k]}) = \delta(-y^{[k]} - F_{CD}(x^{[k]}, u^{[k]}, t_k)) \quad (10.33)$$

Henceforth, assume  $F_{AB}$  and  $F_{CD}$  are as follows. This is called the **linear** case.

$$\begin{cases} F_{AB}(x(t), u(t)) = A(t)x(t) + B(t)u(t) \\ F_{CD}(x(t), u(t)) = C(t)x(t) + D(t)u(t) \end{cases} \quad (10.34)$$

for some matrices  $A(t), B(t), C(t), D(t)$ . In the linear case, the modern model is described by the following equations:

$$\begin{cases} \partial_t x(t) = Ax(t) + Bu(t) \\ y(t) = Cx(t) + Du(t) \end{cases} \quad (10.35)$$

If the matrices  $A(t), B(t), C(t), D(t)$  depend on (resp., are independent of) time  $t$ , we say the system is **time-variant** (resp., **time-invariant**). Next, we solve the differential equation for  $x(t)$ , for both the time-invariant and variant cases.

- time-invariant case

Taking the Laplace transform of the first equation of Eqs.(10.35), we get

$$s\tilde{x}(s) - x(0) = A\tilde{x}(s) + B\tilde{u}(s) \quad (10.36)$$

Hence, the Laplace transform of Eqs.(10.35) is

$$\begin{cases} \tilde{x}(s) = (sI - A)^{-1}x(0) + (sI - A)^{-1}B\tilde{u}(s) \\ \tilde{y}(s) = C\tilde{x}(s) + D\tilde{u}(s) \end{cases} \quad (10.37)$$

If we define the transfer function  $\tilde{H}_{y|u}(s)$  by

$$\underbrace{\tilde{y}(s)}_{\text{output}} = \tilde{H}_{y|u}(s) \underbrace{\tilde{u}(s)}_{\text{input}} \quad (10.38)$$

then, assuming  $x(0) = 0$ ,

$$\tilde{H}_{y|u}(s) = C(sI - A)^{-1}B + D \quad (10.39)$$

Note from the last equation that the set of poles of  $\tilde{H}_{y|u}(s)$  is a subset of the set of eigenvalues of  $A$ .

If we set

$$A = \begin{bmatrix} 0 & 1 & 0 & \cdots & 0 \\ 0 & 0 & 1 & \cdots & 0 \\ \vdots & \vdots & \vdots & & \vdots \\ 0 & 0 & 0 & \cdots & 1 \\ -b_0 & -b_1 & -b_2 & \cdots & -b_{n-1} \end{bmatrix} \quad (10.40)$$

$$B = \begin{bmatrix} 0 \\ 0 \\ \vdots \\ 1 \end{bmatrix} \quad (10.41)$$

$$C = [ a_0 \ a_1 \ \cdots \ a_{m-1} ] \quad (10.42)$$

$$D = 0 \quad (10.43)$$

then one can show that (the laborious part is inverting  $s - A$  algebraically)

$$\tilde{H}_{y|u}(s) = C(sI - A)^{-1}B + D \quad (10.44)$$

$$= \frac{s^m + a_{m-1}s^{m-1} + \cdots + a_0}{s^n + b_{n-1}s^{n-1} + \cdots + b_0} \quad (10.45)$$

This makes it possible to start with a desired transfer function, and build an analog modern model that achieves it.

### Claim 29

$$x(t) = e^{A(t-t_0)}x(t_0) + e^{A(t-t_0)} \int_{t_0}^t d\tau e^{-A(\tau-t_0)} Bu(\tau) \quad (10.46)$$

where

$$e^{At} = \sum_{k=0}^{\infty} \frac{t^k}{k!} A^k \quad (10.47)$$

Hence, setting  $t \geq t_0 = 0$ ,

$$e^{At} = \mathcal{L}^{-1}[(sI - A)^{-1}] \quad (10.48)$$

$$e^{At} \int_0^t d\tau e^{-A\tau} Bu(\tau) = \mathcal{L}^{-1}[(sI - A)^{-1} B \tilde{u}(s)] \quad (10.49)$$

**proof:** To check Eq.(10.46), just take the time derivative of both sides and use  $\partial_t \int_0^t d\tau f(\tau) = f(t)$

**QED**

- time-variant case

### Claim 30

$$x(t) = \mathcal{E}(t, t_0)x(t_0) + \int_{t_0}^t d\tau \mathcal{E}(t, \tau)B(\tau)u(\tau) \quad (10.50)$$

where the state transition matrix (a.k.a. evolution matrix)  $\mathcal{E}(t, t_0)$  satisfies

$$\partial_t \mathcal{E}(t, t_0) = A(t) \quad (10.51)$$

and

$$\mathcal{E}(t, t) = 1 \quad (10.52)$$

**proof:** To prove Eq.(10.50), just differentiate both sides of it with respect to  $t$ , and use  $\partial_t \int_0^t d\tau f(\tau) = f(t)$

**QED**

In the time-invariant case,

$$\mathcal{E}(t, t_0) = e^{A(t-t_0)} \quad (10.53)$$

## 10.4 Classical model (digital)

In this section, we will define the classical model with discrete rather than continuous time.

If we discretize time, then the equivalent of Eqs.(10.6) is

$$\begin{cases} f^{[n]} = (F \circledast y)^{[n]} \\ e^{[n]} = r^{[n]} - f^{[n]} \\ u^{[n]} = (C \circledast e)^{[n]} \\ y^{[n]} = (\Pi \circledast u)^{[n]} \end{cases} \quad (10.54)$$

where  $(x \circledast y)^{[n]}$  denotes a discrete convolution, as defined in Section C.46 on Z-transforms. And if we take the Z-transform of Eqs.(10.54), we get

$$\begin{cases} \tilde{f}(z) = \tilde{F}(z)\tilde{y}(z) \\ \tilde{e}(z) = \tilde{r}(z) - \tilde{f}(z) \\ \tilde{u}(z) = \tilde{C}(z)\tilde{e}(z) \\ \tilde{y}(z) = \tilde{\Pi}(z)\tilde{u}(z) \end{cases} \quad (10.55)$$

The **digital PID controller box**  $\tilde{C}(z)$  is given by

$$\tilde{u}(z) = \underbrace{\left( K_{\Pi} + K_I \frac{T}{2} \left( \frac{z+1}{z-1} \right) + K_D \frac{1}{T} \left( \frac{z-1}{z} \right) \right)}_{\tilde{C}(z), \text{PID controller}} \tilde{e}(z) \quad (\text{assume } e(0^+) = 0) \quad (10.56)$$

## 10.5 Modern model (digital)

In this section, we will define the modern model with discrete rather than continuous time. We will do this 2 different ways. First, we will approximate the time derivatives in all differential equations with a discrete approximation. This approach is interesting and instructive but not perfect, because it's an approximation (i.e., it assumes the sampling time  $T = \Delta t$  is very small). Second, we will replace all differential equations by difference equations, and solve the latter exactly. The second approach is better for most purposes, because it gives exact results (i.e., correct to all orders in  $T$ ), instead of approximations.

### 10.5.1 Discretizing derivatives

If we approximate  $\partial_t x(t)$  by

$$\partial_t x(t) = \lim_{\Delta t \rightarrow 0} \frac{x(t + \Delta t) - x(t)}{\Delta t} \quad (10.57)$$

then Eqs.(10.35) reduce to

$$\begin{cases} x(t + \Delta t) = (1 + \Delta t A)x(t) + \Delta t B u(t) \\ y(t) = Cx(t) + D u(t) \end{cases} \quad (10.58)$$

Using the new notation

$$\hat{A} = e^{A\Delta t} \approx 1 + \Delta t A, \quad (10.59)$$

$$\hat{B} \approx \Delta t B \quad (10.60)$$

$$\Delta t = T, \quad t = nT \quad (10.61)$$

$$X(t) = X(nT) = X^{[n]} \quad \text{for } X = x, u, y \quad (10.62)$$

we get

$$\begin{cases} x^{[n+1]} = \hat{A}x^{[n]} + \hat{B}u^{[n]} \\ y^{[n]} = Cx^{[n]} + Du^{[n]} \end{cases} \quad (10.63)$$

Setting  $t = t_0 + T$  in Eq.(10.46), we get

$$x(t_0 + T) = e^{AT}x(t_0) + e^{AT} \int_{t_0}^{t_0+T} d\tau e^{-A(\tau-t_0)} Bu(\tau) \quad (10.64)$$

$$= e^{AT}x(t_0) + e^{AT} \int_0^T d\tau e^{-A\tau} Bu(\tau + t_0) \quad (\text{substitute } \tau \rightarrow \tau + t_0) \quad (10.65)$$

Now setting

$$t_0 = nT \quad (10.66)$$

and

$$u(\tau + t) \approx u(t) \quad \text{for } \tau \in [0, T] \quad (10.67)$$

we get

$$x^{[n+1]} = \underbrace{e^{AT}}_{\hat{A}} x^{[n]} + \underbrace{e^{AT} \left[ \int_0^T d\tau e^{-A\tau} \right] B u^{[n]}}_{\hat{B}} \quad (10.68)$$

where

$$\hat{A} = e^{AT} \quad (10.69)$$

and

$$\hat{B} = e^{AT} \left[ \int_0^T d\tau e^{-A\tau} \right] B \quad (10.70)$$

$$= e^{AT} (-A)^{-1} (e^{-AT} - I) B \quad (10.71)$$

$$= A^{-1} (\hat{A} - 1) B \quad (10.72)$$

When  $T \ll 1$ ,  $\hat{A} - 1 \approx AT$  so  $A^{-1}(\hat{A} - 1)B \approx BT$ .

### 10.5.2 Solving Difference Equation

- time-invariant case

Consider the following difference equation taken from Eqs.(10.63)

$$x^{[n+1]} = \hat{A}x^{[n]} + \hat{B}u^{[n]} \quad (10.73)$$

To solve this difference equation, we notice that

$$x^{[1]} = \hat{A}x^{[0]} + \hat{B}u^{[0]} \quad (10.74)$$

$$x^{[2]} = \hat{A}x^{[1]} + \hat{B}u^{[1]} \quad (10.75)$$

$$= \hat{A}^2 x^{[0]} + \hat{A}\hat{B}u^{[0]} + \hat{B}u^{[1]} \quad (10.76)$$

$$x^{[3]} = \hat{A}x^{[2]} + \hat{B}u^{[2]} \quad (10.77)$$

$$= \hat{A}^3 x^{[0]} + \hat{A}^2 \hat{B}u^{[0]} + \hat{A}\hat{B}u^{[1]} + \hat{B}u^{[2]} \quad (10.78)$$

The general pattern is clear. In general,

$$x^{[n]} = \hat{A}^n x^{[0]} + \sum_{k=0}^{n-1} \hat{A}^{n-k-1} \hat{B} u^{[k]} \quad (10.79)$$

It is also possible to solve Eqs.(10.63) using Z-transforms (See Section C.46). The Z-transform of the first of those two equations is

$$z(\tilde{x}(z) - x^{[0]}) = \hat{A}\tilde{x}(z) + \hat{B}\tilde{u}(z) \quad (10.80)$$

Therefore, the Z-transform of Eqs.(10.63) is<sup>2</sup>

$$\begin{cases} \tilde{x}(z) = (zI - \hat{A})^{-1} z x^{[0]} + (zI - \hat{A})^{-1} \hat{B} \tilde{u}(z) \\ \tilde{y}(z) = C\tilde{x}(z) + D\tilde{u}(z) \end{cases} \quad (10.81)$$

From this we can get the transfer matrix  $\tilde{H}_{y|u}(z)$ . Assuming  $x^{[0]} = 0$ ,

$$\tilde{y}(z) = \underbrace{\left( \hat{C}(zI - \hat{A})^{-1} \hat{B} + \hat{D} \right)}_{\tilde{H}_{y|u}(z)} \tilde{u}(z) \quad (10.82)$$

As for the analog modern model, it is possible to find for the digital modern model, matrices  $\hat{A}, \hat{B}, \hat{C}, \hat{D}$  that produce a transfer function of a desired form.

- time-variant case

We can also give a discrete version of Claim 30

### Claim 31

$$x^{[n]} = \mathcal{E}^{[n,n_0]} x^{[n_0]} + \sum_{k=0}^{n-1} \mathcal{E}^{[n,k+1]} B^{[k]} u^{[k]} \quad (10.83)$$

where

$$\mathcal{E}^{[n+1,n_0]} = \hat{A}^{[n]} \mathcal{E}^{[n,n_0]} \quad (10.84)$$

and

$$\mathcal{E}^{[n_0,n_0]} = I \quad (10.85)$$

Hence

$$\mathcal{E}^{[n,n_0]} = \hat{A}^{[n-1]} \hat{A}^{[n-2]} \hat{A}^{[n-3]} \dots \hat{A}^{[n_0]} \quad (10.86)$$

$$= \prod_{k \in \mathbb{Z}^{[1,n-n_0]}} \hat{A}^{[n-k]} \quad (10.87)$$

---

<sup>2</sup>Notice the  $z$  factor multiplying  $x^{[0]}$ . There is no counterpart  $s$  factor multiplying  $x(0)$  in the analog case. That's because  $z = e^{sT}$ .

**proof:** Left to reader.

**QED**

## 10.6 Higher than first order differential (or difference) equations

If in the analog, time-invariant modern model, we express  $x(t)$  in terms of  $y(t)$  and  $u(t)$

$$x(t) = C^{-1}[y(t) - Du(t)] \quad (10.88)$$

and then we plug this into the equation for  $\partial_t x(t)$ , we get

$$\partial_t \left( \underbrace{C^{-1}[y(t) - Du(t)]}_{x(t)} \right) = A \underbrace{C^{-1}[y(t) - Du(t)] + Bu(t)}_{x(t)} \quad (10.89)$$

Hence, it appears that this model can only accommodate a first order time derivative of the output  $y(t)$ . Next we give a transformation whereby a model with  $y(t)$  derivatives that are higher than 1st order, can be re-expressed in a form that only has 1st order time derivatives. We will also give an analogous result for the digital (instead of analog) time-invariant modern model; that is, we will show that those digital models can accommodate higher than 1st order time differences.

### 10.6.1 Differential Equations

Let

$$\Omega = \partial_t^3 + a_2 \partial_t^2 + a_1 \partial_t + a_0 \quad (10.90)$$

where  $a_0, a_1, a_2 \in \mathbb{C}$  are independent of time  $t$ , and consider the **linear, constant coefficients (LCC) ordinary differential equation (ODE)**:

$$\Omega y(t) = u(t) \quad (10.91)$$

Assume  $f(t)$  satisfies

$$\Omega f(t) = 0 \quad (10.92)$$

Let

$$\underbrace{\partial_t^3 y(t)}_{\partial_t x_2 + \partial_t^3 f} + a_2 \underbrace{\partial_t^2 y(t)}_{x_2 + \partial_t^2 f} + a_1 \underbrace{\partial_t y(t)}_{x_1 + \partial_t f} + a_0 \underbrace{y(t)}_{x_0 + f} = u(t) \quad (10.93)$$

and

$$x(t) = \begin{bmatrix} x_0(t) \\ x_1(t) \\ x_2(t) \end{bmatrix} \quad (10.94)$$

Then

$$\partial_t x(t) = \underbrace{\begin{bmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ -a_0 & -a_1 & -a_2 \end{bmatrix}}_A x(t) + \underbrace{\begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix}}_B u(t) \quad (10.95)$$

$$y(t) = x_0(t) + f(t) = \underbrace{\begin{bmatrix} 1 & 0 & 0 \end{bmatrix}}_C x(t) + f(t) \quad (10.96)$$

If  $\Omega u = 0$ , we can define  $f = Du$ . Otherwise, define  $f = 0$ .

What's going on here, from a dynamical bnet perspective, is that we are defining the slices to have enough variables so that there only needs to be memory from one slice to the previous slice, instead of, to the previous 3 slices.

### 10.6.2 Difference Equations

Let

$$\underbrace{y^{[n+3]}_{x_3^{[n+1]}}} + a_2 \underbrace{y^{[n+2]}_{x_2^{[n]}}} + a_1 \underbrace{y^{[n+1]}_{x_1^{[n]}}} + a_0 \underbrace{y^{[n]}_{x_0^{[n]}}} = u^{[n]} \quad (10.97)$$

and

$$x^{[n]} = \begin{bmatrix} x_0^{[n]} \\ x_1^{[n]} \\ x_2^{[n]} \end{bmatrix} \quad (10.98)$$

Then

$$x^{[n+1]} = \underbrace{\begin{bmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ -a_0 & -a_1 & -a_2 \end{bmatrix}}_A x^{[n]} + \underbrace{\begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix}}_B u^{[n]} \quad (10.99)$$

$$y^{[n]} = x_0^{[n]} = \underbrace{\begin{bmatrix} 1 & 0 & 0 \end{bmatrix}}_C x^{[n]} \quad (10.100)$$

## 10.7 Time-Invariance, Causality, Stability

A linear system with input  $r(t)$  and output  $y(t)$  has a kernel function  $H(t, \tau)$  such that

$$y(t) = \int_0^{\Lambda} H(t, \tau) r(\tau) \quad (10.101)$$

In general,  $r$  and  $y$  are vectors, so  $H(t, \tau)$  is a matrix.

A system is **time-invariant** if  $H(t, \tau) = H(t - \tau)$ . For time-invariant systems,  $H(t)$  is called the **impulse response** (because  $y(t) = H(t)$  when  $r(\tau) = \delta(\tau)$ ) and its Laplace transform  $\tilde{H}(s)$  is called the **transfer function**.

A system is **causal** if  $\Lambda = t$  (i.e., the output  $y(t)$  depends only on the input  $r(\tau)$  for  $\tau < t$ ).

A system is **stable** if a bounded input  $r(\cdot)$  implies a bounded output  $y(\cdot)$ . (BIBO=Bounded Input, Bounded Output).

Consider the analog time-invariant modern model. Suppose its transfer function is<sup>3</sup>

$$\tilde{H}_{y|u}(s) = K \frac{\mathcal{N}(s)}{\mathcal{D}(s)} \quad (10.102)$$

where  $K \in \mathbb{C}$  is some constant independent of  $s$ ,

$$\mathcal{N}(s) = \prod_{a=1}^A (s - \alpha_a)^{m_a} \quad (10.103)$$

and

$$\mathcal{D}(s) = \prod_{b=1}^B (s - \beta_b)^{n_b} \quad (10.104)$$

and where the polynomials  $\mathcal{N}(s)$  and  $\mathcal{D}(s)$  have no common factors. The  $\{\alpha_a\}_{a=1}^A$  are called the **zeros** of the transfer function, and the  $\{\beta_b\}_{b=1}^B$  are called the **poles** of the transfer function. This system is

- **stable** if the zeros of the transfer function fall on the left half of the  $s$ -plane (i.e., if  $\text{Re}(\beta_b) < 0$  for all  $b$ )
- **marginally stable** if  $\text{Re}(\beta_b) = 0$  for some  $b$  and  $\text{Re}(\beta_b) < 0$  for the others. Marginally stable systems sustain undamped oscillations. They may become unstable if perturbed.

---

<sup>3</sup>We are assuming that the transfer function is a scalar  $1 \times 1$  matrix. If it has row or column dimensions larger than one, one analyzes each entry of the transfer function matrix as if it were a scalar transfer function.

- **unstable** if  $\operatorname{Re}(\beta_b) > 0$  for some  $b$ .

To get some intuition as to why this is so, let's look at the inverse Laplace transform of  $1/(s - \beta_b)$ :

$$\lim_{t \rightarrow \infty} \int_{\gamma-iT}^{\gamma+iT} ds \frac{e^{st}}{s - \beta_b} = K e^{\beta_b t} u_0(t) \quad (10.105)$$

where  $K \in \mathbb{C}$ ,  $\gamma, T \in \mathbb{R}$  and  $\operatorname{Re}(\beta_b) < \gamma$ . At the pole,  $s = \beta_b$ , so

$$e^{st} = e^{\beta_b t} = e^{\operatorname{Re}(\beta_b)t} e^{i\operatorname{Im}(\beta_b)t} \quad (10.106)$$

As  $t \rightarrow \infty$ , the integral blows up if  $\operatorname{Re}(\beta_b) > 0$  and converges if  $\operatorname{Re}(\beta_b) < 0$ . As  $t \rightarrow \infty$ , integration under poles in the left half plane doesn't blow up because it is ultimately damped by a decaying exponential.

An analogous result holds for the digital time-invariant modern model, except that in that case, the transfer function  $\tilde{H}_{y|u}(z)$  is a Z-transform (instead of a Laplace transform), and stability occurs if the poles of the transfer function fall inside the unit circle of the z-plane (instead of the left half plane of the s-plane.)

## 10.8 Controllability, Observability

Suppose  $x, u, y : \mathcal{T} \rightarrow \mathcal{X}$ . where  $\mathcal{T} = [0, \infty)$ .

- $a \in \mathcal{X}$  is **controllable at time**  $t_0 \in \mathcal{T}$  if there exist a time  $t_1 \in \mathcal{T}$  and an input  $u(\cdot)$  such that  $x(t_0) = a$  and  $x(t_1) = 0$ .
- $x(\cdot)$  is **controllable at time**  $t_0 \in \mathcal{T}$  if, for all  $a \in \mathcal{X}$ ,  $a$  is controllable at time  $t_0 \in \mathcal{T}$ .
- $a \in \mathcal{X}$  is **observable at time**  $t_0 \in \mathcal{T}$  if there exists a  $t_1 \in \mathcal{T}$  such that  $x(t_0) = a$  and  $a$  can be determined from the values of  $y(t)$  for  $t \in [t_0, t_1]$ .
- $x(\cdot)$  is **observable at time**  $t_0 \in \mathcal{T}$  if, for all  $a \in \mathcal{X}$ ,  $a$  is observable at time  $t_0 \in \mathcal{T}$ .

## 10.9 Signal Flow Graph

This section on Signal Flow (SF) graphs is based on Ref.[152]. According Ref.[152], SF graphs were invented by Shannon in 1942 to model "differential equation machines". They were later extended and promoted by Mason circa 1955.

SF graphs are very similar to LDEN (Linear Deterministic with External Noise) bnets discussed in Chapter 48. However, there are some important differences between the two, such as: (1) SF graphs have no external random nodes (2) unlike the LDEN considered in Chapter 48, SF graphs can have feedback cycles.

In SF graphs, the multiplicative factors carried by the arrows are called “gains”. In SF graphs, the gains are always Laplace transforms (for the analog case) or Z-transforms (for the digital case). In this section, we will only discuss SF graphs for the analog case, but keep in mind that the digital case is very similar.

Next we will discuss the analog classical and analog (time-invariant) modern models in terms of SF graphs.

- classical model

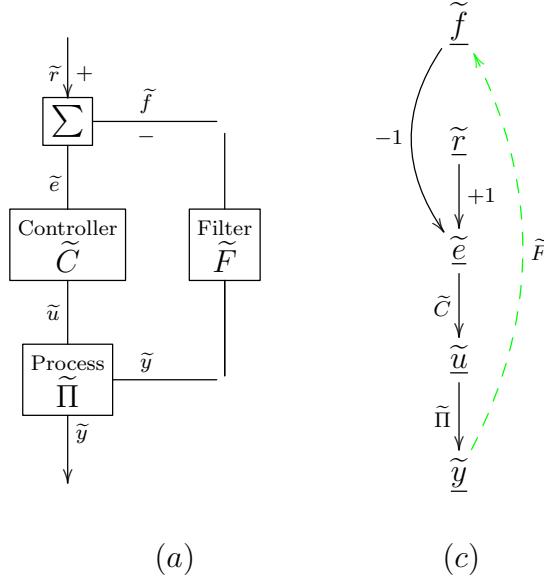


Figure 10.4: This figure is the Laplace transform of classical model Figs.10.2 (a) and (c).

Fig.10.4 is the Laplace transform of Figs.10.2 (a) and (c). Fig.10.4 (c) is an SF graph.

The SF graph of Fig.10.4 implies the following system of equations:

$$\begin{cases} \underline{\tilde{e}} = \underline{\tilde{r}} - \underline{\tilde{f}} \\ \underline{\tilde{u}} = \tilde{C}\underline{\tilde{e}} \\ \underline{\tilde{y}} = \tilde{\Pi}\underline{\tilde{u}} \\ \underline{\tilde{f}} = \tilde{F}\underline{\tilde{y}} \end{cases} \quad (10.107)$$

- time-invariant modern model

Fig.10.5 is the Laplace transform of Figs.10.3 (a) and (c) for the time-invariant case. Fig.10.5 (c) is an SF graph.

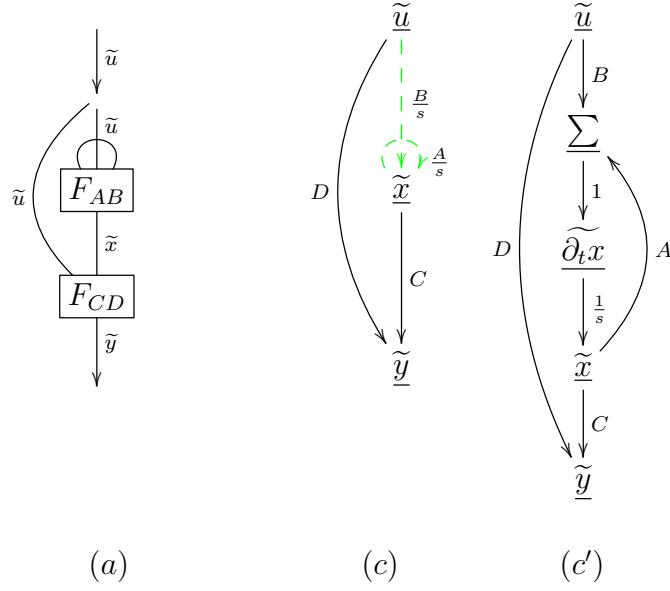


Figure 10.5: This figure is the Laplace transform of modern model Figs.10.3 (a) and (c), for the time-invariant case. Figure (c') is a more detailed version of figure (c).

The SF graph of Fig.10.5 implies the following system of equations:

$$\begin{cases} \tilde{x} = \frac{1}{s}(A\tilde{x} + B\tilde{u}) \\ \tilde{y} = C\tilde{x} + D\tilde{u} \end{cases} \quad (10.108)$$

Next, we shall discuss some properties of the feedback cycles of SF graphs.

An approach that I like is to re-express an SF graph with feedback cycles by one without them that is easier to understand.

**Claim 32** *Eliminating bubbles (i.e., self-feedback cycles)*

$$(10.109)$$

**proof:** From the left hand diagram,

$$\underline{x} = \mu\underline{x} + \alpha\underline{a} + \beta\underline{b} \quad (10.110)$$

Hence,

$$\underline{x} = \frac{\alpha}{1-\mu}\underline{a} + \frac{\beta}{1-\mu}\underline{b} \quad (10.111)$$

**QED**

**Claim 33** *Eliminating 2-node cycles*

$$\begin{array}{ccc}
 \begin{array}{ccccc}
 \begin{array}{c} a \\ \downarrow \alpha \\ \underline{x} \end{array} & \begin{array}{c} b \\ \downarrow \beta \\ \underline{y} \end{array} & = & \begin{array}{ccccc}
 \begin{array}{c} a \\ \downarrow \frac{\alpha}{1-\mu\nu} \\ \underline{x} \end{array} & \begin{array}{c} \frac{\mu\alpha}{1-\mu\nu} \\ \diagup \\ \begin{array}{c} b \\ \downarrow \frac{\beta}{1-\mu\nu} \\ \underline{y} \end{array} \end{array} & & 
 \end{array} & (10.112)
 \end{array}$$

**proof:** From the left hand diagram,

$$\begin{cases} \nu\underline{y} + \alpha\underline{a} = \underline{x} \\ \beta\underline{b} + \mu\underline{x} = \underline{y} \end{cases} \quad (10.113)$$

Hence,

$$\begin{bmatrix} 1 & -\nu \\ -\mu & 1 \end{bmatrix} \begin{bmatrix} \underline{x} \\ \underline{y} \end{bmatrix} = \begin{bmatrix} \alpha\underline{a} \\ \beta\underline{b} \end{bmatrix} \quad (10.114)$$

But

$$\begin{bmatrix} 1 & -\nu \\ -\mu & 1 \end{bmatrix}^{-1} = \frac{1}{1-\mu\nu} \begin{bmatrix} 1 & \nu \\ \mu & 1 \end{bmatrix} \quad (10.115)$$

so

$$\begin{bmatrix} \underline{x} \\ \underline{y} \end{bmatrix} = \frac{1}{1-\mu\nu} \begin{bmatrix} 1 & \nu \\ \mu & 1 \end{bmatrix} \begin{bmatrix} \alpha\underline{a} \\ \beta\underline{b} \end{bmatrix} \quad (10.116)$$

**QED**

We could continue by showing how to eliminate cycles with 3, 4 ... cycle nodes, but the pattern is clear. If there are  $N$  cycle nodes  $\underline{l}_1, \underline{l}_2, \dots, \underline{l}_N$ , then any arrow  $\underline{a} \rightarrow \underline{l}_{k_0}$  in the feedback graph is replaced by  $N$  arrows  $\underline{a} \rightarrow \underline{l}_k$  for  $k = 1, 2, \dots, N$  in the non-feedback graph. Let  $G_{cycle}$  be the product of the gains in the cycle. If  $\alpha_{k_0}$  is the gain of arrow  $\underline{a} \rightarrow \underline{l}_{k_0}$  in the feedback graph, then the gain of  $\underline{a} \rightarrow \underline{l}_k$  in the non-feedback graph equals the product of the gains in the path  $\underline{a} \xrightarrow{\alpha_{k_0}} \underline{l}_{k_0} \rightarrow \dots \rightarrow \underline{l}_k$  divided by  $1 - G_{cycle}$ .

SF graphs with feedback cycles can be used to represent a general system of  $N$  linear equations with  $N$  unknowns (i.e.  $y = Cx$ , where  $C$  is an  $N \times N$  matrix). Fig.10.6 shows an SF graph that does this for  $N = 3$ .

In Fig.10.6,

$$\begin{aligned} \underline{x}_1 &= (c_{11} + 1)\underline{x}_1 + c_{12}\underline{x}_2 + c_{13}\underline{x}_3 - \underline{y}_1 \\ \underline{x}_2 &= c_{21}\underline{x}_1 + (c_{22} + 1)\underline{x}_2 + c_{23}\underline{x}_3 - \underline{y}_2 \\ \underline{x}_3 &= c_{31}\underline{x}_1 + c_{32}\underline{x}_2 + (c_{33} + 1)\underline{x}_3 - \underline{y}_3 \end{aligned} \quad (10.117)$$

so

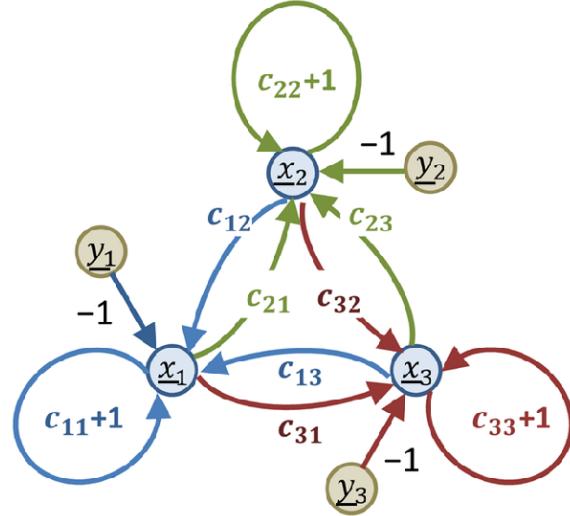


Figure 10.6: SF graph that represents a general system of 3 linear equations with 3 unknowns.

$$\begin{bmatrix} \underline{y}_1 \\ \underline{y}_2 \\ \underline{y}_3 \end{bmatrix} = \begin{bmatrix} c_{11} & c_{12} & c_{13} \\ c_{21} & c_{22} & c_{23} \\ c_{31} & c_{32} & c_{33} \end{bmatrix} \begin{bmatrix} \underline{x}_1 \\ \underline{x}_2 \\ \underline{x}_3 \end{bmatrix} \quad (10.118)$$

$$y = Cx \quad (10.119)$$

Note that the self-feedback cycles in Fig.10.6 can be eliminated using the technique described in Claim 32.

# Chapter 11

## Copula

This chapter is based on Refs.[104] and [7].

A copula in architecture is a domed roof. Here we will discuss a copula in Statistics. Copulas are probably called this in Statistics because their probability density resembles a dome when their domain is the real plane  $\mathbb{R}^2$ . Furthermore, the word “copula” means “connector” or “coupler” in Latin, and both, the copula in Architecture and the one in Statistics, connect the sides (or marginals in the Statistics case) of a geometrical shape.

Let  $x = [x_i]_{i=1}^n \in \mathbb{R}$  be an  $n$  dimensional column vector. Given a probability distribution (actually, a density)  $P(x)$ , we will refer to  $P(\underline{x}_i = x_i)$  for all  $i$  as its **marginals** and to  $P(\underline{x}_i \leq x_i)$  for all  $i$  as its **cumulative marginals** or **c-marginals** for short. This is normally referred to as the **CDF (cumulative distribution function)** of  $\underline{x}_i$ .

Suppose you know the marginals  $P(x_i)$  of  $P(x)$ , but you don't know  $P(x)$  itself. There are infinitely many possible  $P(x)$ 's with those marginals. Informally speaking, a **copula** is one of those  $P(x)$ , a smooth one. The dimension  $n$  of the domain of the copula, is referred to as the **copula dimension**. See Figs. 11.1 and 11.2 for examples of 2-dimensional copulas.

Let  $x = [x_i]_{i=1}^n \in \mathbb{R}^n$  and  $u = [u_i]_{i=1}^n \in \mathbb{R}^n$  be  $n$  dimensional column vectors. Henceforth, will denote the c-marginals of  $\underline{x}_i$  by  $\Phi_{\underline{x}_i}$

$$\Phi_{\underline{x}_i}(x_i) = P(\underline{x}_i \leq x_i) \quad (11.1)$$

and the generalization of this map to vector arguments by  $\Phi_{\underline{x}}$ :

$$x = \begin{bmatrix} x_1 \\ x_2 \\ \dots \\ x_n \end{bmatrix}, \quad \Phi_{\underline{x}}(x) = \begin{bmatrix} \Phi_{\underline{x}_1}(x_1) \\ \Phi_{\underline{x}_2}(x_2) \\ \dots \\ \Phi_{\underline{x}_n}(x_n) \end{bmatrix} \quad (11.2)$$

More precisely, a copula in Statistics is defined as follows. A **copula density** is a probability density  $P(u)$  such that (see Fig.11.3)

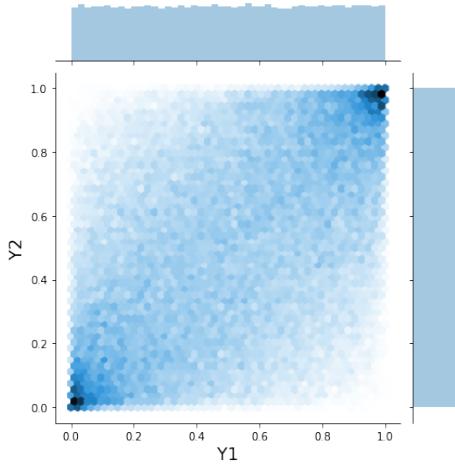


Figure 11.1: Contour plot of a 2-dimensional copula with uniform marginals

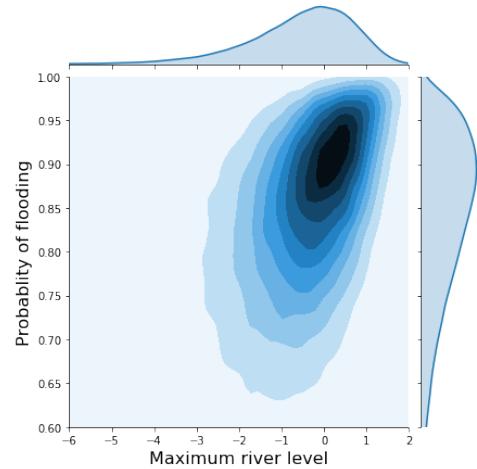


Figure 11.2: Contour plot of a 2-dimensional copula with skewed bell-shaped marginals.

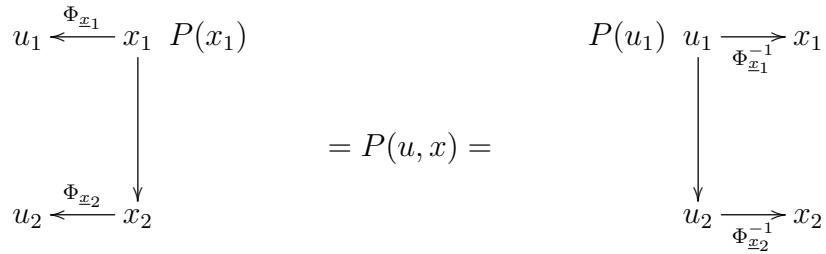


Figure 11.3: Graphical representation of Eq.(11.4) for  $n = 2$ .  $\Phi_{\underline{x}_i}(x_i) = P(\underline{x}_i \leq x_i)$  is the CDF of  $\underline{x}_i$ , and we define  $u_i = \Phi_{\underline{x}_i}(x_i)$

$$\underbrace{P(u|x)}_{\prod_{i=1}^n \delta(u_i - \Phi_{\underline{x}_i}(x_i))} \quad P(x) = P(u, x) = \underbrace{P(x|u)}_{\prod_{i=1}^n \delta(x_i - \Phi_{\underline{x}_i}^{-1}(u_i))} \quad P(u) \quad (11.3)$$

$$P(\underline{x} = x) = \boxed{\left[ \underbrace{P(u = u)}_{\text{copula density}} \right]_{u = \underbrace{\Phi_{\underline{x}}(x)}_{\text{c-marginals}}}} \quad (11.4)$$

A **copula**  $C(u)$  is defined as the CDF of its copula density.

$$C(u) = \prod_{i=1}^n \left\{ \int_{-\infty}^{u_i} du'_i \right\} P(\underline{u} = u') \quad (11.5)$$

$$= \underbrace{P(\forall i : \underline{u}_i \leq u_i)}_{\stackrel{\text{def}}{=} P(\underline{u} \leq u)} \quad (11.6)$$

$$\partial_{u_1} \partial_{u_2} \dots \partial_{u_n} C(u) = P(u) \quad (11.7)$$

There are copulas that are well-defined by Eq.(11.6), but not differentiable, so, technically, without smoothing, their copula density does not exist. For this reason, if possible, it is always best and most general to state copula results in terms of CDFs, instead of probability densities. For example, the boxed Eq.(11.4) stated in terms of CDFs, is

$$P(\underline{x} \leq x) = \left[ \underbrace{P(\underline{u} \leq u)}_{\text{copula}} \right]_{u=\underbrace{\Phi_{\underline{x}}(x)}_{\text{c-marginals}}} \quad (11.8)$$

**Claim 34**  $\underline{u}_i = \Phi_{\underline{x}_i}(\underline{x}_i)$  implies that the marginal  $P(u_i) = 1$  is a uniform distribution on  $[0, 1]$ .

**proof:**

$$\underline{u}_i = \Phi_{\underline{x}_i}(\underline{x}_i) = P(\underline{x}_i \leq \underline{x}_i) = 1 \quad (11.9)$$

If that doesn't convince you, here is another proof.

$$P(\underline{u}_i \leq u_i) = P(\Phi_{\underline{x}_i}(\underline{x}_i) \leq u_i) \quad (11.10)$$

$$= P(\underline{x}_i \leq \Phi_{\underline{x}_i}^{-1}(u_i)) \quad (11.11)$$

$$= \Phi_{\underline{x}_i} \left( \Phi_{\underline{x}_i}^{-1}(u_i) \right) \quad (11.12)$$

$$= u_i \quad (11.13)$$

Hence,

$$P(\underline{u}_i = u_i) = \frac{\partial}{\partial u_i} \int_{-\infty}^{u_i} du'_i P(\underline{u}_i = u'_i) \quad (11.14)$$

$$= \frac{\partial P(\underline{u}_i \leq u_i)}{\partial u_i} \quad (11.15)$$

$$= 1 \quad (11.16)$$

**QED**

## 11.1 Examples

In the following examples,  $n = 2$ , and we sometimes substitute  $(u_1, u_2) = (u, v)$ ,  $(x_1, x_2) = (x, y)$ .

### 1. $\underline{x}_1$ and $\underline{x}_2$ are independent

If  $\underline{x}_1$  and  $\underline{x}_2$  are independent,  $\underline{u}_1$  and  $\underline{u}_2$  are too. Hence,

$$C(u_1, u_2) = P(\underline{u}_1 \leq u_1, \underline{u}_2 \leq u_2) \quad (11.17)$$

$$= P(\underline{u}_1 \leq u_1)P(\underline{u}_2 \leq u_2) \quad (11.18)$$

$$= u_1 u_2 \quad (11.19)$$

$$C(\Phi_{\underline{x}}(x)) = \Phi_{\underline{x}_1}(x_1)\Phi_{\underline{x}_2}(x_2) \quad (11.20)$$

$$\partial_{x_1} \partial_{x_2} C(\Phi_{\underline{x}}(x)) = \partial_{x_1} \partial_{x_2} \Phi_{\underline{x}_1}(x_1)\Phi_{\underline{x}_2}(x_2) \quad (11.21)$$

$$P(x) = P(x_1)P(x_2) \quad (11.22)$$

### 2. $\underline{x}_2 = \alpha \underline{x}_1$ for some $\alpha > 0$

If  $\underline{x}_2 = \alpha \underline{x}_1$  for some parameter  $\alpha > 0$ , then

$$u_1 = \Phi_{\underline{x}_1}(x_1) \quad (11.23)$$

$$= P(\underline{x}_1 \leq x_1) \quad (11.24)$$

$$= P(\alpha x_1 \leq \alpha x_1) \quad (11.25)$$

$$= P(\underline{x}_2 \leq x_2) \quad (11.26)$$

$$= \Phi_{\underline{x}_2}(x_2) \quad (11.27)$$

$$= u_2 \quad (11.28)$$

$$C(u_1, u_2) = P(\underline{u}_1 \leq u_1, \underline{u}_2 \leq u_2) \quad (11.29)$$

$$= P(\underline{u}_1 \leq u_1, u_1 \leq u_2) \quad (11.30)$$

$$= P(\underline{u}_1 \leq \min(u_1, u_2)) \quad (11.31)$$

$$= \min(u_1, u_2) \quad (11.32)$$

3.  $\underline{x}_2 = -\alpha \underline{x}_1$  for some  $\alpha > 0$

If  $\underline{x}_2 = -\alpha \underline{x}_1$  for some parameter  $\alpha > 0$ , then

$$u_1 = \Phi_{\underline{x}_1}(x_1) \quad (11.33)$$

$$= P(\underline{x}_1 \leq x_1) \quad (11.34)$$

$$= P(-\alpha \underline{x}_1 > -\alpha x_1) \quad (11.35)$$

$$= P(\underline{x}_2 > x_2) \quad (11.36)$$

$$= 1 - \Phi_{\underline{x}_2}(x_2) \quad (11.37)$$

$$= 1 - u_2 \quad (11.38)$$

$$C(u_1, u_2) = P(\underline{u}_1 \leq u_1, \underline{u}_2 \leq u_2) \quad (11.39)$$

$$= P(\underline{u}_1 \leq u_1, 1 - \underline{u}_1 \leq u_2) \quad (11.40)$$

$$= P(1 - u_2 \leq \underline{u}_1 \leq u_1) \quad (11.41)$$

$$= \max(u_1 - (1 - u_2), 0) \quad (\text{Area of rectangle } [1 - u_2, u_1] \times [0, 1]) \quad (11.42)$$

The Fréchet–Hoeffding bounds are lower and upper bounds for any  $n$ -dim copula. For  $n = 2$ , these bounds are

$$\underbrace{\max(u_1 + u_2 - 1, 0)}_{\text{case } \underline{x}_2 = -\alpha \underline{x}_1} \leq C(u_1, u_2) \leq \underbrace{\min(u_1, u_2)}_{\text{case } \underline{x}_2 = \alpha \underline{x}_1} \quad (11.43)$$

#### 4. Gaussian copula

Recall that the  $n$ -dimensional multivariate Normal Distribution has a probability density

$$\mathcal{N}(x; \mu, \Sigma) = \frac{\exp\left(-\frac{1}{2}(x - \mu)^T \Sigma^{-1} (x - \mu)\right)}{\sqrt{(2\pi)^n \det(\Sigma)}} \quad (11.44)$$

where  $\mu = E[\underline{x}]$  and  $\Sigma = \langle \underline{x}^T, \underline{x} \rangle$ . For  $n = 2$ ,

$$\Sigma = \langle \underline{x}^T, \underline{x} \rangle \quad (11.45)$$

$$= \begin{bmatrix} \sigma_{\underline{x}_1}^2 & \rho \sigma_{\underline{x}_1} \sigma_{\underline{x}_2} \\ \rho \sigma_{\underline{x}_1} \sigma_{\underline{x}_2} & \sigma_{\underline{x}_2}^2 \end{bmatrix} \quad (\sigma_{\underline{x}_i} = \sqrt{\langle \underline{x}_i, \underline{x}_i \rangle} \text{ and } \rho = \frac{\langle \underline{x}_1, \underline{x}_2 \rangle}{\sigma_{\underline{x}_1} \sigma_{\underline{x}_2}}) \quad (11.46)$$

$$= \underbrace{\begin{bmatrix} 1 & \rho \\ \rho & 1 \end{bmatrix}}_{\stackrel{\text{def}}{=} \Sigma_\rho} \quad (\text{Assume } \sigma_{\underline{x}_1} = \sigma_{\underline{x}_2} = 1) \quad (11.47)$$

$$\Sigma_{\rho}^{-1} = \frac{1}{1-\rho^2} \begin{bmatrix} 1 & -\rho \\ -\rho & 1 \end{bmatrix} \quad (11.48)$$

$$\mathcal{N}(x; \mu = 0, \Sigma = \Sigma_{\rho}) = \frac{\exp\left(-\frac{1}{2(1-\rho^2)}x^T \begin{bmatrix} 1 & -\rho \\ -\rho & 1 \end{bmatrix} x\right)}{\sqrt{(2\pi)^2(1-\rho^2)}} \quad (11.49)$$

$$= \frac{\exp\left(-\frac{1}{2(1-\rho^2)}(x_1^2 + x_2^2 - 2\rho x_1 x_2)\right)}{\sqrt{(2\pi)^2(1-\rho^2)}} \quad (11.50)$$

For each  $i$ , assume the marginal of  $\underline{x}_i$  is a Normal distribution with zero mean and unit variance:

$$P(x_i) = \mathcal{N}(x_i; \mu = 0, \sigma = 1) = \frac{\exp\left(-\frac{x_i^2}{2}\right)}{\sqrt{2\pi}} \quad (11.51)$$

Then

$$\Phi_{\underline{x}_i}(x_i) = P(\underline{x}_i \leq x_i) = \frac{1}{2} \left[ 1 + \operatorname{erf}\left(\frac{x_i}{\sqrt{2}}\right) \right] \quad (11.52)$$

and

$$\Phi_{\underline{x}_i}^{-1}(u_i) = \sqrt{2} \operatorname{erf}^{-1}(1 - 2u_i) \quad (11.53)$$

Besides assuming Gaussian marginals, we will assume a Gaussian copula density

$$C(u) = \prod_{i=1}^2 \left\{ \int_{-\infty}^{u_i} du'_i \right\} P(u') \quad (11.54)$$

where

$$P(u) = \mathcal{N}(x = \Phi_{\underline{x}}^{-1}(u); \mu = 0, \Sigma = \Sigma_{\rho}) \quad (11.55)$$

Hence,

$$P(x) = P(\underline{u} = \Phi_{\underline{x}}(x)) \quad (11.56)$$

$$= \mathcal{N}(x; \mu = 0, \Sigma = \Sigma_{\rho}) \quad (11.57)$$

# Chapter 12

## Counterfactual Reasoning

### 12.1 The 3 Rungs of Causal AI

According to Judea Pearl, there are 3 rungs in the ladder of causal AI. These are (as I see them):

1. **Observing Passively. Answering “What next?”:** Collecting data and fitting curves to it, without any plan designed to investigate Nature’s causal connections. Predicting the future.
2. **Doing causal experiments. Answering “Why?”:** Doing experiments consciously designed to elucidate Nature’s causal connections. Even cats do this!, but current AI doesn’t.
3. **Imagining counterfactual situations, Analogizing. Answering “What if?”:** Imagining gedanken experiments to further understand Nature’s causal connections, and to decide what future courses of action are more likely to succeed, even if those courses of action are unprecedented, and have never been taken before. Making predictions about events that have never happened (“counterfactuals”) is a very Bayesian concern, well out of the purview of frequentists. Nevertheless, humans do such “analogizing” all the time to great advantage. It becomes possible if there is some foreign but similar data that can be transported (transplanted, applied) to the situation of interest.

We will use the term **intervention operator** (or simply “intervention”) to refer to an operator that maps a bnet to another bnet. In Chapter 21, we introduced an intervention operator called the **do operator**  $\mathcal{D}_{\underline{x}=x}$  (this is our notation for what Pearl symbolizes by  $do(\underline{x}) = x$ ). The study of counterfactuals requires that we introduce a new kind of intervention operator that we will call an **imagine operator**, and denote by  $\mathcal{I}_{\underline{x} \rightarrow y}$ . These 2 types of intervention operators will be defined in subsequent sections of this chapter. Usage of the do operator characterizes rung 2, and usage of the imagine operator characterizes rung 3.

Chapter 56 on message passing is about rung 1. Chapter 21 on Do Calculus is about rung 2. This chapter is dedicated to rung 3.

Judea Pearl is fond of discussing rung 3 solely in terms of SCM.<sup>1</sup> In this chapter, we define rung 3 without using SCM, using solely bnets. This gives a more general version of rung 3, because SCM are a subset of bnets.

## 12.2 Do operator

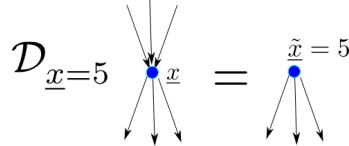


Figure 12.1: Action of “do” operator  $\mathcal{D}_{\underline{x}=5}$  on node  $\underline{x}$ .

The do operator  $\mathcal{D}_{\underline{x}=5}$  is defined graphically in Fig.12.1. The TPM, printed in blue, for node  $\tilde{\underline{x}}$  of Fig.12.1, is as follows.<sup>2</sup>

$$P(\tilde{\underline{x}}; 5) = \delta(5, \tilde{\underline{x}}) \quad (12.1)$$

The do operator  $\mathcal{D}_{\underline{x}=5}$  amputates the incoming arrows of node  $\underline{x}$  and sets the TPM of the new root node  $\tilde{\underline{x}}$  to a delta function  $\delta(\tilde{\underline{x}}, 5)$  (or some state of  $\underline{x}$  other than 5). Sometimes we call the new node  $\mathcal{D}\underline{x}$  instead of  $\tilde{\underline{x}}$ .

The uses of the do operator are discussed in detail in Chapter 21.

## 12.3 Imagine operator

The imagine operator  $\mathcal{I}_{\underline{x} \rightarrow y}(5)$  is defined graphically in Fig.12.2. Note that Fig.12.2 actually defines two types of imagine operators, the one with an argument:  $\mathcal{I}_{\underline{x} \rightarrow y}(5)$ , and the one without an argument:  $\mathcal{I}_{\underline{x} \rightarrow y}$ . The TPMs, printed in blue, for various nodes in Fig.12.2, are as follows.

- For  $\mathcal{I}_{\underline{x} \rightarrow y}(\tilde{\underline{x}})G$

$$P(y|\tilde{\underline{x}}, a.) = P(y|\underline{x} = \tilde{\underline{x}}, a.) \quad (12.2)$$

---

<sup>1</sup>SCM are what we call DEN. DEN (deterministic systems with external noise) are discussed in Chapter 48.

<sup>2</sup>The “;5” in the distribution indicates that 5 is a frequentist parameter of the distribution.

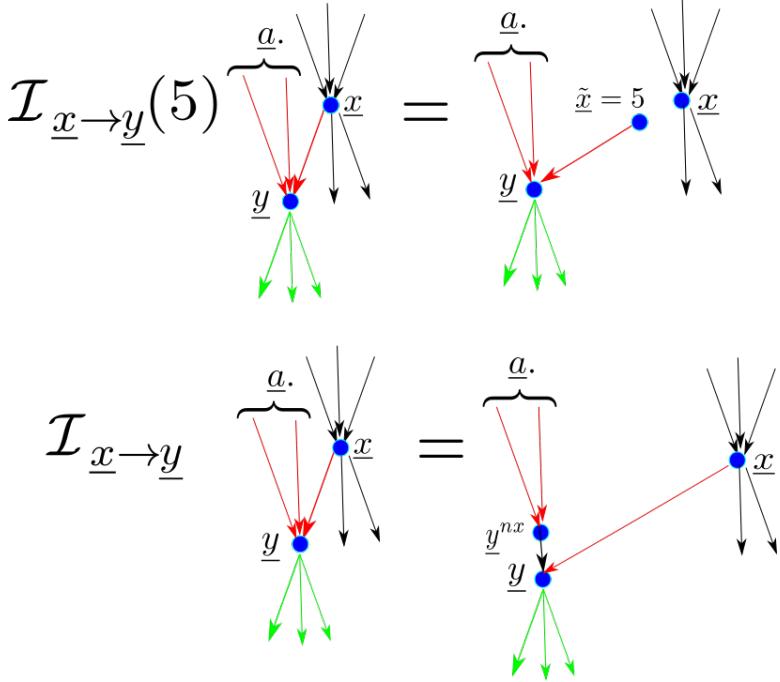


Figure 12.2: Action of “imagine” operators  $\mathcal{I}_{\underline{x} \rightarrow \underline{y}}(5)$  and  $\mathcal{I}_{\underline{x} \rightarrow \underline{y}}$  on arrow  $\underline{x} \rightarrow \underline{y}$ . In this figure,  $y^{nx} = [y(x)]_{\forall x \in S_{\underline{x}}}$ , where  $nx = |S_{\underline{x}}|$  and  $S_{\underline{x}}$  is the set of states of node  $\underline{x}$ .

$$P(\tilde{x}; 5) = \delta(\tilde{x}, 5) \quad (12.3)$$

- For  $\mathcal{I}_{\underline{x} \rightarrow \underline{y}} G$

$$P(y^{nx}|a.) = \prod_{\tilde{x}} P(y(\tilde{x}) = y(\tilde{x})|a.) \quad (12.4)$$

$$P(y|y^{nx}, x) = \delta(y, y(x)) \quad (12.5)$$

The imagine operators  $\mathcal{I}_{\underline{x} \rightarrow \underline{y}}(5)$  and  $\mathcal{I}_{\underline{x} \rightarrow \underline{y}}$  operate on an arrow whereas the  $\mathcal{D}$  operator operates on a node.  $\mathcal{I}_{\underline{x} \rightarrow \underline{y}}(5)$  deletes arrow  $\underline{x} \rightarrow \underline{y}$  and creates a new root node  $\tilde{\underline{x}}$  and a new arrow  $\tilde{\underline{x}} \rightarrow \underline{y}$ . Sometimes we call the new node  $\mathcal{I}_{\underline{y} \rightarrow \underline{x}}$  instead of  $\tilde{\underline{x}}$ .  $\mathcal{I}_{\underline{x} \rightarrow \underline{y}}$  creates a new node  $y^{nx}$  and an arrow  $y^{nx} \rightarrow \underline{y}$ .

Fig.12.3 shows how the imagine operator arises in Potential Outcomes (PO) theory. PO theory is discussed extensively in Chapter 72. As you can see, PO theory only uses a limited version of the 3 rungs of causal inference, because it doesn’t use the do-operator, and it only uses one of 2 possible types of imagine operators. Furthermore, it assumes a very limited triangular DAG.

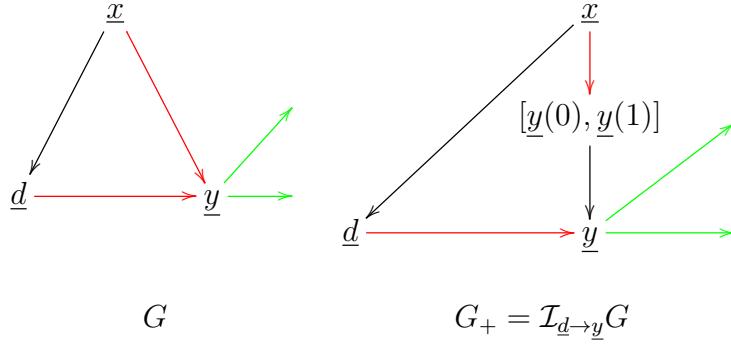


Figure 12.3: How imagine operator arises in Potential Outcomes (PO) theory.

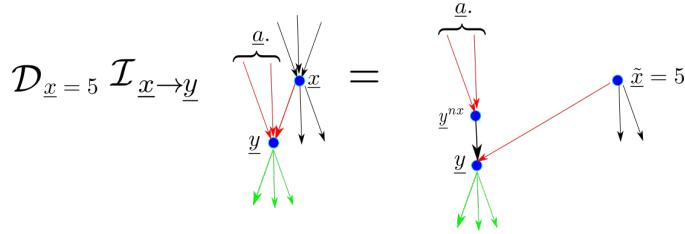


Figure 12.4:  $\mathcal{D}_{\underline{x}=5}\mathcal{I}_{\underline{x} \rightarrow \underline{y}}G$  gives a connection between do and imagine operators.

Fig.12.4 gives a connection between do and imagine operators. We see from that figure that for  $\mathcal{D}_{\underline{x}=\tilde{x}}\mathcal{I}_{\underline{x} \rightarrow \underline{y}}G$ , we have<sup>3</sup>

$$P(y|\mathcal{D}\underline{x} = \tilde{x}, a.) = P(\underline{y}(\tilde{x}) = y|a.) \quad (12.6)$$

One can define a **do-imagine-calculus** whose objective is to express probabilities such as  $P(\underline{y}|\mathcal{D}\underline{r} = r, \mathcal{I}\underline{b}\underline{s} = s, t)$  in terms of observable probabilities that do not contain any do or imagine operators in them. As with Do Calculus, this reduction is not always possible, and we say a probability is  **$\mathcal{D}$ -identifiable**,  **$\mathcal{I}$ -identifiable** or  **$\mathcal{DI}$ -identifiable** if it can be expressed without do, imagine or both operators.

In causal inference, we often consider “counterfactual” random variables  $\underline{y}(0) \in \{0, 1\}$  and  $\underline{y}(1) \in \{0, 1\}$ . They are called counterfactual variables because one of the 2 variables refers to an event that has occurred, whereas the other variable refers to a “counterfactual event”, i.e., an event that has never occurred. For some patients,  $\underline{y}(0)$  has a value but  $\underline{y}(1)$  doesn’t. For other patients, the opposite is the case. There is some disagreement in the community as to which algorithms perform rung 3 operations, and which don’t. This is the convention used in this book. We will say

---

<sup>3</sup>In the notation favored by Pearl, Eq.(12.6) would be

$$P(y|do(X) = \tilde{x}, a.) = P(Y_{\tilde{x}} = y|a.)$$

rung 3 operations are being performed if the counterfactual variables  $\underline{y}(0)$  and  $\underline{y}(1)$  are being used, or, equivalently, if a bnet is being used that includes nodes  $\underline{y}(0)$ , and  $\underline{y}(1)$  that were produced by an imagine operator. Potential Outcomes (PO) theory (see Chapter 72) qualifies as rung 3 according to this convention. However, note that PO theory only does the bare minimum to reach rung 3. In PO theory, one usually evaluates  $ATE = E[\underline{y}(1)] - E[\underline{y}(0)]$ , which entails calculating  $P(\underline{y}(0))$  and  $P(\underline{y}(1))$ . Pearl has extended the reach of rung 3 much further by calculating expected values that require knowledge of the joint distribution  $P(\underline{y}(0), \underline{y}(1))$ .

# Chapter 13

## Cross-Validation

This chapter is based on Ref.[106].

Cross-Validation (CV) is a method of calculating the “**out-of-training-set**” (**OOTs**) error for a classifier. What this means is that the classifier is trained on a training set, and its propensity to err is evaluated on a set different from the training set.

In  **$k$ -fold CV**, the most common CV method, and the only one we will discuss in this chapter, one partitions a dataset into  $k$  disjoint datasets of equal length. One uses  $k - 1$  of those sub-datasets to train a model, and saves the last sub-dataset to validate the model just trained. One actually rotates which of the  $k$  sub-datasets is used for validation purposes, and calculates  $k$  validation errors  $\mathcal{E}_j$  for  $j = 0, 1, \dots, k - 1$ . Then one averages over the  $\mathcal{E}_j$  to obtain a final OOTS error  $\mathcal{E}$ .

CV strongly resembles Jackknife Resampling (JR) (see Chapter 42), but in JR the validation sub-dataset is never used for anything, whereas in CV, it is used for validation purposes, to calculate an OOTS error.

Next, we will explain  $k$ -fold CV more explicitly, using equations and a bnet.

Let  $L = [0, 1, 2, \dots, nsam - 1]$  be a list of individuals (samples) in a population. In this chapter, we will use the notation  $A^\sigma = A[\sigma]$  and  $\vec{A} = [A^\sigma : \sigma \in L]$  for a list (vector, 1-D array) indexed by  $L$ . We will refer to  $DS = (\vec{x}, \vec{y})$  where  $x^\sigma \in S_x$ ,  $y^\sigma \in S_y$ , as a dataset. If  $L_j$  is a list (possibly with duplicate items) such that  $set(L_j) \subset set(L)$ , then define  $DS_j = (\vec{x}, \vec{y})_{L_j} = ((x^\sigma)_{\sigma \in L_j}, (y^\sigma)_{\sigma \in L_j})$ . We will refer to  $DS_j$  as the **restriction of**  $(\vec{x}, \vec{y})$  **to**  $L_j$ .

Let  $J = \{0, 1, 2, \dots, nj - 1\}$ .

Define a **training list(TL), validation list(VL) pair**  $(TL, VL)$  to be a pair of lists such that  $set(TL)$  and  $set(VL)$  are disjoint subsets of  $set(L)$ . Let  $(TL_j, VL_j)$  for  $j \in J$  be  $nj$  such TL-VL pairs.

Fig.13.1 shows the TL-VL pairs that are used when doing  $k$ -fold CV. In that figure,  $k = nj = 4$ . As you can see, in  $k$ -fold CV, one chooses  $nj = k$  list pairs  $(TL_j, VL_j)$  such that all individuals  $\sigma \in L$  appear exactly once, in either  $TL_j$  or  $VL_j$ , but not in both.

We will refer to a function  $Y : S_x \rightarrow S_c$  as a classifier. It maps a vector of

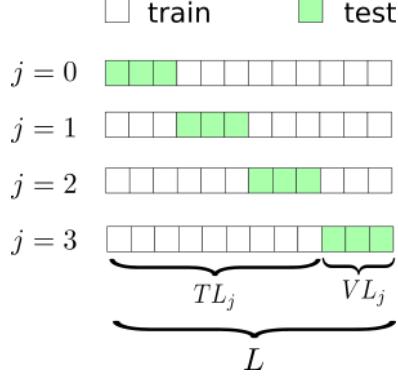


Figure 13.1: 4-fold CV with  $|L| = 12$ . For all  $j$ ,  $|VL_j| = 3$  and  $|TL_j| = 9$ . All individuals  $\sigma \in L$  appear exactly once, in either  $TL_j$  or  $VL_j$ , but not in both.

features  $x$  to a class  $c$ . Let  $Y_j$  for  $j \in J$  denote  $n_j$  classifiers.

If  $Y_j : S_{\underline{x}} \rightarrow S_c$  and  $S_c$  is a discrete set ("categorical"), then define the **OOTs error for the  $j$ th classifier** as:

$$\mathcal{E}_j = \frac{1}{|VL_j|} \sum_{\sigma \in VL_j} \mathbb{1}(y^\sigma \neq Y_j(x^\sigma)) . \quad (13.1a)$$

On the other hand, if  $S_c = \mathbb{R}$ , it makes more sense to define  $\mathcal{E}_j$  as a mean square error:

$$\mathcal{E}_j = \frac{1}{|VL_j|} \sum_{\sigma \in VL_j} (y^\sigma - Y_j(x^\sigma))^2 . \quad (13.1b)$$

Finally, define the **final OOTs error** as

$$\mathcal{E} = \frac{1}{|J|} \sum_{j \in J} \mathcal{E}_j . \quad (13.2)$$

Fig.13.2 gives a bnet that represents the CV algorithm. The TPMs, printed in blue, for the bnet Fig.13.2, are as follows:

$$P((\vec{x}, \vec{y})_{TL_j} | (\vec{x}, \vec{y})) = \mathbb{1}(\text{ } (\vec{x}, \vec{y})_{TL_j} \text{ = restriction of } (\vec{x}, \vec{y}) \text{ to } TL_j. ) \quad (13.3)$$

$$P((\vec{x}, \vec{y})_{VL_j} | (\vec{x}, \vec{y})) = \mathbb{1}(\text{ } (\vec{x}, \vec{y})_{VL_j} \text{ = restriction of } (\vec{x}, \vec{y}) \text{ to } VL_j. ) \quad (13.4)$$

$$P(Y_j | (\vec{x}, \vec{y})_{TL_j}) = \mathbb{1}(\text{ } Y_j \text{ = classifier trained with } (\vec{x}, \vec{y})_{TL_j} ) \quad (13.5)$$

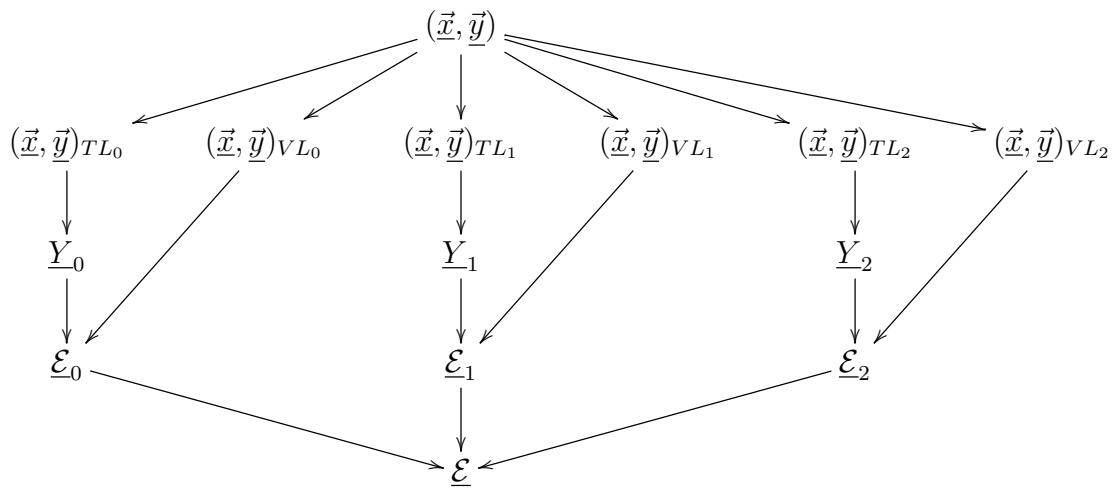


Figure 13.2: Bnet for 3-fold CV.

$$P(\mathcal{E}_j | Y_j, (\vec{x}, \vec{y})_{VL_j}) = \mathbb{1}(\mathcal{E}_j = \text{defined by Eqs.(13.1).}) \quad (13.6)$$

$$P(\mathcal{E} | (\mathcal{E}_j)_{j \in J}) = \mathbb{1}(\mathcal{E} = \text{defined by Eq.(13.2).}) \quad (13.7)$$

## Chapter 14

### DAG Extraction From Text (DEFT)

See my paper and software Ref.[74].

# Chapter 15

## Dataset Shift and Batch Normalization

In this chapter, we will represent Linear Regression (LR) as follows. We list a dataset; i.e., a set of tuples indexed by the individuals  $\sigma$  of a population  $\Sigma$  such that  $|\Sigma| = nsam$ . The independent variables of the LR (i.e.,  $x^\sigma$ ) are unboxed and the dependent variable (a.k.a. target feature) (i.e.,  $y^\sigma$ ) is shown inside a box. Then we show an arrow with the superscript “LR-fit”, followed by the fit function obtained by performing the LR.

$$\{(\sigma, x^\sigma = [x_i^\sigma], \boxed{y^\sigma}) : \sigma \in \Sigma\} \xrightarrow{\text{LR-fit}} \hat{y}(x) = \alpha + \sum_i x_i \beta_i \quad (15.1)$$

Analogously, we represent Supervised Machine Learning (ML) as follows.

$$\{(\sigma, x^\sigma, \boxed{y^\sigma}) : \sigma \in \Sigma\} \xrightarrow{\text{ML-fit}} \hat{y}(x) \quad (15.2)$$

When doing ML, we partition the full population  $\Sigma_{full}$  into two disjoint sets, the **training set**  $\Sigma_{train} = \Sigma(\underline{s} = 0) = \Sigma$  and the **testing set**  $\Sigma_{test} = \Sigma(\underline{s} = 1) = \Sigma^*$ . Then we do two ML fits:

$$\begin{aligned} \text{training: } & \{(\sigma, x^\sigma, \boxed{y^\sigma}) : \sigma \in \Sigma\} \xrightarrow{\text{ML-fit}} \hat{y}(x) \\ \text{testing: } & \{(\sigma, x^\sigma, \boxed{y^\sigma}) : \sigma \in \Sigma^*\} \xrightarrow{\text{ML-fit}} \hat{y}^*(x) \end{aligned} \quad (15.3)$$

Ideally,  $\hat{y}(x)$  and  $\hat{y}^*(x)$ , will be almost equal for all  $x$ . Dataset shift occurs when this is not the case. Equivalently, let

$$\begin{aligned} P_{train}(x, y) &= P(x, y | \underline{s} = 0) = P(x, y) \\ P_{test}(x, y) &= P(x, y | \underline{s} = 1) = P^*(x, y) \end{aligned} \quad (15.4)$$

We say there is a **dataset shift** if

$$P(x, y) \neq P^*(x, y) \quad (15.5)$$

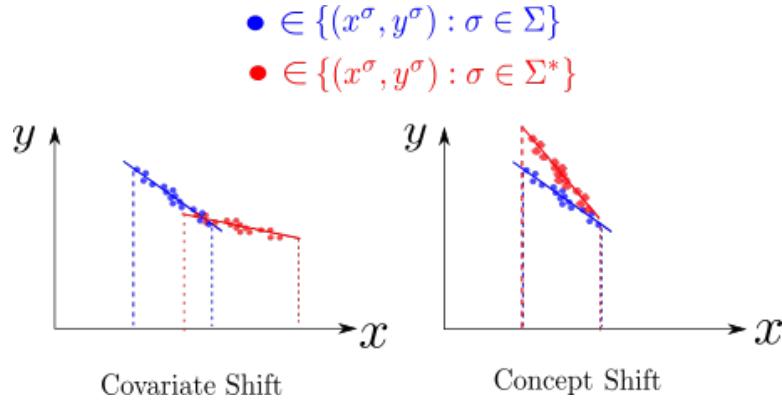


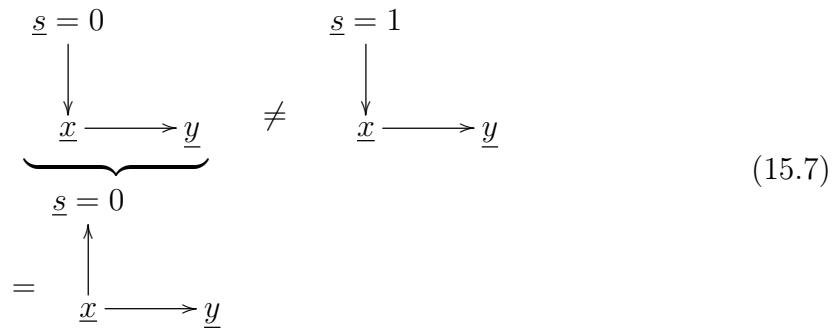
Figure 15.1: For Linear Regression, 2 types of dataset shift: covariate shift and concept shift.

## 15.1 Covariate Shift

We say there is a **covariate shift** if (see Fig.15.1)

$$P(y|x) = P^*(y|x) \text{ but } P(x) \neq P^*(x) \quad (15.6)$$

This can be represented in terms of bnets as follows<sup>1</sup>



## 15.2 Concept Shift

We say there is a **concept shift** if (see Fig.15.1)

$$P(y|x) \neq P^*(y|x) \text{ but } P(x) = P^*(x) \quad (15.8)$$

This can be represented in terms of bnets as follows<sup>2</sup>

<sup>1</sup>See See Chapter 83.

<sup>2</sup>See See Chapter 83.

$$\begin{array}{ccc}
\underline{s} = 0 & & \underline{s} = 1 \\
& \searrow & \downarrow \\
& \underline{x} \longrightarrow \underline{y} & \\
& \underbrace{\quad}_{\underline{s} = 0} & \neq \\
& \uparrow & \\
& \underline{x} \longrightarrow \underline{y} &
\end{array} \tag{15.9}$$

### 15.3 Batch Normalization

Batch Normalization (BN) is a technique that is used to diminish dataset shift in Neural Nets.

Let  $h_i^{\lambda, \sigma}$  be the output, for individual  $\sigma \in \Sigma$ , of the  $i$ th node of layer  $\lambda$  of a Neural Net (NN). Using the notation of Chapter 64,

$$h_i^{\lambda, \sigma} = \mathcal{A}_i^\lambda(z_i^{\lambda, \sigma}) \tag{15.10}$$

where

$$z_i^{\lambda, \sigma} = \sum_j w_{i|j}^\lambda h_j^{\lambda-1, \sigma} + b_i^\lambda \tag{15.11}$$

Activation functions  $\mathcal{A}_i^\lambda : \mathbb{R} \rightarrow \mathbb{R}$  for NNs are discussed in Section 64.1. Suppose the population  $\Sigma$  is partitioned into disjoint batches  $\Sigma^{(b)}$  for  $b = 1, 2, \dots, B$ . Let the set of points  $\{z_i^{\lambda, \sigma} : \sigma \in \Sigma^{(b)}\}$  have mean  $\mu_i^{\lambda(b)}$  and standard deviation  $\sigma_i^{\lambda(b)}$ . For any  $z_i^{\lambda, \sigma}$  with  $\sigma \in \Sigma$ , define the BN activation function  $\mathcal{A}_{i, BN}^\lambda(\cdot)$  by

$$\mathcal{A}_{i, BN}^\lambda(z_i^{\lambda, \sigma}) = \gamma_i^\lambda \left[ \frac{z_i^{\lambda, \sigma} - \mu_i^{\lambda(b)}}{\sigma_i^{\lambda(b)}} \right] + \beta_i^\lambda \quad \text{if } \sigma \in \Sigma^{(b)}, \tag{15.12}$$

where the real valued parameters  $\gamma_i^\lambda$  and  $\beta_i^\lambda$  are learned during the optimization process. If node  $\underline{h}_i^\lambda$  of the NN has activation function  $\mathcal{A}_i^\lambda : \mathbb{R} \rightarrow \mathbb{R}$ , defined a new activation function  $\mathcal{A}_{i, new}^\lambda : \mathbb{R} \rightarrow \mathbb{R}$  by the composition of functions

$$\mathcal{A}_{i, new}^\lambda = \mathcal{A}_i^\lambda \circ \mathcal{A}_{i, BN}^\lambda \tag{15.13}$$

Hence, the BN activation function is applied after the linear transformation Eq.(15.11), but before the nonlinear transformation  $\mathcal{A}_i^\lambda$ .

Intuition on why BN diminishes dataset shift: We discussed in Section 64.1 how nonlinear activation functions have a range that is smaller than their domain. Presumably, BN helps to make the range of the activation functions even more concentrated.

# Chapter 16

## Decision Trees

This chapter is based mainly on Ref.[66].

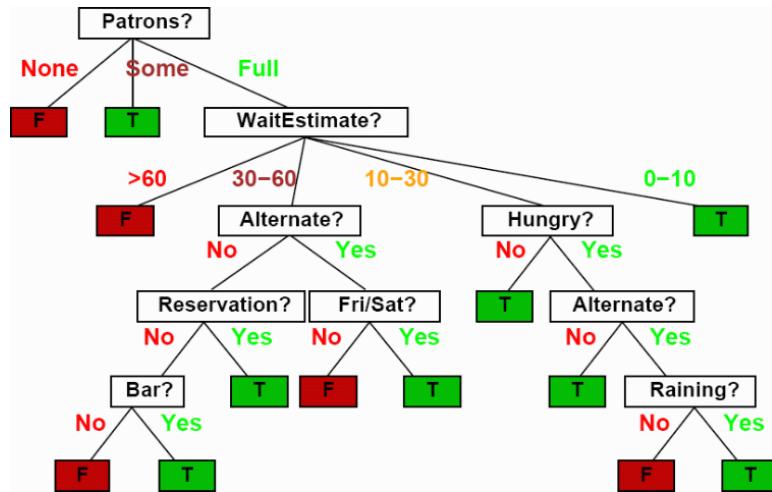


Figure 16.1: Example of dtree taken from Ref.[66]

Fig.16.1 shows a typical decision tree (dtree). This example was taken from Ref.[66], where it is analyzed in detail. As you can see, a dtree contains two main types of nodes: the non-leaf nodes, and the leaf nodes. The **non-leaf nodes** pose **questions**. In general, the **answers**<sup>1</sup> to those questions can be multiple choices with two or more choices. For each of those choices, a tree branch labeled by the choice comes down from the question node. The **leaf nodes** represent endpoints, goals, final conclusions, etc. Dtress can be viewed as classifiers. They take in a large amount of information about a population and compress that information to just a few classes. If  $S_c$  is the set of distinct leaf node labels, then we call each  $c \in S_c$  a **class of the classifier**. In the case of Fig.16.1,  $S_c = \{False, True\}$ .

<sup>1</sup>The **question-answer pairs** in dtrees are also called **attribute-value pairs**. Attributes are also called **features**.

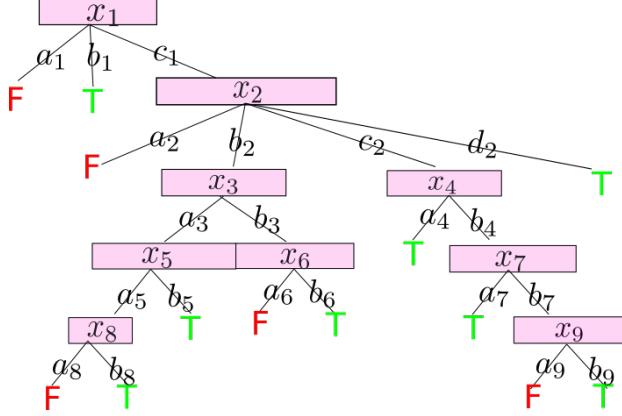


Figure 16.2: Fig.16.1 with abridged labels.

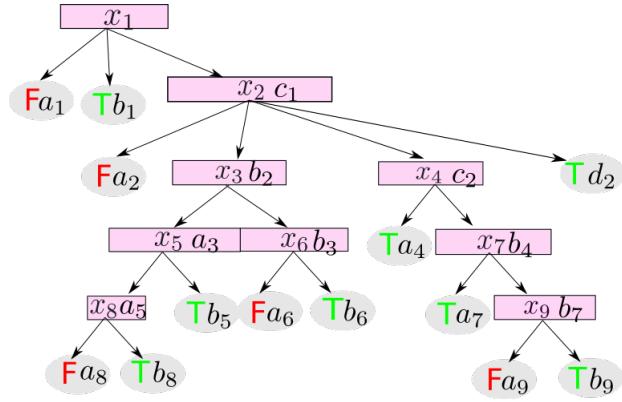


Figure 16.3: Fig.16.2 converted to a bnet.

Dtrees can be used with probabilities attached to each node, or without probabilities (as a plain undirected graph(UG)). This is analogous to bnets, which can be used with probabilities attached to each node (as DAGs with TPMs specified for each node) or without probabilities (as plain DAGs). Dtrees differ from bnets in that their tree branches are labelled, whereas bnet arrows aren't labelled. Also, whereas the nodes of a bnet carry a matrix of probabilities (the TPM), the nodes of a dtree carry just a column vector of probabilities which represents a single probability distribution. Henceforth, we will refer to the column vector of probabilities carried by each node of a dtree as its **Transition Probability Vector (TPV)**. Without the TPVs, a dtree can be used as a deterministic classifier, to classify inputs. With the TPVs, it can be used as a probabilistic sampler (to generate random samples.)

$P(x a)$	$a = a_0$	$a \in S_{\underline{a}}^- - \{a_0\}$	$null$
0	$p_0$	0	0
1	$p_1$	0	0
$\vdots$	$\vdots$	0	0
$N_{\underline{x}}^- - 1$	$p_{N_{\underline{x}}^- - 1}$	0	0
$null$	0	1	1

Table 16.1: TPM of a node of a dtree image bnet.

## 16.1 Transforming a dtree into a bnet

A trivial observation that is seldom made in the dtree pedagogical literature is that every dtree maps into a special bnet, let's call it its "image" bnet, in a very natural way. We use the dtree of Fig.16.1 as an example to show how to do this. As a first step, we go from Fig.16.1 to Fig.16.2 by replacing all the labels of the nodes and of the branches of the dtree by abridged symbols. Next, we go from Fig.16.2 to Fig.16.3, by replacing all tree branches by arrows pointing down, and by moving the tree branch labels down so that they become a suffix to the question that the tree branch leads to. At this point, we have created Fig.16.3, which constitutes the DAG of the image bnet. It remains for us to define a TPM for each node of this DAG.

Table 16.1 gives the TPM  $P(x|a)$  for a node  $\underline{x}$  with single parent  $\underline{a}$  of a dtree image bnet. Say node  $\underline{x}$  has a set  $S_{\underline{x}}^-$  of possible tree branches coming out of it. Let  $N_{\underline{x}}^- = |S_{\underline{x}}^-|$ . Let  $S_{\underline{x}} = S_{\underline{x}}^- \cup \{null\}$  and  $N_{\underline{x}} = |S_{\underline{x}}| = N_{\underline{x}}^- + 1$ . Define  $S_{\underline{a}}^-, N_{\underline{a}}^-, S_{\underline{a}}$  and  $N_{\underline{a}}$  analogously for node  $\underline{a}$ . In Table 16.1,  $S_{\underline{x}}^- = \{0, 1, \dots, N_{\underline{x}}^- - 1\}$  and  $a_0$  is the value of node  $\underline{a}$  which labels the tree branch connecting nodes  $\underline{a}$  and  $\underline{x}$ .  $\vec{p} = (p_0, p_1, \dots, p_{N_{\underline{x}}^- - 1})$  is a probability distribution associated with node  $\underline{x}$ , its TPV. TPVs can be learned from a dataset following the dtree Structure Learning (SL) algorithm discussed in Section 16.2.

Table 16.1 also applies when node  $\underline{x}$  is a leaf node, except that for leaf nodes,  $\vec{p}$  is one hot (i.e., all components are zero except for one component which is 1). Also, all leaf nodes  $\underline{x}$  have the same  $S_{\underline{x}}^-$ , namely  $S_c$ .

Adding a null state to the set of states (SOS) of each node of the image bnet is necessary because, once  $null$  is added to the SOS of any node, it must be added to the SOS of all descendant nodes.  $null$  must be added to the SOS of the children of the root node to take care of the situations when those first children don't receive the state they were expecting from their parent, i.e., the root node.

When drawing dtrees, some people put info like explanations and probabilities on the branches of the dtree. That info can all be preserved in the TPM and the node names and node state names of the image bnet nodes. One can also place info inside tool tips attached to the node name and node state names. Often, the pedagogical literature states that dtrees are more explicit and carry more info than their image bnets, but if one follows the above prescriptions, both can carry the same info.

A naive Bayes (NB) bnet (see Chapter 63) consists of a single “class node” with states  $S_c$  that fans out with arrows pointing to the “feature nodes”. If each leaf node of a NB bnet fans out into a set of new leaf nodes, and those new leaf nodes also fan out and so on, we get a generalized NB bnet. Let’s call this type of tree bnet an  $NB^*$  bnet. An  $NB^*$  bnet has the same graph structure as the image bnet of a dtree, but it’s more general, because its TPMs are more general. Each TPM of a  $NB^*$  bnet can have several non-trivial columns instead of just one  $\text{TPV} = \vec{p}$ .

## 16.2 Structure Learning for Dtrees

Let

$J_0 = \{0, 1, \dots, nj - 1\}$   
 $\Sigma = \{0, 1, 2, \dots, nsam - 1\}$   
 $DS = \{(\sigma, x^\sigma, c^\sigma) : \sigma \in \Sigma\}$  be a dataset  
 $\sigma \in \Sigma$  be an individual (a sample) from a population,  
 $x^\sigma \in S_{\underline{x}}$  be the **feature (attributes, questions) vector**.  $S_{\underline{x}} = S_{x_0} \times S_{x_1} \times \dots \times S_{x_{nj-1}}$ ,  $x = (x_0, x_1, \dots, x_{nj-1}) \in S_{\underline{x}}$ ,  $x_j \in S_{x_j}$   
 $c^\sigma \in S_c$  be a **classification class**  
We will assume  $S_{\underline{x}}$  and  $S_c$  are finite sets.

Building a **classifier**  $Y$  (curve fit) for a dtree means finding a deterministic function  $Y : S_{\underline{x}} \rightarrow S_c$  such that  $c^\sigma \approx Y(x^\sigma)$  for all  $\sigma \in \Sigma$ . If we divide the population  $\Sigma$  into two large disjoint sets, a **training set**  $\Sigma_{train}$  and a **validation set**  $\Sigma_{vali}$ , and if  $c^\sigma \approx Y(x^\sigma)$  very closely for  $\sigma \in \Sigma_{train}$  but fits poorly for  $\sigma \in \Sigma_{vali}$ , then we say the classifier  $Y$  suffers from **overfitting**. We can learn the structure and TPVs of a dtree from a dataset  $DS$ , by using the dtree **Structure Learning (SL)** algorithm that we will discuss in detail later. However, that algorithm is prone to produce a classifier  $Y$  that overfits. Two techniques commonly used to reduce the effects of overfitting are **pruning** and **Random Forest (RF)** (see Chapter 74). Pruning just means somehow removing nodes that are too specific. An RF is an ensemble of dtrees that one averages over. In this chapter, we will only deal with a single dtree, not an ensemble of them.

Dtree SL was invented in 1984-1986 so it is fairly old. Many in the AI community consider dtrees old fashioned compared to neural nets. But dtrees are **interpretable** whereas neural nets aren’t.<sup>2</sup> Bnets are interpretable too.

Below, we give the standard algorithm for SL of a dtree, in the form of pseudo-code. But first, we define two quantities, Information Gain and Gini, that are used in that pseudo-code.

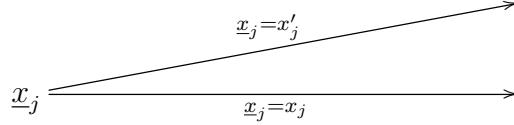
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<sup>2</sup>To be precise, only plain dtrees without boosting or bagging are interpretable. Dtrees used within boosting (see Chapter 1 on AdaBoost and Chapter 101 on XGBoost) or bagging (see Chapter 74 on Random Forest) gain much accuracy but lose **interpretability**.

### 16.2.1 Information Gain, Gini

This section uses various Shannon Information Theory entropies. Our notation for those entropies is described in Chapter C.

Call a **separation ability measure** (SAM) a measure used to decide, when constructing a dtree from a dataset, in what order to ask the questions about the feature vector  $x$ . The question order is decided by searching over all so far unused questions for the question with the largest SAM.<sup>3</sup>



$$\{N_j(c, x_j)\}_{c \in S_{\underline{c}}, x_j \in S_{\underline{x}_j}}$$

$$\sum_{c \in S_{\underline{c}}} N_j(c, x_j) = N_j(x_j)$$

$$\sum_{x_j \in S_{\underline{x}_j}} N_j(c, x_j) = N_j(c) \quad \sum_{c \in S_{\underline{c}}} N_j(c) = \sum_{x_j \in S_{\underline{x}_j}} N_j(x_j) = N_j$$

Figure 16.4: Some population numbers associated with the nodes of a dtree.  $N_j(c, x_j)$  is the number of individuals  $\sigma$  in the population that reaches node  $j$ , belonging to class  $c$  and having  $\underline{x}_j = x_j$ .

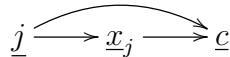


Figure 16.5: Bnet derived from population numbers in Fig.16.4

Fig.16.4 defines some population numbers associated with the nodes of a dtree. From these population numbers, we can define the bnet in Fig.16.5. The TPMs, printed in blue, for the (non-root) nodes of this bnet, are as follows

$$P(c|x_j, j) = \frac{N_j(c, x_j)}{N_j(x_j)} \tag{16.1}$$

---

<sup>3</sup>SAM is also called, somewhat confusingly, the splitting criterion and Gain.

$$P(x_j|j) = \frac{N_j(x_j)}{N_j} \quad (16.2)$$

where  $j \in J_0$ ,  $x_j \in S_{\underline{x}_j}$ , and  $c \in S_c$  is a class node.

One can define the following information theory quantities<sup>4</sup> associated with the bnet Fig.16.5.

$$INFO\_fin_j = - \sum_c P(c|j) \ln P(c|j) \quad (16.3)$$

$$= H(\underline{c}|j) \quad (16.4)$$

$$= H(\underline{c}|\underline{x}_j, j) \quad (16.5)$$

$$INFO\_init_j = \sum_{x_j \in S_{\underline{x}_j}} P(x_j|j) H(\underline{c}|x_j, j) \quad (16.6)$$

$$= H(\underline{c}|\underline{x}_j, j) \quad (16.7)$$

$$IG_j = INFO\_fin_j - INFO\_init_j \quad (16.8)$$

$$= H(\underline{c}|j) - H(\underline{c}|\underline{x}_j, j) \quad (16.9)$$

$$= H(\underline{c} : \underline{x}_j | j) \quad (16.10)$$

$IG_j$  is called the **information gain for node  $\underline{x}_j$** . Maximizing this mutual information produces a node  $\underline{x}_j$  that has a large correlation to a class  $c$ . If the goal is to reach a point where each leaf node is closely correlated to a different class, then maximizing the Information Gain of each new node is a greedy move towards that goal. Thus, Information Gain is a good SAM for dtree SL.

Note that if we approximate

$$\ln P(c|x_j) \approx \ln[1 + P(c|x_j) - 1] \quad (16.11)$$

$$\approx P(c|x_j) - 1 \quad (16.12)$$

in  $H(\underline{c}|x_j)$ , we get what is called the **Gini (or Gini Index) for node  $\underline{x}_k$** :

---

<sup>4</sup>The average of  $H(\underline{c} : b)$  over  $b$  is  $H(\underline{c} : \underline{b}) = \sum_b P(b)H(\underline{c} : b)$ . Likewise, the average of  $H(\underline{c}|b)$  over  $b$  is  $H(\underline{c}|b) = \sum_b P(b)H(\underline{c}|b)$ .  $H(\underline{c} : \underline{b})$  becomes  $H(\underline{c} : b)$  and  $H(\underline{c}|b)$  becomes  $H(\underline{c}|b)$  when there is no  $b$ -prior (i.e.,  $P(b)$  is a delta function).

$$H(\underline{c}|x_j) = - \sum_c P(c|x_j) \ln P(c|x_j) \quad (16.13)$$

$$\approx 1 - \sum_{c \in S_{\underline{c}}} P(c|x_j)^2 \stackrel{\text{def}}{=} Gini_{x_j} \quad (16.14)$$

$Gini_{x_j}$  is a fairly good polynomial approximation to  $H(\underline{c}|x_j)$ . It is computationally much less expensive than  $H(\underline{c}|x_j)$ , because it does not require computing a log.

We say a probability distribution  $P_{\underline{x}}$ , is **pure** (i.e., **deterministic**) if  $P_{\underline{x}}(x) = \delta(x, x_0)$ .  $Gini_{x_j}$  and  $H(\underline{c}|x_j)$  are both always non-negative. They both vanish iff  $P(c|x_j)$  is pure. Thus,  $Gini_{x_j}$  and  $H(\underline{c}|x_j)$  are both good measures of **class impurity**.

The **average Gini of node  $\underline{x}_j$**  is defined as

$$AGini_j = \sum_{x_j \in S_{\underline{x}_j}} P(x_j|j) Gini_{x_j}. \quad (16.15)$$

It measure the average impurity of the children of node  $\underline{x}_j$ .

In practice, the SL algorithm is done recursively. Each recursion step decides which feature  $x_j$  will be the root node of the current tree. For all "candidate" features (i.e., all  $\underline{x}_j$  that haven't been used yet as tree nodes), one calculates  $IG_j$ , either exactly or approximately via Gini's, using the following formula:

$$IG_j = \underbrace{H(\underline{c}|j)}_{\approx Gini_j} - \sum_{x_j \in S_{\underline{x}_j}} P(x_j|j) \underbrace{H(\underline{c}|x_j)}_{\approx Gini_{x_j}} \quad (16.16)$$

One then chooses  $j = \operatorname{argmax}_j IG_j$ . This maximizes the  $\underline{c} - \underline{x}_j$  correlation.

Alternatively, some software programs use the average Gini  $AGini_j$  as their SAM. They choose as root node  $j = \operatorname{argmin}_j AGini_j$ . This minimizes the average impurity of the children of node  $j$ . Since  $IG_j$  differs from  $AGini_j$  by  $H(\underline{c}|j)$ , maximizing  $IG_j$  and minimizing  $AGini_j$  might lead to different results.

---

### Example of calculation of $AGini_j$ and $IG_j$

Suppose we deduce from a dataset the numbers in the yellow cells in Table 16.2. These numbers are repeated in Fig.16.6. Then we can calculate the white cells as follows:

- Gini(hot)=  $1 - (3/4) - (1/4) = 0.375$
- Gini(med)=  $1 - (3/5)^2 - (2/5)^2 = 0.48$
- Gini(cold)=  $1 - (3/5)^2 - (2/5)^2 = 0.48$
- AGini =  $(4/14)(0.375) + (5/14)(0.48) + (5/14)(0.48) = 0.45$

$j = \text{temp?}$	$x_j = \text{hot}$	$x_j = \text{med}$	$x_j = \text{cold}$
$c = \text{play}$	3	3	3
$c = \text{stay}$	1	2	2
$Gini$	0.375	0.48	0.48
$AGini = 0.45$			
$H(\underline{c} x_j)$	$\approx 0.375$	$\approx 0.48$	$\approx 0.48$
$IG \approx 0$			

Table 16.2: Evaluating AGini and IG for node  $\text{temp}$ .

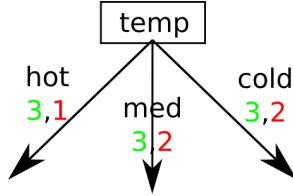


Figure 16.6: Tree stump corresponding to Table 16.2.

- $IG \approx [1 - (6/9)^2 - (3/9)^2] - AGini = 0.44 - 0.45 \approx 0$

This gives the AGini and IG for just one candidate root node. We would have to calculate AGini (or IG) for all possible candidates and choose the candidate with the lowest AGini (or highest IG).

### 16.3 Information Gain Ratio

The Information Gain Ratio (IGR) is an alternative SAM.

$$IGR_j = \frac{IG_j}{H(\underline{x}_j|j)} \quad (16.17)$$

$$= \frac{H(\underline{c} : \underline{x}_j|j)}{H(\underline{x}_j|j)} \quad (16.18)$$

$$= \frac{H(\underline{x}_j|j) - H(\underline{x}_j|\underline{c}, j)}{H(\underline{x}_j|j)} \quad (16.19)$$

$$= 1 - \frac{H(\underline{x}_j|\underline{c}, j)}{H(\underline{x}_j|j)} \quad (16.20)$$

$$0 \leq IGR_j \leq 1$$

$$IGR_j = 0 \text{ iff } H(\underline{x}_j|\underline{c}, j) = H(\underline{x}_j|j).$$

### 16.3.1 Pseudo-code

Below, we give the standard algorithm for SL of a dtree, in the form of pseudo-code. The strategy employed by the algo is to assume an incoming population into the current root node, then determine the feature  $x_j$  that best separates that incoming population. The feature  $x_j$  is chosen so as to maximize  $IG_j$  (or minimize  $AGini_j$ ). This process is repeated by nominating the end of each new branch to be the current root node. Features can appear as a node more than once, so the order in which nodes are split does not matter. In essence, what we are doing is performing a top-down, greedy search through the space of possible dtrees.

The pseudo-code below describes the following historically important software programs:

- CART (Classification and Regression Trees), invented by Breiman et al in 1984. Uses  $AGini_j$  as SAM.
- ID3 (Iterative Dichotomiser 3) invented by Quinlan in 1986. Uses  $IG_j$  as SAM. C4.5/C5.0 are successors to ID3.

Thus, CART and ID were invented independently around the same time. The main difference between them is the SAM being used.

The pseudo-code below uses the majority function defined in Chapter C.

---

**Algorithm 1:** Pseudo-code for learning a dtree from a dataset

---

**Input :**

- dataset  $DS = \{(\sigma, x^\sigma, c^\sigma) : \sigma \in \Sigma\}$
- set of currently available node indices  $J$ , where  $J \subset J_0$

**Output:**

- tree  $T$ ,
- population numbers  $\{(r, c, x_r, N_r(c, x_r)) : r \in J_0, c \in S_c, x_r \in S_{x_r}\}$  stored globally

From  $DS$ , calculate  $J_0, S_c, S_{x_i}$  for each  $i$   
 $c^\sigma$  is called the target feature/attribute.

$J \leftarrow J_0$

**Function** `learn_dtreete(DS, J):`

```

 $\Sigma \leftarrow$  set of all  $\sigma$  in  $DS$ 
if  $\{c^\sigma : \sigma \in \Sigma\} = \{c\}$  then
     $T \leftarrow$  one node tree with leaf node label=  $c$ 
else if  $J = \emptyset$  then
     $T \leftarrow$  one node tree with leaf node label= majority( $[c^\sigma : \sigma \in \Sigma]$ )
else
     $r \leftarrow \underset{j \in J}{\operatorname{argmax}} IG_j(DS)$  // or replace  $\operatorname{argmax} IG_j$  by  $\underset{j \in J}{\operatorname{argmin}} AGini_j$ 
    from  $DS$ , calculate  $\{(r, c, x_r, N_r(c, x_r)) : c \in S_c, x_r \in S_{x_r}\}$  and store it
        globally
    for  $v \in S_{x_r}$  do
        /* Notice that  $J$  is the same every time repeat this loop, so
           order in which  $v \in S_{x_r}$  are called does not matter.
           Furthermore, this means that multiple tree nodes may be
           labeled by same feature. */
        On current tree  $T$ , add a branch below  $x_r$  with label " $x_r = v$ "
         $DS|_{x_r=v} \leftarrow$  subset of  $DS$  with  $x_r = v$ 
        if  $DS|_{x_r=v} = \emptyset$  then
            below the new branch add a
            leaf node labeled = majority( $[c^\sigma : \sigma \in \Sigma]$ )
        else
            below the new branch add
            subtree = learn_dtreete( $DS|_{x_r=v}, J - \{r\}$ )
    return  $T$ 

```

---

# Chapter 17

Decisions Based on Rungs 2 and 3:  
COMING SOON

# Chapter 18

## Difference-in-Differences

This chapter is based on Ref.[12].

The Difference-in-Differences (DID) method was first used by John Snow in an 1854 report that argued that cholera in London was being transmitted by sewage polluted water rather than, as others at the time believed, by air (in fetid vapors called miasmas). In general, one can apply DID to discover causal effects in historical data. By **historical data** (a.k.a. a **natural experiment**. See Ref.[144]) we mean data that is collected long after the treatment (rather than during it) and is thus not subject to active intervention by the experimenter.

This chapter assumes that the reader has read Chapter 72 on Potential Outcomes (PO). The DID method applies the basic single-time PO theory described in Chapter 72, to 2 well separated times in which different conditions prevail.

### 18.1 John Snow, DID and a cholera transmission pathway

Let

$$\begin{aligned} d &\in \{0, 1\} \\ t &\in \{t_0, t_1\}, t_0 < t_1 \\ y &= f(d, t) \in \mathbb{R}. \end{aligned}$$

Define

$$\Delta_t f(d, t) = f(d, t_1) - f(d, t_0), \quad (18.1)$$

$$\Delta_d f(d, t) = f(1, t) - f(0, t), \quad (18.2)$$

$$DID = \delta = \Delta_d \Delta_t f(d, t). \quad (18.3)$$

DID is illustrated in Fig.18.1.

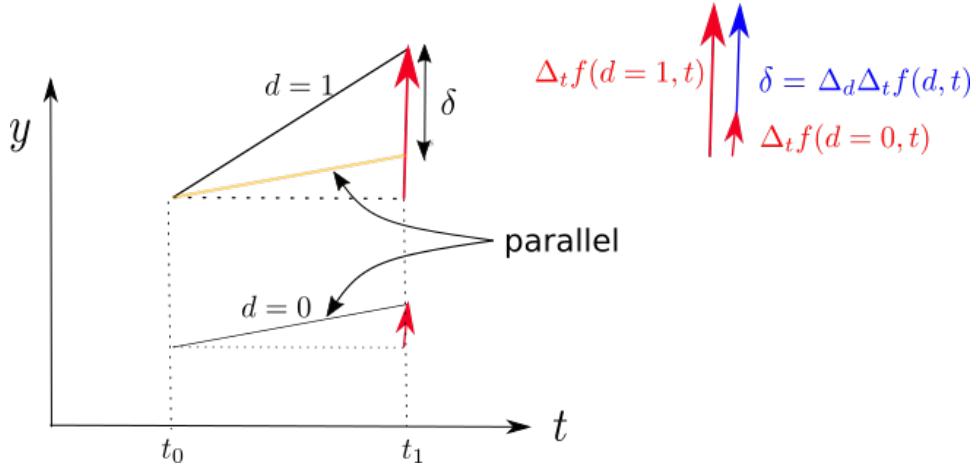


Figure 18.1: Pictorial representation of Difference-in-differences (DID) as a difference of two differences (i.e., a difference of two slopes).

A **time series** is any function of time for which the domain is a discrete set of times.

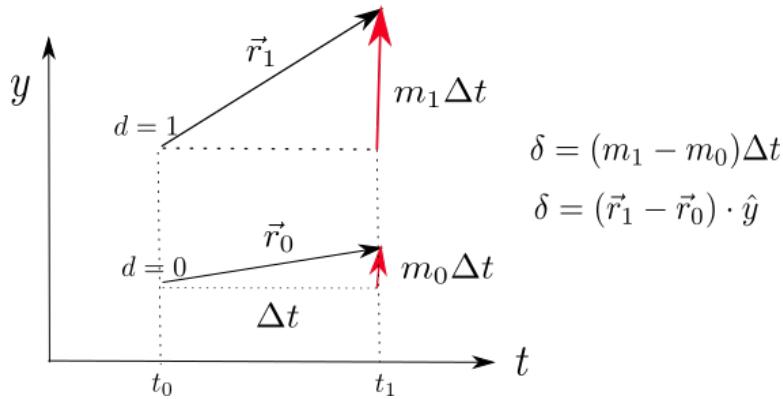


Figure 18.2:  $DID = \delta$  expressed as difference of slopes or difference of vectors.

Note that, as shown Fig.18.2,  $DID = \delta$  can also be expressed as a difference of 2 slopes times  $\Delta t = t_1 - t_0$ . Let  $\hat{y}$  be a unit in the  $y$  direction.  $\delta$  can also be expressed as the dot product of a difference of 2 vectors dotted with  $\hat{y}$ .

A condensation of the data collected by John Snow in 1854 is given in Table 18.1. From that data, we find that

$$\delta = \Delta_d \Delta_t f(d, t) = (19 - 85) - (147 - 135) = -66 - 12 = -78 \quad (18.4)$$

	$t = t_0$ (1849)	$t = t_1$ (1854)
$d = 1$ (town 1)	85 deaths, polluted DW	19 deaths, unpolluted DW
$d = 0$ (town 0)	135 deaths, polluted DW	147 deaths, polluted DW

Table 18.1: A condensation of the data collected by John Snow in 1854, to test the hypothesis that cholera in London was being spread by polluted drinking water (DW).

## 18.2 PO analysis

In this section, we show how to analyze the DID method using the formalism of PO theory.

We will speak of a treatment outcome  $\underline{y}_{t,g}^\sigma(c^\sigma, x^\sigma)$  for individual  $\sigma$  that depends, not just on the treatment dose  $c^\sigma \in \{0, 1\}$  and the confounder state  $x^\sigma$ , but also on a group parameter (i.e., which population or town)  $g^\sigma \in \{0, 1\}$  and on a time parameter  $t \in \{t_0, t_1\}$  (note  $t$  is independent of  $\sigma$ ). Actually, we will assume  $g^\sigma = c^\sigma$ , so we will just speak of  $\underline{y}_t^\sigma(c^\sigma, x^\sigma)$  with no explicit  $g^\sigma$  dependence. As usual for PO theory, we will consider expected values of  $\underline{y}_t^\sigma$ :

$$E_{\sigma|d,x}[\underline{y}_t^\sigma(c)] = E_{\underline{y}_t(c)|d,x}[\underline{y}_t(c)] = \mathcal{Y}_{c|d,x}(t) \quad (18.5)$$

To calculate these expected values, we need a “model” with probability distributions. In this case, the needed model and probability distributions are provided by the bnets depicted in Fig.18.3. The TPMs, printed in blue, for the bnet  $G_{t,+}$  in Fig.18.3, are as follows. Note that the TPMs for the bnet  $G_{t,+}$  are defined in terms of the TPMs for the bnet  $G_t$ .

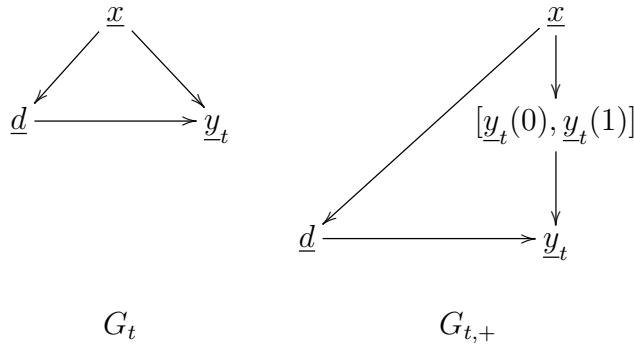


Figure 18.3:  $t \in \{t_0, t_1\}$ . Bnet  $G_{t,+}$  is obtained by adding two new nodes  $\underline{y}_t(0)$  and  $\underline{y}_t(1)$  to bnet  $G_t$ .

$$P(x) = P_{\underline{x}}(x) \quad (18.6)$$

$$P(d|x) = P_{d|\underline{x}}(d|x) \quad (18.7)$$

$$P(y_t|y_t(0), y_t(1), d) = \mathbb{1}(y_t = y_t(d)) \quad (18.8)$$

$$P(y_t(c)|x) = P(y_t(c)|d, x) = \text{given} \quad (18.9)$$

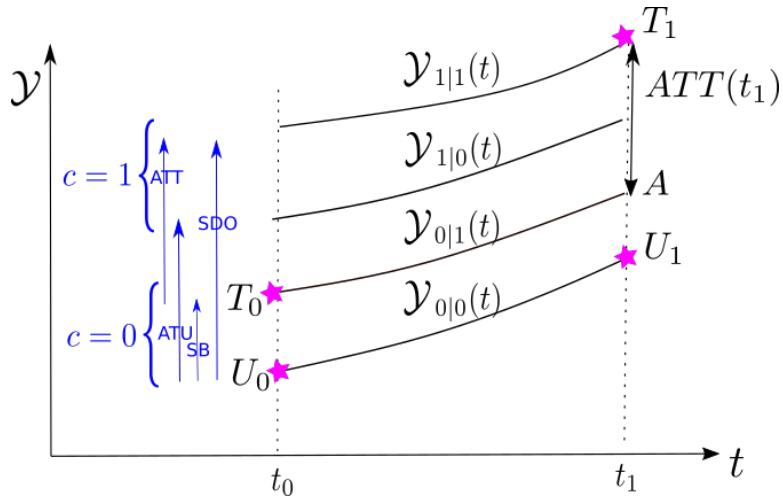


Figure 18.4: Four different time-dependent expected values  $\mathcal{Y}_{c|d}(t)$  of  $y_t^\sigma$  for bnet  $G_{t,+}$ . The 4 magenta stars represent the 4 DID measurements.

We define the function  $c(t)$  for  $t = t_0, t_1$  by

$$c(t) = \begin{cases} 0 & \text{if } t = t_0 \\ d & \text{if } t = t_1 \end{cases} \quad (18.10)$$

Now we claim that the DID  $\delta$  calculated in the previous section for John Snow's data, can be expressed in PO formalism as follows:

$$\delta = \Delta_d \Delta_t \mathcal{Y}_{c(t)|d}(t) . \quad (18.11)$$

Fig.18.4 depicts the four functions  $\mathcal{Y}_{c|d}(t)$  for  $t$  in the interval  $[t_0, t_1]$  and for  $c, d \in \{0, 1\}$ . The  $\mathcal{Y}$  coordinates of the four magenta stars in Fig.18.4 can be calculated using bnet  $G_t$ .

Define the **parallel trends** (PT) by

$$PT = \Delta_d \Delta_t \mathcal{Y}_{0|d}(t) . \quad (18.12)$$

We will say the **parallel trends assumption (PTA)** holds if  $PT = 0$ .

Next we prove that the DID  $\delta$  equals the sum of an ATT<sup>1</sup> and PT.

$$\delta = \Delta_d \Delta_t \mathcal{Y}_{c(t)|d}(t) \quad (18.13)$$

$$= [\Delta_t \mathcal{Y}_{c(t)|1}(t) - \Delta_t \mathcal{Y}_{c(t)|0}(t)] \quad (18.14)$$

$$= \mathcal{Y}_{1|1}(t_1) - \mathcal{Y}_{0|1}(t_0) - \{\mathcal{Y}_{0|0}(t_1) - \mathcal{Y}_{0|0}(t_0)\} \quad (18.15)$$

$$= \mathcal{Y}_{1|1}(t_1) - \mathcal{Y}_{0|1}(t_0) - \{\mathcal{Y}_{0|0}(t_1) - \mathcal{Y}_{0|0}(t_0)\} + \underbrace{\{\mathcal{Y}_{0|1}(t_1) - \mathcal{Y}_{0|1}(t_1)\}}_{\text{zero}} \quad (18.16)$$

$$= \underbrace{\mathcal{Y}_{1|1}(t_1) - \mathcal{Y}_{0|1}(t_1)}_{ATT(t_1)} - \mathcal{Y}_{0|1}(t_0) - \{\mathcal{Y}_{0|0}(t_1) - \mathcal{Y}_{0|0}(t_0)\} + \mathcal{Y}_{0|1}(t_1) \quad (18.17)$$

$$= ATT(t_1) - \Delta_t \mathcal{Y}_{0|0}(t) + \Delta_t \mathcal{Y}_{0|1}(t) \quad (18.18)$$

$$= ATT(t_1) + \underbrace{\Delta_d \Delta_t \mathcal{Y}_{0|d}(t)}_{\text{zero if PTA holds}} \quad (18.19)$$

## 18.3 Linear Regression

In this section, we show how to apply linear regression (LR) to the PO analysis of DID.

As before, let  $y_t^\sigma(c^\sigma)$  be the treatment outcome for individual  $\sigma$ , who receives a treatment dose  $c^\sigma$  at times  $t \in \{t_0, t_1\}$ .  $y_t^\sigma(c^\sigma)$  can be fitted as follows. Here  $\epsilon^\sigma$  is the residual for individual  $\sigma$ , and  $b_0, m_0, b_1, m_1 \in \mathbb{R}$  are the fit parameters.

$$y_t^\sigma = [b_0 + m_0(t - t_0)](1 - c^\sigma) + [b_1 + m_1(t - t_0)]c^\sigma + \epsilon^\sigma. \quad (18.20)$$

Note that Eq.(18.20) yields a straight line in the  $y_t^\sigma - t$  plane for  $c^\sigma = 0$ , and another straight line for  $c^\sigma = 1$ . We are using the standard symbols  $b$  to denote the y-intercept, and  $m$  to denote the slope of a straight line.

Taking the expected value of Eq.(18.20), we get

$$\mathcal{Y}_{c|d}(t) = [b_0 + m_0(t - t_0)](1 - d) + [b_1 + m_1(t - t_0)]d. \quad (18.21)$$

If  $\Delta t = t_1 - t_0$ , then

$$\mathcal{Y}_{d|d}(t_1) = [b_0 + m_0 \Delta t](1 - d) + [b_1 + m_1 \Delta t]d, \quad (18.22)$$

and

$$\mathcal{Y}_{0|d}(t_0) = b_0. \quad (18.23)$$

---

<sup>1</sup>ATT stands for the average treatment effect of the treated. ATT is defined in Chapter 72

Thus,

$$\delta = \Delta_d \Delta_t \mathcal{Y}_{c(t)|d}(t) \quad (18.24)$$

$$= \Delta_d [\mathcal{Y}_{d|d}(t_1) - \mathcal{Y}_{0|d}(t_0)] \quad (18.25)$$

$$= (m_1 - m_0) \Delta t. \quad (18.26)$$

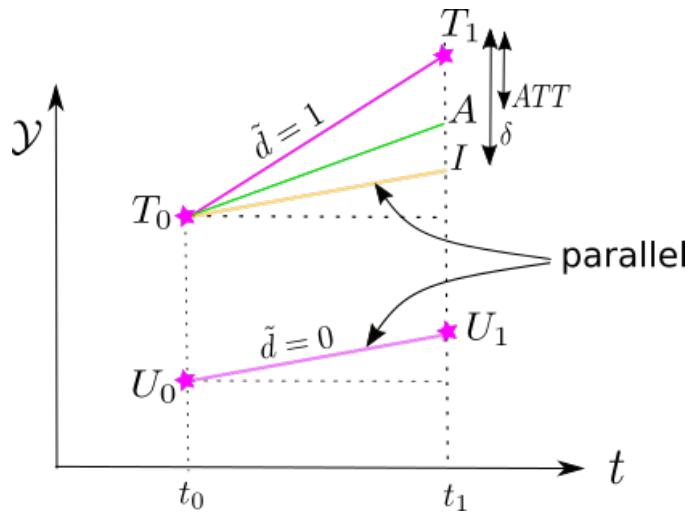


Figure 18.5: We use Linear Regression to fit a straight line between points  $U_0$  and  $U_1$ , and between points  $T_0$  and  $T_1$ . ( $U$ =untreated,  $T$ =treated, subscript refers to times  $t_0, t_1$ ).  $U_0, T_0, U_1, T_1$  are the measurement points. Point  $I$  is an image of point  $U_1$ .

	$t = t_0$	$t = t_1$
$d = 1$	$\mathcal{Y}(T_0) = \mathcal{Y}_{0 1}(t_0)$	$\mathcal{Y}(T_1) = \mathcal{Y}_{1 1}(t_1)$
$d = 0$	$\mathcal{Y}(U_0) = \mathcal{Y}_{0 0}(t_0)$	$\mathcal{Y}(U_1) = \mathcal{Y}_{0 0}(t_1)$

Table 18.2:  $\mathcal{Y}$  coordinates of points  $U_0, T_0, U_1, T_1$  in Figs.18.4 and 18.5.

Figs.18.4 and 18.5 define points  $U_0, T_0, U_1, T_1, I, A$ . The  $\mathcal{Y}$  coordinates of points  $U_0, T_0, U_1, T_1$  are given by Table 18.2. The  $\mathcal{Y}$  coordinates of points  $A, I$  are given by Eqs.18.27.

$$\mathcal{Y}(A) = \mathcal{Y}_{0|1}(t_1) \quad (18.27a)$$

$$\mathcal{Y}(I) = \mathcal{Y}(U_1) + [\mathcal{Y}(T_0) - \mathcal{Y}(U_0)] \quad (18.27b)$$

We can express  $ATT$  and the  $\delta$  for DID in terms of the  $\mathcal{Y}$  of the points  $U_0, T_0, U_1, T_1, I, A$ . Indeed,

$$\delta = \mathcal{Y}(T_1) - \mathcal{Y}(I) \quad (18.28)$$

$$= \mathcal{Y}(T_1) - \mathcal{Y}(U_1) - [\mathcal{Y}(T_0) - \mathcal{Y}(U_0)] \quad (18.29)$$

$$ATT = \mathcal{Y}(T_1) - \mathcal{Y}(A) \quad (18.30)$$

Hence,

$$\delta = ATT \iff \mathcal{Y}(I) = \mathcal{Y}(A) \iff \text{PTA holds} \quad (18.31)$$

# Chapter 19

## Diffusion Models

This chapter is based on Ref.[85]

Diffusion Models (DM) are a way of generating fake images from an original image. They are a competitor to GANs (see Chapter 33), and are used in DALL-E (OpenAI's computer program that generates images from text).

DM works by subjecting each degree of freedom of the image to a forward Markov chain of transformations labeled  $t = 0, 1, 2, \dots, T$  and a reverse Markov chain of transformations labeled  $t = T - 1, T - 2, \dots, 0$ . Each step of the forward chain multiplies each degree of freedom of the image by a constant and adds white noise to it. The last image ( $t = T$ ) of the forward chain is changed to the point that it looks like a normal distribution. The reverse chain tries to undo, as well as possible, the alterations to the original image done by the forward chain. Full, faithful restoration is impossible because the forward chain is an irreversible process.

Of course, a DM is only a small part of the magic of DALL-E. I haven't studied DALL-E's algorithm, but my guess is that it works roughly as follows. Given a text description of an image, such as "A hedgehog using a calculator painted in the style of Vincent van Gogh", it uses a neural net trained on a vast corpus of words and images, to match separate words in the description with an image for each word. Then it uses a second neural net to create a pastiche/superposition from the set of images created in the first stage. Then, it uses a DM to smooth the transitions of the pastiche or assign different weights to the elements of the superposition. Finally, it modifies the image at this point by passing it through a photoshop-like stylistic filter that can be specified in the initial description.

### 19.1 Bnet for DM

For  $t \in 1, 2, \dots, T$ , let

$$0 < \alpha^t < 1, \beta^t = 1 - \alpha^t \quad (19.1)$$

$$\pi_1^t \alpha = \prod_{\tau=1}^t \alpha^\tau \quad (19.2)$$

Let

$\underline{x}^t, \tilde{\underline{x}}^t \in \mathbb{R}^{df}$  for  $t = 0, 1, 2, \dots, T$  be column vectors describing an image. Here  $df$  is the number of degrees of freedom of the image.  $\underline{x}^0$  will denote the initial Original image,  $\underline{x}^T = \tilde{\underline{x}}^T$  will denote an image which is very close to a normal distribution, and  $\tilde{\underline{x}}^0$  will denote the final Fake image.

$I \in \mathbb{R}^{df \times df}$  is the identity matrix

$\underline{w}^t, \underline{a}^t, \underline{n}_\theta^t \in \mathbb{R}^{df}$

Fig.19.1 shows a bnet for DM, and 19.2 shows the same bnet in more detail.<sup>1</sup>

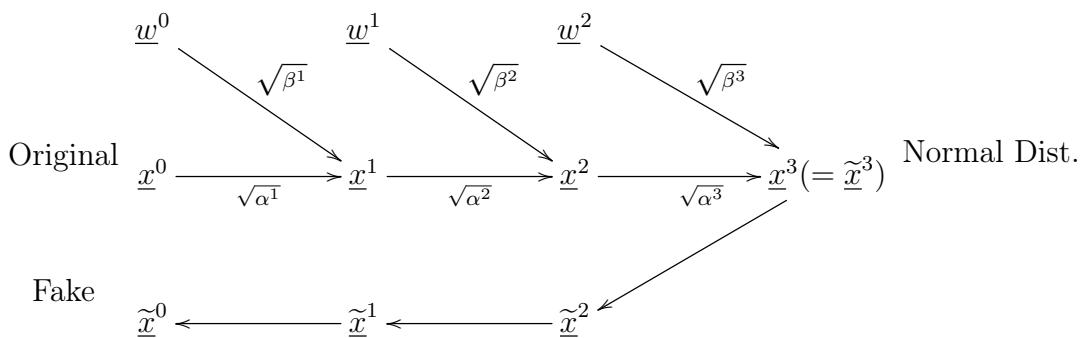


Figure 19.1: Bnet for DM with  $T = 3$ . See Chapter 48 for an explanation of LDEN notation.

The TPMs, printed in blue, for the bnet of Fig.19.1 are as follows:

$$P(x^0) = \delta(x^0, X^0) \quad (\text{original image}) \quad (19.3)$$

$$P(x^t|x^{t-1}, w^t) = \mathbb{1}(x^t = \sqrt{\alpha^t} x^{t-1} + \sqrt{\beta^t} w^{t-1}) \quad (19.4)$$

$$P(w^t) = \mathcal{N}(w^t; \mu = 0, \sigma^2 = I) \quad (\text{white noise}) \quad (19.5)$$

---

<sup>1</sup>Ref.[85] uses  $\underline{z}^t$  instead of  $\underline{w}^t$  for white noise. Note that the time index of  $\underline{w}^t$  often does not matter because  $\underline{w}^t \sim \mathcal{N}(0, I)$  for all  $t$ . This does not mean that we can drop the time index of  $\underline{w}^t$ , because  $\underline{w}^{t_1}$  and  $\underline{w}^{t_2}$  are uncorrelated for  $t_1 \neq t_2$ , so we can get into trouble if we assume  $\underline{w}^{t_1} = \underline{w}^{t_2} = \underline{w}$ .

$$P(\underline{\tilde{x}}^{t-1} = x^{t-1} | \underline{\tilde{x}}^t = x^t) = \tilde{P}_\theta(x^{t-1} | x^t) \quad (19.6)$$

$$= \mathcal{N}(x^{t-1}; \mu = M_\theta^{t-1}(x^t), \sigma^2 = \Sigma_\theta^{t-1}(x^t)) \quad (19.7)$$

We will assume that

$$\Sigma_\theta^{t-1}(x^t) = (\sigma^{t-1})^2 I \quad (19.8)$$

where  $\sigma^{t-1} \in \mathbb{R}$ .

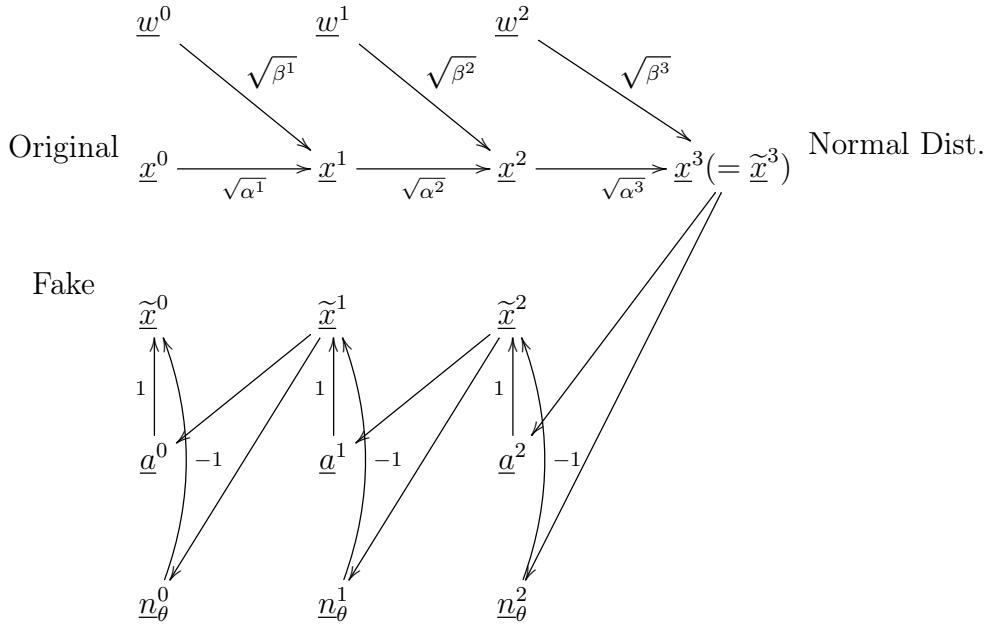


Figure 19.2: The bnet of Fig.19.1 shown in more detail.

The TPMs, printed in blue, for the bnet of Fig.19.2 are as follows:

$$P(n_\theta^t) = \mathcal{N}(n_\theta^t; \mu = M_\theta^t(x^{t+1}), \sigma = \sigma^t) \quad (19.9)$$

$$P(a^t | \underline{\tilde{x}}^{t+1} = x^{t+1}) = \mathbb{1}(a^t = M^t(x^{t+1})) \quad (19.10)$$

$$P(\underline{\tilde{x}}^t = x^t | a_t, n_\theta^t) = \mathbb{1}(x^t = a^t - n_\theta^t) \quad (19.11)$$

Note that these TPMs for the bnet Fig.19.2 imply that

$$\underbrace{P(\underline{\tilde{x}}^t = x^t | \underline{\tilde{x}}^{t+1} = x^{t+1})}_{\text{call this } \tilde{P}_\theta(x^t | x^{t+1})} = \mathcal{N}(x^t; \mu = M^t(x^{t+1}) - M_\theta^t(x^{t+1}), \sigma = \sigma^t) \quad (19.12)$$

## 19.2 Mean Values $M^{t-1}(x^t)$ and $M_\theta^{t-1}(x^t)$

**Claim 35**

$$\boxed{\underline{x}^t = \sqrt{\pi_1^t \alpha} \underline{x}^0 + \sqrt{1 - \pi_1^t \alpha} \underline{w}^t} \quad (19.13)$$

$$\begin{array}{ccc} & \underline{w}^t & \\ & \downarrow & \\ \underline{x}^0 & \xrightarrow[\sqrt{\pi_1^t \alpha}]{} & \underline{x}^t \end{array} \quad (19.14)$$

**proof:**

Suppose  $\underline{x}_1$  and  $\underline{x}_2$  are independent random variables with variances  $V_1$  and  $V_2$ , respectively. Then the variance  $V$  of  $\underline{x} = \underline{x}_1 + \underline{x}_2$  is

$$V = \langle \underline{x}, \underline{x} \rangle \quad (19.15)$$

$$= \langle \underline{x}_1 + \underline{x}_2, \underline{x}_1 + \underline{x}_2 \rangle \quad (19.16)$$

$$= \langle \underline{x}_1, \underline{x}_1 \rangle + \langle \underline{x}_2, \underline{x}_2 \rangle \quad (19.17)$$

$$= V_1 + V_2 \quad (19.18)$$

By similar reasoning, the mean of  $\underline{x}$  equals the sum of the means of  $\underline{x}_1$  and  $\underline{x}_2$ . It's also true that if both  $\underline{x}_1$  and  $\underline{x}_2$  are normally distributed, then  $\underline{x}$  is too. We will refer to a sum of independent normals as a SIN.

Let  $\underline{w} \sim \mathcal{N}(0, I)$ .

$$\underline{x}^t = \sqrt{\alpha^t} \underline{x}^{t-1} + \sqrt{1 - \alpha^t} \underline{w}^{t-1} \quad (19.19)$$

$$= \sqrt{\alpha^t} [\sqrt{\alpha^{t-1}} \underline{x}^{t-2} + \sqrt{1 - \alpha^{t-1}} \underline{w}^{t-2}] + \sqrt{1 - \alpha^t} \underline{w}^{t-1} \quad (19.20)$$

$$= \sqrt{\alpha^t \alpha^{t-1}} \underline{x}^{t-2} + [\sqrt{\alpha^t(1 - \alpha^{t-1})} \underline{w}^{t-2} + \sqrt{1 - \alpha^t} \underline{w}^{t-1}] \quad (19.21)$$

$$= \sqrt{\alpha^t \alpha^{t-1}} \underline{x}^{t-2} + \sqrt{1 - \alpha^t \alpha^{t-1}} \underline{w} \quad (\text{because it's a SIN}) \quad (19.22)$$

$$= \dots \quad (19.23)$$

$$= \sqrt{\pi_1^t \alpha} \underline{x}^0 + \sqrt{1 - \pi_1^t \alpha} \underline{w} \quad (19.24)$$

Now replace  $\underline{w}$  by  $\underline{w}^t$ . This is justified because they are both  $\mathcal{N}(0, I)$ , and, when  $t_1 \neq t_2$ , we want the  $\underline{w}$  for  $\underline{x}^{t_1}$  to be independent from the  $\underline{w}$  for  $\underline{x}^{t_2}$ .

**QED**

Solving Eq.(19.13) for  $\underline{x}^0$ , we get

$$\boxed{\underline{x}^0 = \frac{1}{\sqrt{\pi_1^t \alpha}} \underline{x}^t - \frac{\sqrt{1 - \pi_1^t \alpha}}{\sqrt{\pi_1^t \alpha}} \underline{w}^t} \quad (19.25)$$

$$\begin{array}{ccc}
& \frac{\sqrt{1-\pi_1^t \alpha}}{\sqrt{\pi_1^t \alpha}} & \underline{w}^t \\
& \swarrow & \nearrow \\
\underline{x}_0 & \xleftarrow[\frac{1}{\sqrt{\pi_1^t \alpha}}]{} & \underline{x}^t
\end{array} \tag{19.26}$$

**Claim 36**

$$P(x^{t-1}|x^t, x^0) = P(x^t|x^{t-1}) \frac{P(x^{t-1}|x^0)}{P(x^t|x^0)} \tag{19.27}$$

**proof:**

This is a simple consequence of Bayes rule. We will prove this in two ways: algebraically and graphically.

The algebraic proof goes as follows.

$$P(x^{t-1}|x^t, x^0)P(x^t|x^0) = \overbrace{P(x^t|x^{t-1}, x^0)}^{P(x^t|x^{t-1})} P(x^{t-1}|x^0) \tag{19.28}$$

The graphical proof, although longer, is more intuitive. Start by noticing that

$$\begin{aligned}
& \sum w^0 \quad \dots \quad \sum w^{t-2} \quad \sum w^{t-1} \\
& \downarrow \qquad \qquad \downarrow \qquad \qquad \downarrow \\
x^0 & \longrightarrow \sum x^1 \longrightarrow \dots \longrightarrow x^{t-1} \longrightarrow x^t \\
= & \quad x^0 \longrightarrow x^{t-1} \longrightarrow x^t \text{ (diagram A)} \tag{19.29} \\
= & \quad x^0 \xrightarrow[0]{\quad} x^{t-1} \xrightarrow{\quad} x^t \quad (\text{make fully connected}) \\
= & \quad x^0 \xrightarrow[0]{\quad} x^{t-1} \xleftarrow{\quad} x^t \quad (\text{reverse arrow}) \text{ (diagram B)}
\end{aligned}$$

Therefore,

$$\underbrace{P(x^{t-1}|x^t, x^0)P(x^t|x^0)}_{\text{diagram B of Eq.19.29}} = \underbrace{P(x^t|x^{t-1})P(x^{t-1}|x^0)}_{\text{diagram A of Eq.19.29}} \tag{19.30}$$

**QED**

Define the following mean value:

$$M^{t-1}(x^t) = \sum_{x^{t-1}} x^{t-1} P(x^{t-1}|x^t, x^0) \tag{19.31}$$

**Claim 37**

$$M^{t-1}(x^t) = \frac{\sqrt{\alpha^t}(1 - \pi_1^{t-1}\alpha)}{1 - \pi_1^t\alpha} x^t + \frac{\sqrt{\pi_1^{t-1}\alpha} \beta^t}{1 - \pi_1^t\alpha} x^0 \quad (19.32)$$

**proof:**

By Claim 36, we know that  $\mathcal{Q} = P(x^{t-1}|x^t, x^0)$  can be expressed as a product of two Gaussians  $P(x^t|x^{t-1})$  and  $P(x^{t-1}|x^0)$ , divided by a third Gaussian  $P(x^t|x^0)$ , and all 3 of these Gaussians have been calculated in closed form previously in this chapter. So it's just a matter of algebra to express  $\mathcal{Q}$  as a Gaussian, complete the square inside the exponent of  $\mathcal{Q}$ , and thus obtain its mean value  $M^{t-1}(x^t)$ . We leave the algebra to the reader. If in doubt, the algebra can be found in Ref.[85].

**QED**

**Claim 38**

$$M^{t-1}(x^t) = \frac{1}{\sqrt{\alpha^t}} \left( x^t - \frac{\beta^t}{\sqrt{1 - \pi_1^t\alpha}} w^t \right) \quad (19.33)$$

**proof:**

Use Eq.(19.25) to replace  $x^0$  in Eq.(19.32).

**QED**

Let us parameterize  $M_\theta^{t-1}(x^t)$  by

$$M_\theta^{t-1}(x^t) = \frac{1}{\sqrt{\alpha^t}} \left( x^t - \frac{\beta^t}{\sqrt{1 - \pi_1^t\alpha}} n_\theta^{t-1}(x^t) \right) \quad (19.34)$$

If we define

$$C^t = \frac{-\beta^t}{\sqrt{\alpha^t(1 - \pi_1^t\alpha)}} , \quad (19.35)$$

then

$$M^{t-1}(x^t) - M_\theta^{t-1}(x^t) = C^t [w^t - n_\theta^{t-1}(x^t)] \quad (19.36)$$

$$= C^t [w^t - n_\theta^{t-1}(\sqrt{\pi_1^t\alpha} x^0 + \sqrt{1 - \pi_1^t\alpha} w^t)] \quad (19.37)$$

### 19.3 Loss function $\mathcal{L}$

Note that<sup>2</sup>

$$0 \leq D_{KL}(P(x^{1:T}|x^0) \parallel \tilde{P}_\theta(x^{1:T}|x^0)) \quad (19.38)$$

$$= \sum_{x^{1:T}} P(x^{1:T}|x^0) \ln \frac{P(x^{1:T}|x^0)}{\tilde{P}_\theta(x^{1:T}|x^0)} \quad (19.39)$$

$$= \ln \tilde{P}_\theta(x^0) + \sum_{x^{1:T}} P(x^{1:T}|x^0) \ln \frac{P(x^{1:T}|x^0)}{\tilde{P}_\theta(x^{0:T})} \quad (19.40)$$

$$\underbrace{- \sum_{x^0} P(x^0) \ln \tilde{P}_\theta(x^0)}_{-E_{x^0}[\ln \tilde{P}_\theta(x^0)]} \leq \underbrace{\sum_{x^{0:T}} P(x^{0:T}) \ln \frac{P(x^{1:T}|x^0)}{\tilde{P}_\theta(x^{0:T})}}_{E_{x^{0:T}}\left[\ln \frac{P(x^{1:T}|x^0)}{\tilde{P}_\theta(x^{0:T})}\right]} = \mathcal{L}(\theta) = \text{loss function} \quad (19.41)$$

Henceforth, expected values  $E_{x^{0:T}}$  are to be understood as being with respect to  $P(x^{0:T})$ .

The left hand side of the inequality Eq.(19.41) is expected to be a small positive constant, because we expect  $\tilde{P}_\theta(x^0) \approx P(x^0) \approx \delta(x^0, X^0)$ . Thus, we are justified in defining the right hand side of Eq.(19.41) as loss function  $\mathcal{L} = \mathcal{L}(\theta)$  to be minimized.

**Claim 39**

$$\mathcal{L} = \sum_{t=0}^T \mathcal{L}^t \quad (19.42)$$

$$\mathcal{L}^0 = -\ln \tilde{P}_\theta(x^0|x^1) \quad (19.43)$$

$$\mathcal{L}^{t-1} = E_{x^{0:T}} \left[ \ln \frac{P(x^{t-1}|x^t, x^0)}{\tilde{P}_\theta(x^{t-1}|x^t)} \right] \quad \text{for } t = 2, 3, \dots, T \quad (19.44)$$

$$\mathcal{L}^T = E_{x^{0:T}} \left[ \ln \frac{P(x^T|x^0)}{\tilde{P}_\theta(x^T)} \right] \quad (19.45)$$

---

<sup>2</sup> $D_{KL}$  is the Kullback-Leibler divergence. It's defined in Chapter C.

**proof:**

$$\mathcal{L} = E_{x^{0:T}} \left[ \ln \frac{P(x^{1:T}|x^0)}{\tilde{P}_\theta(x^{0:T})} \right] \quad (19.46)$$

$$= E_{x^{0:T}} \left[ \ln \frac{\prod_{t=1}^T P(x^t|x^{t-1})}{\tilde{P}_\theta(x^T) \prod_{t=1}^T \tilde{P}_\theta(x^{t-1}|x^t)} \right] \quad (19.47)$$

$$= E_{x^{0:T}} \left[ \ln \frac{P(x^1|x^0) \prod_{t=2}^T \overbrace{P(x^t|x^{t-1})}^{P(x^t|x^{t-1}, x^0)}}{\tilde{P}_\theta(x^T) \tilde{P}_\theta(x^0|x^1) \prod_{t=2}^T \tilde{P}_\theta(x^{t-1}|x^t)} \right] \quad (19.48)$$

$$= E_{x^{0:T}} \left[ \ln \frac{P(x^1|x^0) \prod_{t=2}^T P(x^{t-1}|x^t, x^0) \frac{P(x^t|x^0)}{P(x^{t-1}|x^0)}}{\tilde{P}_\theta(x^T) \tilde{P}_\theta(x^0|x^1) \prod_{t=2}^T \tilde{P}_\theta(x^{t-1}|x^t)} \right] \quad (19.49)$$

$$= E_{x^{0:T}} \left[ \ln \frac{P(x^1|x^0) \frac{P(x^T|x^0)}{P(x^1|x^0)} \prod_{t=2}^T P(x^{t-1}|x^t, x^0)}{\tilde{P}_\theta(x^T) \tilde{P}_\theta(x^0|x^1) \prod_{t=2}^T \tilde{P}_\theta(x^{t-1}|x^t)} \right] \quad (19.50)$$

$$= E_{x^{0:T}} \left[ \ln \frac{1}{\tilde{P}_\theta(x^0|x^1)} \cdot \frac{P(x^T|x^0)}{\tilde{P}_\theta(x^T)} \cdot \frac{\prod_{t=2}^T P(x^{t-1}|x^t, x^0)}{\prod_{t=2}^T \tilde{P}_\theta(x^{t-1}|x^t)} \right] \quad (19.51)$$

**QED**

We expect  $\tilde{P}_\theta(x^0|x^1)$  in  $\mathcal{L}^0$  to depend only very weakly on  $\theta$  because it comes at the end of the reverse Markov chain. Likewise, we expect  $\tilde{P}_\theta(x^T)$  in  $\mathcal{L}^T$  to be approximately a normal distribution independent of  $\theta$ , because it comes at the beginning of the reverse Markov chain. Hence, we are justified in using  $\mathcal{L}' = \sum_{t=2}^T \mathcal{L}^{t-1}$  as the new loss function to me minimized with respect to  $\theta$ .

**Claim 40**

$$\mathcal{L}^{t-1} = E_{x^t} \left[ \frac{1}{2(\sigma^{t-1})^2} [M^{t-1}(x^t) - M_\theta^{t-1}(x^t)]^2 \right] \quad (19.52)$$

$$= E_{x^0, w^t} \left[ \frac{(C^t)^2}{2(\sigma^{t-1})^2} \left[ w^t - n_\theta^{t-1} (\sqrt{\pi_1^\alpha} x^0 + \sqrt{1 - \pi_1^\alpha} w^t) \right]^2 \right] \quad (19.53)$$

**proof:**

Eq.(19.53) follows trivially from Eq.(19.37) and Eq.(19.52).

To show Eq.(19.52), recall that

$$\mathcal{L}^{t-1} = E_{x^{0:T}} \left[ \ln \frac{P(x^{t-1}|x^t, x^0)}{\tilde{P}_\theta(x^{t-1}|x^t)} \right] \quad (19.54)$$

The denominator  $\tilde{P}_\theta(x^{t-1}|x^t)$  is one of the TPMs for the bnet Fig.19.2 , and it's a normal distribution with mean  $M_\theta^{t-1}(x^t)$ . The numerator  $P(x^{t-1}|x^t, x^0)$  is a normal distribution too; it was calculated in the proof of Claim 37, where its mean was called  $M^{t-1}(x^t)$ . Hence, after some algebra which is left to the reader, one can show Eq.(19.52).

**QED**

Eq.(19.53) for  $\mathcal{L}^{t-1}$  is usually simplified to

$$\mathcal{L}_{simple} = E_{x^0, w^t} \left[ \left[ w^t - n_\theta^{t-1}(\sqrt{\pi_1^t \alpha} x^0 + \sqrt{1 - \pi_1^t \alpha} w^t) \right]^2 \right] \quad (19.55)$$

## 19.4 Algorithms for training and sampling DM

---

**Algorithm 2:** Algorithm for training DM (i.e., finding optimum  $\theta$ )

---

**Input :**  $\{\beta^t\}_{t=1}^T$ ,  $0 < \epsilon < 1$ ,  $n_\theta^t(x)$  function,  $\theta_{in}$ ,  $\Delta\theta_{in}$ ,  $P(x^0)$ ,  $T$ ,  $\eta > 0$

**Output:**  $\theta_{next}$  = optimal  $\theta$

$\Delta\theta = \Delta\theta_{in}$

$\theta_{next} = \theta_{in}$

**while**  $|\Delta\theta| > \epsilon$  **do**

    Choose  $x^0 \sim P(x^0)$

    Choose  $t \sim Uniform(\{1, 2, \dots, T\})$

    Choose  $w \sim \mathcal{N}(0, I)$

$\theta = \theta_{next}$

    // Gradient descent for simple loss function given by Eq.(19.55).

$\theta_{next} = \theta + \eta \partial_\theta \left[ w - n_\theta^{t-1}(\sqrt{\pi_1^t \alpha} x^0 + \sqrt{1 - \pi_1^t \alpha} w) \right]^2$

$\Delta\theta = \theta_{next} - \theta$

**return**  $\theta_{next}$

---

---

**Algorithm 3:** Algorithm for sampling DM (i.e., finding fake image  $x^0$ )

---

**Input :**  $n_\theta^t(x)$ , where  $\theta$  is optimal,  $T$ ,  $\{\alpha^t\}_{t=1}^T$ ,  $\{\sigma^t\}_{t=1}^T$

**Output:**  $x^0$  = fake image

Choose  $x^T \sim \mathcal{N}(0, I)$

**for**  $t = T, T - 1, \dots, 2, 1$  **do**

Choose  $w \sim \mathcal{N}(0, I)$  if  $t > 1$ , else  $w = 0$

*// See Eq.19.33*

$$x^{t-1} = \frac{1}{\sqrt{\alpha^t}} \left( x^t - \frac{\beta^t}{\sqrt{1-\pi_1^t \alpha}} n_\theta^{t-1}(x^t) \right) + \sigma^t w$$

**return**  $x^0$

---

# Chapter 20

## Digital Circuits

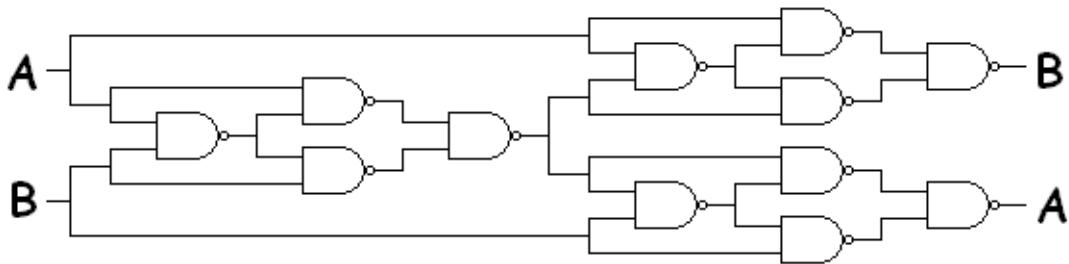


Figure 20.1: Typical digital circuit of NAND gates.

**Digital (logic) gate:** node with  $na$  input ports and  $nx$  output ports which represents a function

$$f : \{0, 1\}^{na} \rightarrow \{0, 1\}^{nx}. \quad (20.1)$$

Suppose

$$a^{na} = (a_i)_{i=0,1,\dots,na-1} \text{ where } a_i \in \{0, 1\},$$

$$x^{nx} = (x_i)_{i=0,1,\dots,nx-1} \text{ where } x_i \in \{0, 1\}.$$

$f$  maps  $a^{na}$  into  $x^{nx}$ .

**Digital circuit (dcircuit)** = circuit of digital gates.

### 20.1 Mapping any dcircuit to a bnet

#### 20.1.1 Option A of Fig.20.2

1. Replace every dcircuit gate described by Eq.(20.1) by  $nx$  bnet nodes  $\underline{x}_i$  for  $i = 0, 1, \dots, nx - 1$  such that

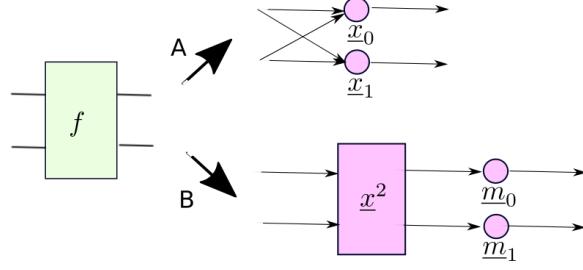


Figure 20.2: 2 options for mapping dcircuit node with multiple output ports into bnet.

$$P(x_i|a^{na}) = \delta(x_i, f_i(a^{na})) \quad (20.2)$$

2. Replace all connectors of the dcircuit by arrows pointing in the direction of the bit flow.

### 20.1.2 Option B of Fig.20.2

1. Replace every dcircuit gate described by Eq.(20.1) with one bnet node called  $x^{nx}$  and, if  $nx > 0$ ,  $nx$  “marginalizer nodes”  $\underline{m}_i$  for  $i = 0, 1, \dots, nx - 1$ , such that

$$P(x^{nx}|a^{na}) = \delta(x^{nx}, f(a^{na})) , \quad (20.3)$$

and

$$P(m_i|x^{nx}) = \delta(m_i, x_i) . \quad (20.4)$$

2. Replace all connectors of the dcircuit by arrows pointing in the direction of the bit flow.

---

Options A and B don't work for digital circuits with feedback loops such as flip-flops. Those could probably be modeled with dynamical bnets.

# Chapter 21

## Do Calculus

The Do Calculus and associated ideas were invented by Judea Pearl and collaborators. This chapter is based on Judea Pearl's books (see Chapter A).

When doing Do Calculus, it is convenient to separate the nodes of a bnet into 2 types: **observed**, and **hidden** (i.e., **unobserved**, **latent**, **unmeasured**, **non-visible**), depending on whether data describing the state of that node is available (i.e., measured) or not. In this chapter, every hidden node will be indicated in a bnet diagram by either: (1) enclosing its random variable in a dashed circle or (2) making the arrows coming out of it dashed. Accordingly, the 3 diagrams in Fig.21.1 all mean the same thing.

A **confounder node**  $\underline{c}$  for nodes  $\underline{x}$  and  $\underline{y}$  is a root node with arrows pointing from it to both  $\underline{x}$  and  $\underline{y}$ . Thus,  $\underline{c}$  acts as a **common cause** of  $\underline{x}$  and  $\underline{y}$ . In general, confounders can be either observed or hidden nodes. The word "confounder" itself just means that it confuses the analysis. It says nothing about whether it is hidden or not. The node  $\underline{c}$  in Fig.21.1) is a **hidden confounder**.

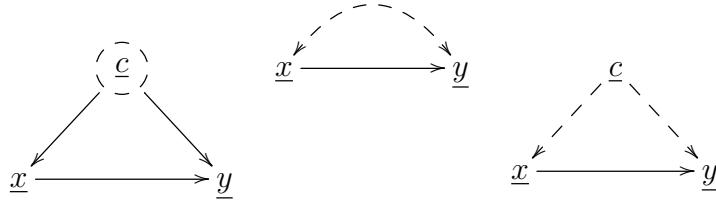


Figure 21.1: These 3 diagrams are equivalent. They mean that node  $\underline{c}$  is hidden. Node  $\underline{c}$  is implicit in the middle diagram.

Let  $\mathcal{D}_{\underline{x}}$  be an operator that acts on a graph  $G$  with a node  $\underline{x}$  by deleting all the arrows entering  $\underline{x}$ , thus converting  $\underline{x}$  into a new node  $\mathcal{D}\underline{x}$  that is a root node. Let  $\mathcal{L}_{\underline{x}}$  be an operator that acts on a graph  $G$  with a node  $\underline{x}$  by deleting all the arrows leaving  $\underline{x}$ , thus converting  $\underline{x}$  into a new node  $\mathcal{L}\underline{x}$  that is a leaf node.  $\mathcal{D}_{\underline{x}}$  and  $\mathcal{L}_{\underline{x}}$  are depicted in Fig.21.2.<sup>1</sup>

---

<sup>1</sup>Pearl uses  $\mathcal{D}_X G = G_{\overline{X}}$  and  $\mathcal{L}_X G = G_{\underline{X}}$  for a random variable  $X$  in a graph  $G$ . The way I

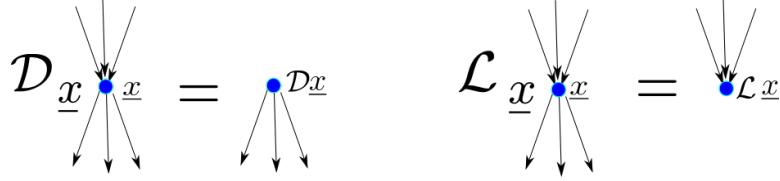


Figure 21.2: The do operator  $\mathcal{D}_{\underline{x}}$  converts node  $\underline{x}$  into a root node  $\mathcal{D}\underline{x}$ . The leaf operator  $\mathcal{L}_{\underline{x}}$  converts node  $\underline{x}$  into a leaf node  $\mathcal{L}\underline{x}$ .

If you don't know yet what we mean by a multi-node  $\underline{a}.$ , see Chapter D.

Given a bnet  $G$ , we define as follows the operators  $\mathcal{D}_{\underline{a}.}$  and  $\mathcal{L}_{\underline{a}.}$  for a multi-node  $\underline{a}..$

$$\mathcal{D}_{\underline{a}.}G = \left[ \prod_j \mathcal{D}_{\underline{a}_j} \right] G, \quad \mathcal{L}_{\underline{a}.}G = \left[ \prod_j \mathcal{L}_{\underline{a}_j} \right] G. \quad (21.1)$$

Consider a bnet whose totality of nodes is labeled  $\underline{X}..$ . Recall that

$$P(\underline{X}.) = \prod_j P(X_j | (X_k)_{k: \underline{X}_k \in pa(\underline{X}_j)}). \quad (21.2)$$

Define an operator  $\mathcal{D}$  that acts as follows<sup>2</sup>: Let  $\underline{X}. - a. = (X_k)_{k: \underline{X}_k \notin a..}$

$$P(\underline{X}. - a. | \mathcal{D}\underline{a}. = a.) = \mathcal{N}(!(\underline{X}. - a.)) \frac{P(\underline{X}.)}{\prod_{j: \underline{X}_j \in a.} P(X_j | (X_k)_{k: \underline{X}_k \in pa(\underline{X}_j)})} \quad (21.3)$$

$$= \mathcal{N}(!(\underline{X}. - a.)) \prod_{j: \underline{X}_j \notin a.} P(X_j | (X_k)_{k: \underline{X}_k \in pa(\underline{X}_j)}) \quad (21.4)$$

$$\neq P(\underline{X}. - a. | \underline{a}. = a.). \quad (21.5)$$

Also,

$$P(\mathcal{D}\underline{a}. = a.) = \delta(a', a.). \quad (21.6)$$

In words, we replace the TPM for multinode  $\underline{a}.$  by a delta function.

For instance, for the bnet

$$\underline{r} \longrightarrow \underline{x} \longrightarrow \underline{y} \quad (21.7)$$

with

$$P(r, x, y) = P(y|x)P(x|r)P(r), \quad (21.8)$$

---

remember Pearl's notation is top-in (as in topping), and bottom-out (as in butt-out).

<sup>2</sup>As usual,  $\mathcal{N}(!x)$  denotes a constant that is independent of  $x$ .

one has

$$P(r, y | \mathcal{D}\underline{x} = x) = P(y|x)P(r) \quad (21.9)$$

Hence,

$$P(y | \mathcal{D}\underline{x} = x) = P(y|x) \quad (21.10)$$

For the bnet



with

$$P(x, y, c) = P(y|x, c)P(x|c)P(c), \quad (21.12)$$

one has

$$P(y, c | \mathcal{D}\underline{x} = x) = P(y|x, c)P(c). \quad (21.13)$$

Hence,

$$P(y | \mathcal{D}\underline{x} = x) = \sum_c P(y|x, c)P(c). \quad (21.14)$$

This is called **adjusting the parents of  $\underline{x}$** .

For  $\underline{b} \subset \underline{X} - \underline{a}$ , define

$$P(b. | \mathcal{D}\underline{a} = a.) = \sum_{X. - a. - b.} P(X. - a. | \mathcal{D}\underline{a} = a.). \quad (21.15)$$

and for  $\underline{s} \subset \underline{X} - \underline{a} - \underline{b}$ , define

$$P(b. | \mathcal{D}\underline{a} = a., s.) = \frac{P(b., s. | \mathcal{D}\underline{a} = a.)}{P(s. | \mathcal{D}\underline{a} = a.)}. \quad (21.16)$$

$P(b. | \mathcal{D}\underline{a} = a., s.)$  is denoted by Pearl by  $P(b. | do(\underline{a} = a.), s.)$ . I prefer to use  $\mathcal{D}$  instead of  $do()$ . I will still call  $\mathcal{D}$  a **do operator**.

In  $P(y | \mathcal{D}\underline{x} = x)$ , node  $\underline{x}$  is turned into a root node. This guarantees that there is no confounding node connecting  $\underline{x}$  and  $\underline{y}$ . Such confounding nodes are unwelcomed when calculating causal effects between the 2 variables  $\underline{x}$  and  $\underline{y}$  because they introduce non-causal correlations between the two. This is also what happens in a **Randomized Controlled Trial (RCT)**. In an RCT with treatment  $\underline{x}$ , the value of  $\underline{x}$  for each patient is determined by a coin toss, effectively turning  $\underline{x}$  into a root node. Hence, the do operator mimics an RCT.

$P(b \cdot | \mathcal{D}\underline{a} = a, s)$  is said to be **do-identifiable** (i.e., expressible without `do()`) if it can be expressed in terms of probability distributions that only depend on observed variables, and that have no do operators in them.<sup>3</sup>

For  $\underline{x}, \underline{y} \in \{0, 1\}$ , the **average causal effect (ACE)** is defined as

$$ACE = P(y = 1 | \mathcal{D}\underline{x} = 1) - P(y = 1 | \mathcal{D}\underline{x} = 0) \quad (21.17)$$

and the **Risk Difference (RD)** is defined as

$$RD = P(y = 1 | \underline{x} = 1) - P(y = 1 | \underline{x} = 0). \quad (21.18)$$

## 21.1 3 Rules of Do Calculus

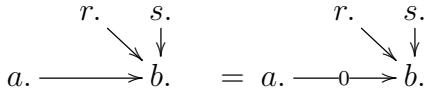
Throughout this section, suppose  $\underline{a}, \underline{b}, \underline{r}, \underline{s}$  are disjoint multinodes in a bnet  $G$ .

Recall from Chapter 23 on d-separation, that  $(\underline{b} \perp_G \underline{a} | \underline{r}, \underline{s})$  means that we have established from the d-separation rules that all paths in  $G$  from  $\underline{a}$  to  $\underline{b}$  are blocked if we condition on  $\underline{r} \cup \underline{s}$ . Recall also that:

**Rule 0:** Insertion or deletion of observations, without do operators.

If  $(\underline{b} \perp \underline{a} | \underline{r}, \underline{s})$  in  $G$ , then

✓  $P(b \cdot | \underline{a} \cdot, \underline{r} \cdot, \underline{s} \cdot) = P(b \cdot | \underline{r} \cdot, \underline{s} \cdot)$  (i.e.,  $\underline{a} = a \leftrightarrow 1$ )



✓  $H(\underline{b} \cdot : \underline{a} \cdot | \underline{r} \cdot, \underline{s} \cdot) = 0$

Zeroing an arrow is the same as deleting it. The 3 rules of Do Calculus can be presented in the same format.

- **Rule 1:** Insertion or deletion of observations

If  $(\underline{b} \perp \underline{a} | \underline{r}, \underline{s})$  in  $\mathcal{D}_{\underline{r}} G$ , then

✓  $P(b \cdot | \underline{a} \cdot, \mathcal{D}\underline{r} \cdot = r \cdot, \underline{s} \cdot) = P(b \cdot | \mathcal{D}\underline{r} \cdot = r \cdot, \underline{s} \cdot)$  (i.e.,  $\underline{a} = a \leftrightarrow 1$ )



✓  $H(\underline{b} \cdot : \underline{a} \cdot | \mathcal{D}\underline{r} \cdot, \underline{s} \cdot) = 0$

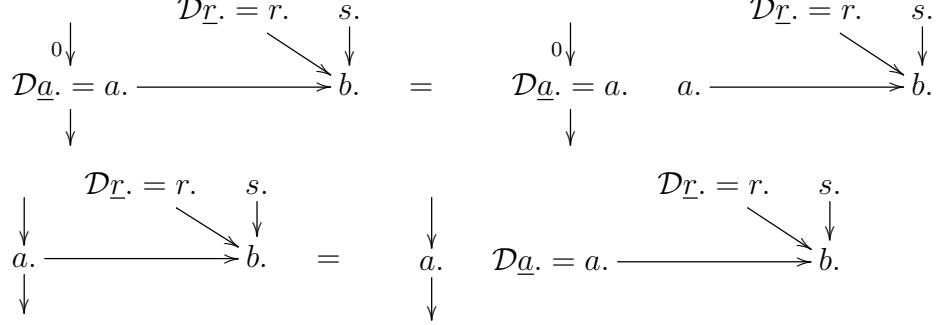
- **Rule 2:** Action or observation exchange

If  $(\underline{b} \perp \underline{a} | \underline{r}, \underline{s})$  in  $\mathcal{L}_{\underline{a}} \mathcal{D}_{\underline{r}} G$ , then

---

<sup>3</sup>In Statistics, one says a probability distribution  $P(x; \theta)$  of  $x$  that depends on a parameter  $\theta$  is **identifiable** if  $P(x; \theta_1) = P(x; \theta_2)$  implies  $\theta_1 = \theta_2$ .

$$\checkmark P(b | \mathcal{D}\underline{a}_. = a., \mathcal{D}\underline{r}_. = r., s.) = P(b | a., \mathcal{D}\underline{r}_. = r., s.) \quad (\text{i.e., } \mathcal{D}\underline{a}_. = a. \leftrightarrow a. = a.)$$



In this rule, the node is split into a  $\mathcal{D}\underline{a}_. = a.$  node and a  $a.$  node. The original node keeps the arrows, and the new node is a root node.

$$\checkmark H(\underline{b}_. : \mathcal{D}\underline{a}_. | \mathcal{D}\underline{r}_., \underline{s}_.) = H(\underline{b}_. : \underline{a}_. | \mathcal{D}\underline{r}_., \underline{s}_.)$$

- **Rule 3:** Insertion and deletion of actions

If  $(\underline{b}_. \perp \underline{a}_. | \underline{r}_., \underline{s}_.)$  in  $\mathcal{D}_{\underline{a}_.-an(\underline{s}_.)} \mathcal{D}\underline{r}_. G$ , then

$$\checkmark P(b | \mathcal{D}\underline{a}_. = a., \mathcal{D}\underline{r}_. = r., s.) = P(b | \mathcal{D}\underline{r}_. = r., s.) \quad (\text{i.e., } \mathcal{D}\underline{a}_. = a. \leftrightarrow 1)$$



$$\checkmark H(\underline{b}_. : \mathcal{D}\underline{a}_. | \mathcal{D}\underline{r}_., \underline{s}_.) = 0$$

See Fig.21.3 for a pictorial representation of these rules.

These rules have been proven to be sufficient for removing all do operators from an expression for which it is possible to do so.

Next we discuss two formulae that can be proven using Do Calculus: the backdoor and the frontdoor adjustment formulae.

The backdoor formula adjusts one multinode and the frontdoor formula adjusts two.

## 21.2 Parent Adjustment Formula

Suppose that  $\underline{x}_., \underline{y}_., \underline{z}_.$  are disjoint multinodes and their union equals the totality of all nodes of a bnet. Suppose we have data available that allows us to estimate  $P(\underline{x}_., \underline{y}_., \underline{z}_.).$  Hence, all nodes of the bnet are observable. Furthermore, suppose  $\underline{z}_. = pa(\underline{x}_.).$  In other words, we are considering the bnet



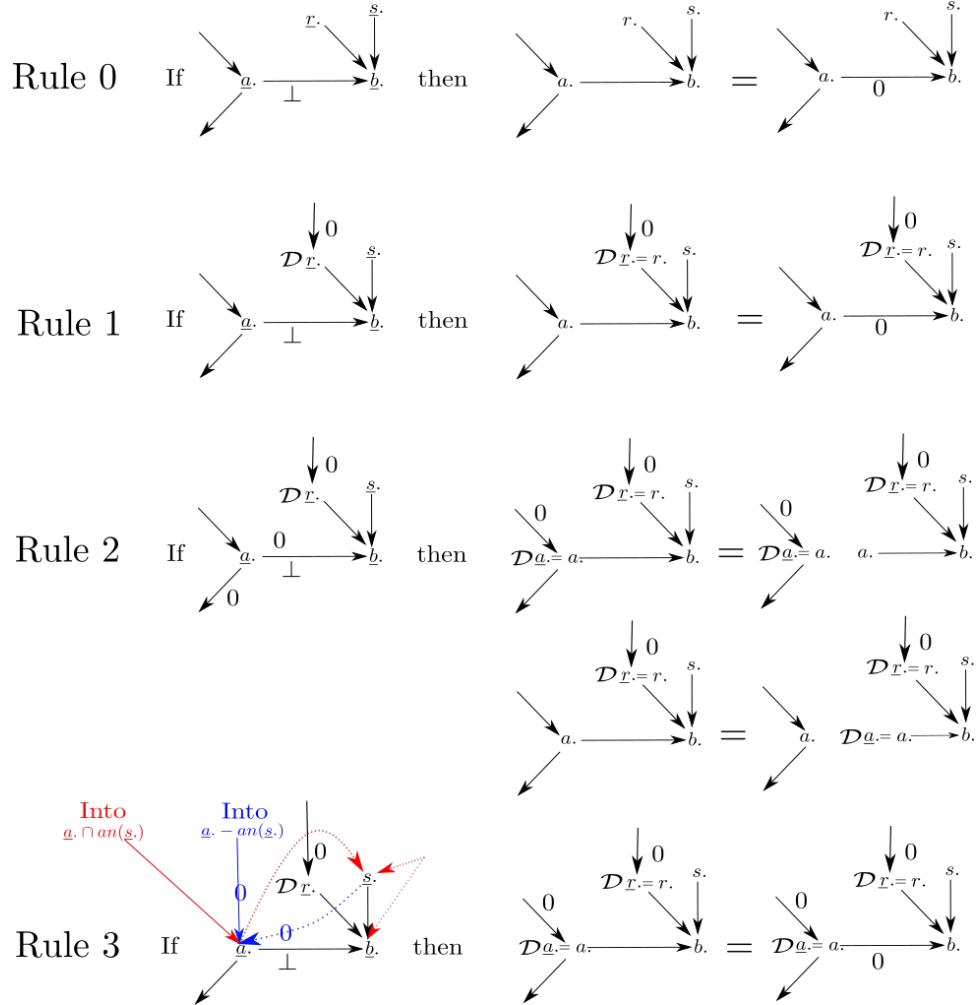


Figure 21.3: Pictorial representation of the rules of Do Calculus.  $an(\underline{s})$  stands for the ancestors of  $\underline{s}$ . In Rule 2, we zero the arrows leaving  $\underline{a}$ . and ascertain that there is no flow of info between  $\underline{a}$ . and  $\underline{b}$ . under those circumstances. In Rule 3, as shown by the dotted arrows, conditioning on  $\underline{s}$ . is enough to block paths going from  $\underline{b}$ . into  $\underline{a} \cap an(\underline{s})$ , but it is not sufficient to block paths going from  $\underline{b}$ . into  $\underline{a} \cup an(\underline{s})$ . In the example with red dotted arrows, conditioning on  $\underline{s}$ . opens a path between  $\underline{a}$ . and  $\underline{b}$ . in which  $\underline{s}$ . is a collider. That is the reason for zeroing arrows going into  $\underline{a} \cap an(\underline{s})$ , but not zeroing arrows going into  $\underline{a} \cup an(\underline{s})$ .

Then

$$P(y., z.| \mathcal{D}\underline{x}. = x.) = P(y.| x., z.)P(z.) \quad (21.20)$$

so

$$P(y.|D\underline{x}. = x.) = \sum_{z.} P(y.|x., z.)P(z.). \quad (21.21)$$

This is called **adjusting the parents** of  $\underline{x}.$ .

We say that we are **adjusting or controlling a node  $\underline{a}$**  if we condition a probability on  $\underline{a}$  and then we average that probability over  $\underline{a}$ . More generally, we can adjust a whole multinode  $\underline{a}$  together.

Next, we will introduce a generalization of this parent adjustment formula called the backdoor adjustment formula. In a backdoor adjustment formula, the adjusted multinode is not necessarily the parents of  $\underline{x}.$ .

## 21.3 Backdoor Adjustment Formula

See Chapter 4 for examples of the use of the backdoor adjustment formula. In this section, we shall mainly be concerned with proving this theorem using Do Calculus.

For any two disjoint multinodes  $\underline{x}.$  and  $\underline{y}.$ , we define a **backdoor path** from  $\underline{x}.$  to  $\underline{y}.$  as a path from  $\underline{x}.$  and  $\underline{y}.$  that starts with an arrow pointing into  $\underline{x}.$ ,

Suppose that we have access to data that allows us to estimate a probability distribution  $P(x., y., z.).$  Hence, the variables  $\underline{x}., \underline{y}., \underline{z}.$  are ALL observed (i.e, not hidden). Then we say that the backdoor  $\underline{z}.$  satisfies the **backdoor adjustment criterion** relative to  $(\underline{x}., \underline{y}.)$  if

1. All backdoor paths from  $\underline{x}.$  to  $\underline{y}.$  are blocked by conditioning on  $\underline{z}..$
2.  $\underline{z}_. \cap de(\underline{x}.) = \emptyset.$

**Motivation for BD criterion:** Part 1 rules out paths from  $\underline{x}$  to  $\underline{y}$  containing a fork node (confounder) which, if not blocked by conditioning on  $\underline{z}.$ , would introduce a non-causal correlation (confounder bias). Part 2 rules out a directed path from  $\underline{x}$  to  $\underline{y}$  that has a mediator node blocked by conditioning on  $\underline{z}.$  or a collider node unblocked by conditioning on  $\underline{z}..$

**Claim 41** (*Backdoor Adjustment Formula*)

If  $\underline{z}.$  satisfies the backdoor criterion relative to  $(\underline{x}., \underline{y}.)$ , then

$$P(y.|D\underline{x}. = x.) = \sum_{z.} P(y.|x., z.)P(z.) \quad (21.22)$$

$$= \sum_{z.} z. \quad (21.23)$$

$x. \xrightarrow{\hspace{1cm}} y.$

where  $\sum z.$  means node  $\underline{z}.$  is summed over.

**proof:**

For simplicity, let us omit the dots from the multinodes. If  $z$  satisfies the backdoor criterion relative to  $(\underline{x}, \underline{y})$ , then  $\underline{x}, \underline{y}, \underline{z}$  might have the following structure.



See Claim 45 for a proof of this claim for the special case Eq.(21.24).

**QED**

Note that the backdoor adjustment formula can be written as

$$P(y | \mathcal{D}\underline{x} = x.) = \sum_{z.} P(y | x., z.) P(z.) \quad (21.25)$$

$$= \sum_{z.} \frac{P(y., x., z.)}{P(x.|z.)} \quad (21.26)$$

This assumes  $P(x.|z.) \neq 0$  for all  $x., z..$  This assumption is referred to as **positivity**, and is violated if  $P(x.|z.) = \delta(x., x.(z.))$ .  $P(x.|z.)$  is called the **propensity score** of  $x.$  given  $z..$  This equation does **inverse probability weighting**. One can approximate  $P(x.|z.)$  in this equation to get an approximation to  $P(y | \mathcal{D}\underline{x} = x)$ .

## 21.4 Frontdoor Adjustment Formula

See Chapter 29 for examples of the use of the frontdoor adjustment formula. In this section, we shall mainly be concerned with proving this theorem using Do Calculus.

Suppose that we have access to data that allows us to estimate a probability distribution  $P(x., m., y.)$ . Hence, the variables  $\underline{x}, \underline{m}, \underline{y}$  are ALL observed (i.e, not hidden). Then we say that the frontdoor  $\underline{m}$  satisfies the **frontdoor adjustment criterion** relative to  $(\underline{x}, \underline{y})$  if

1. All directed paths from  $\underline{x}.$  to  $\underline{y}.$  are intercepted by (i.e., have a node in)  $\underline{m}..$
2. All backdoor paths from  $\underline{x}.$  to  $\underline{m}.$  are blocked.
3. All backdoor paths from  $\underline{m}.$  to  $\underline{y}.$  are blocked by conditioning on  $\underline{x}..$

**Claim 42 (Frontdoor Adjustment Formula)**

If  $\underline{m}.$  satisfies the frontdoor criterion relative to  $(\underline{x}, \underline{y})$ , and  $P(x., m.) > 0$ , then

$$P(y_{\cdot} | \mathcal{D}\underline{x}_{\cdot} = x_{\cdot}) = \sum_{m_{\cdot}} \underbrace{\left[ \sum_{x'_{\cdot}} P(y_{\cdot} | x'_{\cdot}, m_{\cdot}) P(x'_{\cdot}) \right]}_{P(y_{\cdot} | \mathcal{D}\underline{m}_{\cdot} = m_{\cdot})} \underbrace{P(m_{\cdot} | x_{\cdot})}_{P(m_{\cdot} | \mathcal{D}\underline{x}_{\cdot} = x_{\cdot})} \quad (21.27)$$

$$= \sum_{x'_{\cdot}} \xrightarrow{x_{\cdot} \longrightarrow \sum m_{\cdot} \longrightarrow y_{\cdot}} \quad (21.28)$$

where  $\sum x'_{\cdot}$ . and  $\sum m_{\cdot}$  means nodes  $\underline{x}'_{\cdot}$ . and  $\underline{m}_{\cdot}$  are summed over.

**proof:**

For simplicity, let us omit the dots from the multinodes. If  $\underline{m}$  satisfies the frontdoor criterion relative to  $(\underline{x}, \underline{y})$ , then  $\underline{x}, \underline{m}, \underline{y}$  might have the following structure, where node  $\underline{c}$  is unobserved.



See Claim 46 for a proof of this claim for the special case Eq.(21.29).

See also Ref.[47] for a proof by Pearl of the Frontdoor Adjustment Formula without using Do Calculus.

**QED**

## 21.5 Comparison of Backdoor and Frontdoor adjustment formulae

Define a **direct effect path** for a query  $P(y | \mathcal{D}\underline{x} = x, z_{\cdot})$  as a directed path that starts at  $\underline{x}$  and ends at  $\underline{y}$ . A backdoor path (i.e., one that connects  $\underline{x}$  and  $\underline{y}$  starting with an arrow pointing into  $\underline{x}$ ), is not a direct effect path; it's an **indirect effect path**.

Note that in the backdoor AF (adjustment formula), we can find a possibly empty observed multinode  $\underline{z}_{\cdot}$  such that if we condition on  $\underline{z}_{\cdot}$ , all indirect effect paths are blocked. In the frontdoor AF, we can't find a multinode  $\underline{z}_{\cdot}$  that blocks all indirect effect paths. Despite this, in the frontdoor scenario, the do-query is identifiable and an adjustment formula exists. How is that possible? The frontdoor AF uses the backdoor AF once and then it uses the backdoor AF again, a second time, on the result of the first use. The frontdoor AF replaces a sum over an unobserved node by a sum over an observed one.

## 21.6 Do operator for DEN diagrams

Recall that the structural equations for a linear DEN, as given by Eq.(48.48) of Chapter 48, are:

$$\underline{x} = A\underline{x} + \underline{u}. \quad (21.30)$$

Therefore,

$$\underline{x} = (1 - A)^{-1}\underline{u} \quad (21.31)$$

which can be represented for both linear and non-linear DEN diagrams by:

$$\underline{x}_i = x_i(\underline{u}) \quad (21.32)$$

If now we apply the operator  $\mathcal{D}_{\underline{a}=a}$  to the diagram described by the structural equations Eqs.21.30, we get the following new structural equations:

$$\underline{x}_i^* = \begin{cases} \sum_{j < i} A_{i|j} \underline{x}_j^* + \underline{u}_i & \text{if } \underline{x}_i \neq \underline{a} \\ a & \text{if } \underline{x}_i = \underline{a} \end{cases}, \quad (21.33)$$

where we are calling  $\underline{x}_i^*$  the nodes of the DEN diagram post intervention.

Eqs.(21.33) can be expressed in matrix notation as follows. Define  $\pi_{\underline{a}}$  to be the  $nx \times nx$  matrix with all entries equal to zero except for the  $(i_0, i_0)$  entry, which is 1. And define  $e_{\underline{a}}$  to be the column vector with all entries zero except for the  $i_0$ 'th one, which is 1. Here  $i_0$  is defined so that  $\underline{x}_{i_0} = \underline{a}$ . In other words,  $\pi_{\underline{a}}$  and  $e_{\underline{a}}$  are defined by

$$(\pi_{\underline{a}})_{i,j} = \mathbb{1}(i = j, \underline{a} = \underline{x}_i) \quad (21.34)$$

and

$$(e_{\underline{a}})_i = \mathbb{1}(\underline{a} = \underline{x}_i), \quad (21.35)$$

for  $i, j \in \{0, 1, \dots, nx - 1\}$ . Next define

$$\pi_{!\underline{a}} = 1 - \pi_{\underline{a}}, \quad (21.36)$$

$$A^* = \pi_{!\underline{a}} A, \quad (21.37)$$

and

$$\underline{u}_{!\underline{a}} = \pi_{!\underline{a}} \underline{u}. \quad (21.38)$$

The effect of pre-multiplying the matrix  $A$  and the column vector  $\underline{u}$  by  $\pi_{!\underline{a}}$  is to leave all rows intact except for the  $i_0$  row, which is set to zero. Here  $i_0$  is defined by  $\underline{a} = \underline{x}_{i_0}$ .

Finally, using all of the variables just defined, we can express the structural equations of the linear DEN diagram, post intervention, as

$$\underline{x}^* = A^* \underline{x}^* + \underline{u}_{!a} + ae_a . \quad (21.39)$$

Thus,

$$\underline{x}^* = (1 - A^*)^{-1}(\underline{u}_{!a} + ae_a) . \quad (21.40)$$

which can be represented for both linear and non-linear DEN diagrams by:

$$\underline{x}_i^* = x_i^*(\underline{u}_{!a}, a) . \quad (21.41)$$

For any bnet,

$$P(y = y | \underline{x} = x) = P_G(y = y | \underline{x} = x) \quad (21.42)$$

$$P(\underline{y} = y | \mathcal{D}\underline{x} = x) = P_{\mathcal{D}_{\underline{x}=x}G}(\underline{y} = y) \quad (21.43)$$

**Claim 43** *For a non-linear DEN diagram,*

$$P(y | \mathcal{D}\underline{x} = x) = E [\delta[y, y(\underline{u}_{!x}, x)]] . \quad (21.44)$$

**proof:**

$$P(\underline{y} = y | \mathcal{D}\underline{x} = x) = P_{\mathcal{D}_{\underline{x}=x}G}(\underline{y} = y) \quad (21.45)$$

$$= \sum_{u_{!x}} P(u_{!x}) P_{\mathcal{D}_{\underline{x}=x}G}(\underline{y} = y | u_{!x}) \quad (21.46)$$

$$= \sum_{u_{!x}} P(u_{!x}) \delta[y, y(u_{!x}, x)] \quad (21.47)$$

$$= E_{u_{!x}} [\delta[y, y(u_{!x}, x)]] \quad (21.48)$$

$$= E[\delta[y, y(\underline{u}_{!x}, x)]] \quad (21.49)$$

**QED**

**Claim 44** *For a nonlinear DEN diagram,*

$$E[\underline{y} | \mathcal{D}\underline{x} = x] = E[y(\underline{u}_{!x}, x)] . \quad (21.50)$$

**proof:**

$$E[\underline{y}|\mathcal{D}\underline{x} = x] = \sum_y y P(\underline{y} = y|\mathcal{D}\underline{x} = x) \quad (21.51)$$

$$= \sum_y y E[\delta[y, y(u_{!\underline{x}}, x)]] \quad (21.52)$$

$$= E[y(u_{!\underline{x}}, x)] \quad (21.53)$$

**QED**

For any bnet

$$P(y|\mathcal{D}\underline{x} = x, z) = \frac{P(y, z|\mathcal{D}\underline{x} = x)}{P(z|\mathcal{D}\underline{x} = x)} = P_{\mathcal{D}_{\underline{x}=x}G}(y|x, z) \quad (21.54)$$

For a nonlinear DEN diagram,

$$P(y, z|\mathcal{D}\underline{x} = x) = \sum_{u_{!\underline{x}}} P(u_{!\underline{x}}) \delta[y, y(u_{!\underline{x}}, x)] \delta[z, z(u_{!\underline{x}}, x)] \quad (21.55)$$

$$P(z|\mathcal{D}\underline{x} = x) = \sum_{u_{!\underline{x}}} P(u_{!\underline{x}}) \delta[z, z(u_{!\underline{x}}, x)]. \quad (21.56)$$

# Chapter 22

## Do Calculus proofs

In Chapter 21, we explained Do Calculus, but referred to this chapter for proofs of claims that use Do Calculus. In this chapter, we've aggregated all proofs, from throughout the book, of claims that use Do Calculus.

Note that even though the 3 rules of Do Calculus are great for proving adjustment formulae for general classes of DAGs, they are sometimes overkill for proving adjustment formulae for a single specific DAG. Indeed, since the 3 rules of Do Calculus are a consequence of the d-separation theorem, it follows that all adjustment formulae should be provable from first principles, assuming only the d-separation theorem and the standard rules of probability theory.

In this chapter, we use the following conventions for bnet diagrams.

Random variables are underlined and their values are not. For example,  $\underline{a} = a$  means the random variable  $\underline{a}$  takes the value  $a$ . A diagram with all its nodes underlined represents a Bayesian Network (bnet), whereas the same diagram with the letters not underlined represents a specific **instantiation** of that bnet. For example  $\underline{a} \rightarrow \underline{b} \rightarrow \underline{c}$  represents the bnet with full probability distribution  $P(c|b)P(b|a)P(a)$ , whereas  $a \rightarrow b \rightarrow c$  represents  $P(c|b)P(b|a)$ . Note that, for convenience, we define  $a \rightarrow b \rightarrow c$  to exclude the priors of root nodes such as  $P(a)$ .

If  $\underline{a}$  is a root node, then  $\sum a$  signifies a weighted sum  $\sum_a P(a)$ . For example,

$$\sum a \rightarrow b \rightarrow c = \sum_a P(c|b)P(b|a)P(a) \quad (22.1)$$

If  $\underline{a}$  is not a root node, then  $\sum a$  signifies a simple unweighted sum  $\sum_a$ . For example,

$$x \rightarrow \sum a \rightarrow y = \sum_a P(y|a)P(a|x) \quad (22.2)$$

Two bnets are equated if their full probability distributions (i.e., their full instantiations) are equal numerically. For example,

$$\underline{a} \rightarrow \underline{b} \rightarrow \underline{c} = P(c|b)P(b|a)P(a) = \underline{a} \leftarrow \underline{b} \leftarrow \underline{c} \quad (22.3)$$

Unobserved (a.k.a. hidden, latent) nodes are indicated in a bnet by enclosing their label in a dashed circle. For example,  $\langle u \rangle$ . Alternatively, they are indicated by using dashed arrows for all arrows emanating from the unobserved node.

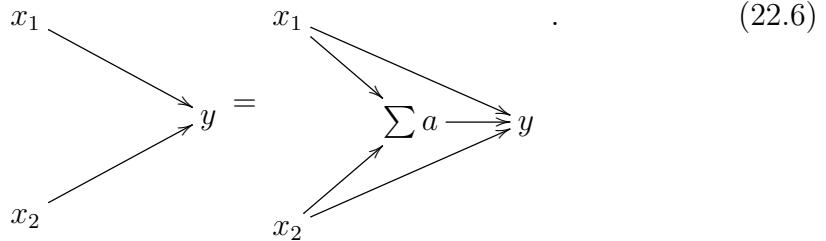
Selection diagrams with switch nodes are discussed in Chapter 96. In a selection diagram with a switch node  $s \in \{0, 1\}$ , if a node  $\underline{x}$  has parents  $pa(\underline{x})$  where  $s \notin pa(\underline{x})$ , then the TPM of  $\underline{x}$  is  $P(x|pa(\underline{x}))$ . If, on the other hand,  $\underline{x}$  has parents  $pa(\underline{x}) = pa'(\underline{x}) \cup s$ , where  $pa'(\underline{x}) = pa(\underline{x}) - s$ , then the TPM of  $\underline{x}$  is

$$P(x|pa'(\underline{x}), s) = \begin{cases} P(x|pa'(\underline{x})) & \text{if } s = 0 \\ P^*(x|pa'(\underline{x})) & \text{if } s = 1 \end{cases} \quad (22.4)$$

Some identities that are used in this chapter:

1.

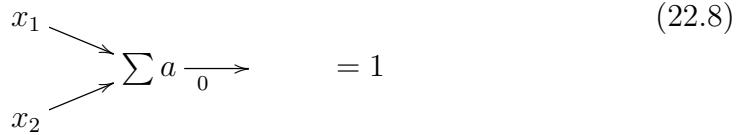
$$P(y|x_1, x_2) = \sum_a P(y|a, x_1, x_2)P(a|x_1, x_2). \quad (22.5)$$



One can describe this identity as “giving  $y$  a universal backdoor”, because  $\sum a$  is a backdoor (i.e., input) to  $y$ , and  $\sum a$  is universal in the sense that it is entered by every arrow that enters  $y$  except  $\sum a$  itself.

2.

$$\sum_a P(a|x_1, x_2) = 1 \quad (22.7)$$



One can describe this identity as “summing over the values of a collider node which has no emerging arrows”<sup>1</sup>. Eq.(22.8) can be understood as an edge case (when  $y = \emptyset$ ) of Eq.(22.6).

3.

$$\sum_a P(x_2|a)P(a|x_1) = P(x_2|x_1) \quad (22.9)$$

---

<sup>1</sup>A zeroed arrow means the same as no arrow.

$$x_1 \longrightarrow \sum a \longrightarrow x_2 = x_1 \longrightarrow x_2 \quad (22.10)$$

One can describe this identity as “summing over the values of a mediator node”.

4.

$$P(x) = \sum_a P(x|a)P(a) = \sum_b P(x|b)P(b) \quad (22.11)$$

$$P(x) = \underset{0}{\longrightarrow} \sum a \longrightarrow x = \underset{0}{\longrightarrow} \sum b \longrightarrow x \quad (22.12)$$

One can describe this identity as “averaging over different priors”. Eq.(22.12) can be understood as an edge case of Eq.(22.10).

A **do-adjustment formula** expresses a **do-query** (i.e., a conditional probability with do operators in its condition) by an equivalent expression without do operators. The equivalent expression must satisfy 2 constraints to be discussed below. If a do-adjustment formula exists for a particular do-query, then we say the do-query is **do-identifiable (DI)**. A **do-transport formula** is a relationship between 2 do-queries. This chapter deals with both do-adjustment and do-transport formulae.

See Fig.22.1 for some simple examples of bnets for which the do-query  $P(y|\mathcal{D}\underline{x} = x)$  is DI and non-DI.

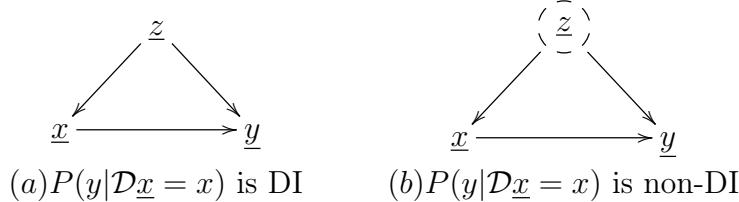


Figure 22.1: Examples of bnets for which the do-query  $P(y|\mathcal{D}\underline{x} = x)$  is DI and non-DI.

Let  $G$  be a graph before amputation of the arrows entering node  $\underline{x}$ , and let  $G_x = \mathcal{D}_{\underline{x}=x}G$  be the same graph after amputation. Also let  $P_G() = P()$  be the full probability distribution for graph  $G$ , and  $P_{G_x}()$  be that for  $G_x$ . In general, the following is always true, whether it applies to a bnet with or without hidden nodes:<sup>2</sup>

$$P(y|\mathcal{D}\underline{x} = x) = P_{G_x}(y|x) \quad (22.13)$$

---

<sup>2</sup>Note that  $P_{G_x}(y|x) \neq P_G(y|x) = P(y|x)$ . In fact,  $P_{G_x}(y|x) = P(y|x)$  iff there is no confounding, so  $P_{G_x}(y|x) \neq P(y|x)$  indicates confounding.

However, the right hand side of this equation is not a valid adjustment formula for this query because it's not expressed in terms of  $P()$ . We define a valid adjustment formula for query  $P(y|\mathcal{D}\underline{x} = x)$  to be a bnet instantiation diagram that satisfies the following 2 constraints:

1. **(structural constraint)**

The adjustment formula must be representable by a bnet instantiation that has a DAG structure identical to the DAG structure of  $G$ , except that arrows entering node  $\underline{x}$  have been amputated. All nodes of that instantiation, except nodes  $x$  and  $y$ , must be summed over.

2. **(probabilistic constraint)**

- If  $G$  has hidden nodes, these must be renamed and assigned a TPM that can be constructed from the *observable* TPMs of  $G$ .
- The observable nodes of  $G$  with hidden parents, must also be assigned a TPM that can be constructed from the *observable* TPMs of  $G$ .
- The observable nodes of  $G$  with no hidden parents, must be assigned the same TPM as they have in  $G$ .

The reason for these 2 constraints is that we want an adjustment formula to show exactly how it is calculated from the full probability distribution  $P()$ . If we don't show exactly how it is calculated (i.e., whether with or without the amputated arrows), it is impossible to distinguish between marginals of  $P()$  and  $P_{G_x}()$  such as  $P(y|x)$  and  $P_{G_x}(y|x)$ .

Based on these 2 constraints, we can easily see why the query  $P(y|\mathcal{D}\underline{x} = x)$  is DI (resp., non-DI) for bnet (a) (resp., bnet (b)) of Fig.22.1. For bnet (a), after amputating arrow  $z \rightarrow x$  and summing over node  $z$ , we get

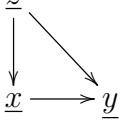
$$P(y|\mathcal{D}\underline{x} = x) = \sum z \quad (22.14)$$

The right hand side of Eq.(22.14) is a valid adjustment formula because it satisfies both constraints. For bnet (b), if we amputate arrow  $z \rightarrow x$  and sum over node  $z$ , we get

$$P(y|\mathcal{D}\underline{x} = x) = \left( \sum z \right) \quad (22.15)$$

The right hand side of Eq.(22.15) is not a valid adjustment formula because it violates the second constraint. Furthermore, try as we may, there is no way to replace the sum over hidden node  $z$  by a sum over an observed node, such that constraint 2 is satisfied.

**Claim 45** (*Backdoor Adjustment Formula*)

If  then

$$P(y|\mathcal{D}\underline{x} = x) = \sum_z P(y|x, z)P(z) \quad (22.16)$$

$$= \sum_z \begin{array}{c} z \\ \searrow \\ x \longrightarrow y \end{array} \quad (22.17)$$

**proof:**

\* **proof 1:**

$$P(y|\mathcal{D}\underline{x} = x) = \sum_z \begin{array}{c} z \\ \searrow \\ x \longrightarrow y \end{array} \quad (22.18)$$

\* **proof 2:**

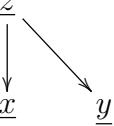
$$P(y|\mathcal{D}\underline{x} = x) = \sum_z P(y|\mathcal{D}\underline{x} = x, z)P(z|\mathcal{D}\underline{x} = x)$$

by Probability Axioms

$$= \sum_z P(y|x, z)P(z|\mathcal{D}\underline{x} = x)$$

$$P(y|\mathcal{D}\underline{x} = x, z) \rightarrow P(y|x, z)$$

by Rule 2: If  $(\underline{b} \perp \underline{a} | \underline{r}, \underline{s})$  in  $\mathcal{L}_{\underline{a}} \mathcal{D}_{\underline{r}} G$ , then  
 $\mathcal{D}_{\underline{a}} = a \leftrightarrow \underline{a} = a$ .

$\underline{y} \perp \underline{x} | \underline{z}$  in  $\mathcal{L}_{\underline{x}} \mathcal{D}_{\emptyset} G$  : 

$$= \sum_z P(y|x, z)P(z)$$

$$P(z|\mathcal{D}\underline{x} = x) \rightarrow P(z)$$

by Rule 3: If  $(\underline{b} \perp \underline{a} | \underline{r}, \underline{s})$  in  $\mathcal{D}_{\underline{a}-an(\underline{s})} \mathcal{D}_{\underline{r}} G$ , then  
 $\mathcal{D}_{\underline{a}} = a \leftrightarrow 1$

$$\underline{z} \perp \underline{x} \text{ in } \mathcal{D}_{\underline{x}} \mathcal{D}_{\emptyset} G : \underline{z} \searrow \underline{x} \longrightarrow \underline{y}$$

QED

**Claim 46** (*Frontdoor Adjustment Formula*)

$$\text{If } \begin{array}{c} (\bar{c}) \\ \diagdown \quad \diagup \\ x \longrightarrow m \longrightarrow y \end{array} \text{ then}$$

$$P(y|\mathcal{D}\underline{x} = x) = \sum_m \left[ \sum_{x'} P(y|x', m) P(x') \right] P(m|x) \quad (22.19)$$

$$= \sum x' \quad (22.20)$$

$$x \longrightarrow \sum m \longrightarrow y$$

**proof:**

\* **proof 1:**

$$P(y|\mathcal{D}\underline{x} = x) = \begin{array}{c} (\sum \bar{c}) \\ \diagdown \quad \diagup \\ x \longrightarrow \sum m \longrightarrow y \end{array} \quad (22.21)$$

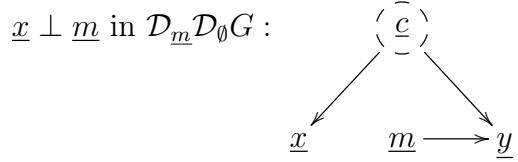
$$= \sum x' \longrightarrow \begin{array}{c} (\sum \bar{c}) \\ \diagdown \quad \diagup \\ x \longrightarrow \sum m \longrightarrow y \end{array} \quad (22.22)$$

$$= \sum x' \quad (22.23)$$

$$x \longrightarrow \sum m \longrightarrow y$$

\* **proof 2:**

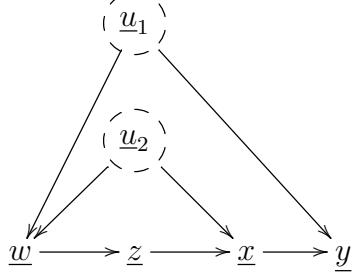
$$\begin{aligned}
P(y|\mathcal{D}\underline{x} = x) &= \sum_m P(y|\mathcal{D}\underline{x} = x, m)P(m|\mathcal{D}\underline{x} = x) \\
&\quad \text{by Probability Axioms} \\
&= \sum_m P(y|\mathcal{D}\underline{x} = x, \mathcal{D}\underline{m} = m)P(m|\mathcal{D}\underline{x} = x) \\
&\quad P(y|\mathcal{D}\underline{x} = x, m) \rightarrow P(y|\mathcal{D}\underline{x} = x, \mathcal{D}m = m) \\
&\quad \text{by Rule 2: If } (\underline{b} \perp \underline{a} | \underline{r}, \underline{s}) \text{ in } \mathcal{L}_{\underline{a}} \mathcal{D}_{\underline{r}} G, \text{ then} \\
&\quad \mathcal{D}\underline{a} = a \leftrightarrow \underline{a} = a. \\
&y \perp \underline{m} | \underline{x} \text{ in } \mathcal{L}_{\underline{m}} \mathcal{D}_{\underline{x}} G : \quad \begin{array}{c} \swarrow \quad \searrow \\ \underline{x} \longrightarrow m \end{array} \quad \begin{array}{c} \swarrow \quad \searrow \\ \underline{y} \end{array} \\
&= \sum_m P(y|\mathcal{D}\underline{x} = x, \mathcal{D}\underline{m} = m)P(m|x) \\
&\quad P(m|\mathcal{D}\underline{x} = x) \rightarrow P(m|x) \\
&\quad \text{by Rule 2: If } (\underline{b} \perp \underline{a} | \underline{r}, \underline{s}) \text{ in } \mathcal{L}_{\underline{a}} \mathcal{D}_{\underline{r}} G, \text{ then} \\
&\quad \mathcal{D}\underline{a} = a \leftrightarrow \underline{a} = a. \\
&\underline{m} \perp \underline{x} \text{ in } \mathcal{L}_{\underline{x}} \mathcal{D}_{\emptyset} G : \quad \begin{array}{c} \swarrow \quad \searrow \\ \underline{x} \quad \underline{m} \longrightarrow \underline{y} \end{array} \\
&= \sum_m P(y|\mathcal{D}\underline{m} = m)P(m|x) \\
&\quad P(y|\mathcal{D}\underline{x} = x, \mathcal{D}\underline{m} = m) \rightarrow P(y|\mathcal{D}\underline{m} = m) \\
&\quad \text{by Rule 3: If } (\underline{b} \perp \underline{a} | \underline{r}, \underline{s}) \text{ in } \mathcal{D}_{\underline{a}-an(\underline{s})} \mathcal{D}_{\underline{r}} G, \text{ then} \\
&\quad \mathcal{D}\underline{a} = a \leftrightarrow 1 \\
&y \perp \underline{x} | \underline{m} \text{ in } \mathcal{D}_{\underline{x}} \mathcal{D}_{\underline{m}} G : \quad \begin{array}{c} \swarrow \quad \searrow \\ \underline{x} \quad \underline{m} \longrightarrow \underline{y} \end{array} \\
&= \sum_{x'} \sum_m P(y|\mathcal{D}\underline{m} = m, x')P(x'|\mathcal{D}\underline{m} = m)P(m|x) \\
&\quad \text{by Probability Axioms} \\
&= \sum_{x'} \sum_m P(y|m, x')P(x'|\mathcal{D}\underline{m} = m)P(m|x) \\
&\quad P(y|\mathcal{D}\underline{m} = m, x') \rightarrow P(y|m, x') \\
&\quad \text{by Rule 2: If } (\underline{b} \perp \underline{a} | \underline{r}, \underline{s}) \text{ in } \mathcal{L}_{\underline{a}} \mathcal{D}_{\underline{r}} G, \text{ then} \\
&\quad \mathcal{D}\underline{a} = a \leftrightarrow \underline{a} = a. \\
&y \perp \underline{m} | \underline{x} \text{ in } \mathcal{L}_{\underline{m}} \mathcal{D}_{\emptyset} G : \quad \begin{array}{c} \swarrow \quad \searrow \\ \underline{x} \longrightarrow \underline{m} \end{array} \quad \begin{array}{c} \swarrow \quad \searrow \\ \underline{y} \end{array} \\
&= \sum_{x'} \sum_m P(y|m, x')P(x')P(m|x) \\
&\quad P(x'|\mathcal{D}\underline{m} = m) \rightarrow P(x') \\
&\quad \text{by Rule 3: If } (\underline{b} \perp \underline{a} | \underline{r}, \underline{s}) \text{ in } \mathcal{D}_{\underline{a}-an(\underline{s})} \mathcal{D}_{\underline{r}} G, \text{ then} \\
&\quad \mathcal{D}\underline{a} = a \leftrightarrow 1
\end{aligned}$$



QED

**Claim 47** (*Napkin problem from Ref.[56]*)

If then



$$P(y|\mathcal{D}\underline{x} = x) = \sum_{w,z,z',x'} P(y|x, z') P(w|z', x') P(z') P(x') P(z|w) \quad (22.24)$$

$$= \begin{array}{ccc} \sum z' & & \\ \sum x' & & \\ \sum w \longrightarrow \sum z & & x \longrightarrow y \end{array} \quad (22.25)$$

Note that  $x'$  and  $z'$  can be swapped, and we still get a valid adjustment formula. So there can be more than one adjustment formula!

**proof:**

$$P(y|\mathcal{D}\underline{x} = \underline{x}) = \begin{array}{c} (\sum u_1) \\ \swarrow \quad \searrow \\ \sum w \longrightarrow \sum z \end{array} \quad (22.26)$$

$$= \begin{array}{c} (\sum u_1) \leftarrow \sum z' \\ \swarrow \quad \searrow \\ (\sum u_2) \end{array} \quad (22.27)$$

$$= \begin{array}{c} (\sum u_1) \leftarrow \sum x' \\ \swarrow \quad \searrow \\ (\sum u_2) \end{array} \quad (22.28)$$

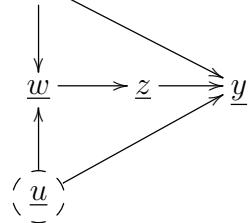
$$\begin{array}{c} \sum z' \\ \swarrow \quad \searrow \\ \sum w \longrightarrow \sum z \end{array}$$

$$x \longrightarrow \underline{y}$$

QED

**Claim 48** (from Ref.[56])

If  $\begin{array}{c} \underline{x} \\ \downarrow \\ w \longrightarrow z \longrightarrow \underline{y} \\ \uparrow \\ (\underline{u}) \end{array}$  then



$$P(y|\mathcal{D}\underline{z} = z, \underline{x}) = \sum_w P(y|z, \underline{x}, w)P(w) \quad (22.29)$$

$$= \begin{array}{c} x \\ \searrow \\ \sum w \end{array} \quad (22.30)$$

$$\begin{array}{c} z \\ \searrow \\ \sum w \end{array} \quad z \longrightarrow \underline{y}$$

**proof:**

$$P(y|\mathcal{D}\underline{z} = z, x) = \begin{array}{c} x \\ \downarrow \\ \sum w \\ \uparrow \\ (\sum u) \\ \bar{x} \\ \downarrow \\ \sum w \\ \uparrow \\ (\sum u) \end{array} \quad (22.31)$$

$$= \begin{array}{c} x \\ \downarrow \\ \sum w \\ \uparrow \\ (\sum u) \\ \bar{x} \\ \downarrow \\ \sum w \\ \uparrow \\ (\sum u) \end{array} \quad (22.32)$$

$$= \begin{array}{c} x \\ \downarrow \\ \sum w \\ \uparrow \\ (\sum u) \\ \bar{x} \\ \downarrow \\ \sum w' \\ \uparrow \\ (\sum u) \end{array} \quad (22.33)$$

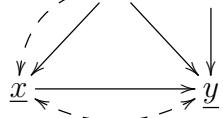
$$= \begin{array}{c} x \\ \downarrow \\ \sum w \\ \uparrow \\ (\sum w') \\ \bar{x} \\ \downarrow \\ \sum w \\ \uparrow \\ (\sum w') \end{array} \quad (22.34)$$

$$\sum w \quad z \rightarrow\!\!\! \rightarrow y$$

QED

**Claim 49** (*Trivial Memoryless Transportability, from Ref.[54]*)

If  $\underline{z} \rightarrow\!\!\! \rightarrow \underline{s}$  where  $\underline{s} \in \{0, 1\}$  is a switch node, then

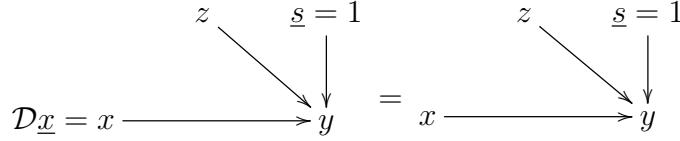


$$P^*(y|\mathcal{D}\underline{x} = x, z) = P^*(y|x, z) \quad (\text{replace } \mathcal{D} \text{ by } 1, \text{ keep } P^*) \quad (22.35)$$

$$\mathcal{D}\underline{x} = x \xrightarrow{\quad} y \quad = \quad x \xrightarrow{\quad} y \quad (22.36)$$

**proof:**

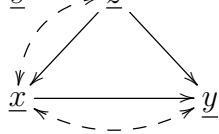
$$P(y|\mathcal{D}\underline{x} = x, z, \underline{s} = 1) = P(y|x, z, \underline{s} = 1)$$



**QED**

**Claim 50** (*Direct Transportability, a.k.a. External Validity, from Ref.[54]*)

If  $\underline{s} \xrightarrow{\quad} z$  where  $\underline{s} \in \{0, 1\}$  is a switch node, then



$$P^*(y|\mathcal{D}\underline{x} = x, z) = P(y|\mathcal{D}\underline{x} = x, z) \quad (\text{replace } P^* \text{ by } P, \text{ keep } \mathcal{D}) \quad (22.37)$$

$$\begin{array}{ccc} \underline{s} = 1 \longrightarrow z & & z \\ \swarrow & \searrow & \downarrow \\ \mathcal{D}\underline{x} = x \longrightarrow y & = & \mathcal{D}\underline{x} = x \longrightarrow y \end{array} \quad (22.38)$$

Furthermore,

$$P^*(y|\mathcal{D}\underline{x} = x) = \sum_z P(y|\mathcal{D}\underline{x} = x, z)P^*(z) \quad (22.39)$$

$$\begin{array}{ccc} \underline{s} = 1 & & \underline{s} = 1 \longrightarrow \sum z \\ \searrow & & \swarrow \\ \mathcal{D}\underline{x} = x \longrightarrow y & = & \mathcal{D}\underline{x} = x \longrightarrow y \end{array} \quad (22.40)$$

**proof:**

$$P(y|\mathcal{D}\underline{x} = x, z, \underline{s} = 1) = P(y|\mathcal{D}\underline{x} = x, z)$$

$$\begin{array}{ccc} \underline{s} = 1 \longrightarrow z & & z \\ \swarrow & \searrow & \downarrow \\ \mathcal{D}\underline{x} = x \longrightarrow y & = & \mathcal{D}\underline{x} = x \longrightarrow y \end{array} \quad \text{Because } \underline{s} \perp \underline{y} | \underline{z}$$

Furthermore,

$$P(y|\mathcal{D}\underline{x} = x, \underline{s} = 1) = \sum_z P(y|\mathcal{D}\underline{x} = x, z)P(z|\underline{s} = 1)$$

$\underline{s} = 1 \longrightarrow \sum z$   
  
 $\mathcal{D}\underline{x} = x \longrightarrow y$

QED

**Claim 51** (*S-Admissible Transportability, from Ref.[54]*)

If  $\underline{s} \xrightarrow{\text{---}} (\underline{z}) \xrightarrow{\text{---}} \underline{a}$  where  $\underline{s} \in \{0, 1\}$  is a switch node, then

$\underline{x} \xrightarrow{\text{---}} y$

$$P^*(y|\mathcal{D}\underline{x} = x) = \sum_a P(y|\mathcal{D}\underline{x} = x, a)P^*(a) \quad (22.41)$$

$$\begin{array}{ccc} \underline{s} = 1 & & \underline{s} = 1 \longrightarrow \sum a \\ \searrow & & \downarrow \\ \mathcal{D}\underline{x} = x \longrightarrow y & = & \mathcal{D}\underline{x} = x \longrightarrow y \end{array} \quad (22.42)$$

proof:

$$P(y|\mathcal{D}\underline{x} = x, \underline{s} = 1) = \sum_a P(y|\mathcal{D}\underline{x} = x, a)P(a|\underline{s} = 1)$$

$\underline{s} = 1 \longrightarrow (\sum z) \longrightarrow \sum a$   
  
 $\mathcal{D}\underline{x} = x \longrightarrow y$

QED

**Claim 52** (*Non-transportability, from Ref.[54]*)

If  $\underline{s} \xrightarrow{\text{---}} (\underline{h}) \xrightarrow{\text{---}} \underline{s}$  where  $\underline{s} \in \{0, 1\}$  is a switch node, then

$\underline{x} \longrightarrow y$

$$P^*(y|\mathcal{D}\underline{x} = x) = P^*(y|\mathcal{D}\underline{x} = x) \quad (22.43)$$

$$\begin{array}{ccc}
 & \underline{s} = 1 & \\
 & \downarrow & \\
 \mathcal{D}\underline{x} = x & \xrightarrow{\hspace{2cm}} & y = \text{same}
 \end{array} \tag{22.44}$$

**proof:**

$$P^*(y|\mathcal{D}\underline{x} = x) = P^*(y|\mathcal{D}\underline{x} = x)$$

$$\begin{array}{ccc}
 & \left( \sum h \right) & \underline{s} = 1 \\
 & \swarrow \searrow & \downarrow \\
 \mathcal{D}\underline{x} = x & \xrightarrow{\hspace{2cm}} & y = \mathcal{D}\underline{x} = x \xrightarrow{\hspace{2cm}} y \quad \underline{s} = 1
 \end{array}$$

Can't replace  $\mathcal{D}\underline{x} = x$  by  $x$  because  $y \not\perp \underline{x}$  in  $\mathcal{L}_{\underline{x}}G$ . Hence, Rule 2 not satisfied.

**QED**

**Claim 53** (*from Ref.[54]*)

$$\begin{array}{c}
 \text{If } \underline{s} \xrightarrow{\hspace{1cm}} \left( \sum h \right) \xrightarrow{\hspace{1cm}} z \text{ where } \underline{s} \in \{0, 1\} \text{ is a switch node, then} \\
 \begin{array}{c}
 \xrightarrow{\hspace{1cm}} \left( \sum h \right) \xrightarrow{\hspace{1cm}} z \\
 \swarrow \quad \searrow \\
 x \xrightarrow{\hspace{1cm}} y
 \end{array}
 \end{array}$$

$$P^*(y|\mathcal{D}\underline{x} = x) = P(y|\mathcal{D}\underline{x} = x) \tag{22.45}$$

$$\underline{s} = 1 \quad \mathcal{D}\underline{x} = x \xrightarrow{\hspace{2cm}} y = \mathcal{D}\underline{x} = x \xrightarrow{\hspace{2cm}} y \tag{22.46}$$

$$\mathcal{D}\underline{x} = x \xrightarrow{\hspace{2cm}} y = \mathcal{D}\underline{x} = x \xrightarrow{\hspace{2cm}} y$$

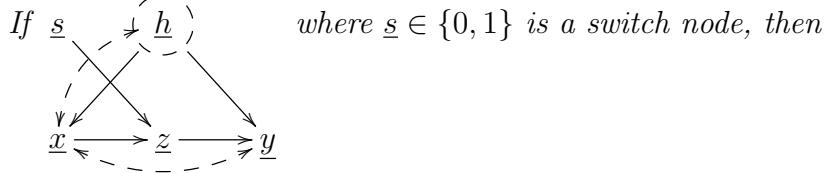
**proof:**

$$P(y|\mathcal{D}\underline{x} = x, \underline{s} = 1) = \sum_h P(y|\mathcal{D}\underline{x} = x, h)P(h)$$

$$\begin{array}{ccc}
 & \underline{s} = 1 \xrightarrow{\hspace{1cm}} \left( \sum h \right) \xrightarrow{\hspace{1cm}} \sum z & \\
 & & \left( \sum h \right) \xrightarrow{\hspace{1cm}} y \\
 & \mathcal{D}\underline{x} = x \xrightarrow{\hspace{2cm}} y & = \mathcal{D}\underline{x} = x \xrightarrow{\hspace{2cm}} y \\
 & = P(y|\mathcal{D}\underline{x} = x) & \\
 & = \mathcal{D}\underline{x} = x \xrightarrow{\hspace{2cm}} y &
 \end{array}$$

**QED**

**Claim 54** (from Ref.[54])

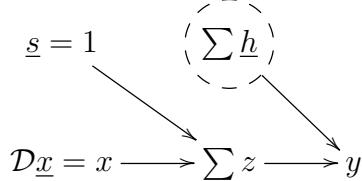


$$P^*(y|\mathcal{D}\underline{x} = x) = \sum_z P(y|\mathcal{D}\underline{x} = x, z)P^*(z|x) \quad (22.47)$$

$$\begin{array}{ccc} \underline{s} = 1 & \mathcal{D}\underline{x} = x & \underline{s} = 1 \\ \searrow & \downarrow & \searrow \\ & y & \\ = & & \\ & x \longrightarrow \sum z \longrightarrow y & \end{array} \quad (22.48)$$

**proof:**

$$P(y|\mathcal{D}\underline{x} = x, \underline{s} = 1) = \sum_h \sum_z P(y|h, z)P(h)P(z|\mathcal{D}\underline{x} = x, \underline{s} = 1)$$

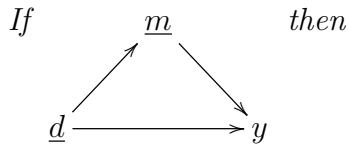


$$= \sum_h \sum_z P(y|h, z)P(h|\mathcal{D}\underline{x} = x)P(z|x, \underline{s} = 1)$$

$$\begin{array}{ccc} \underline{s} = 1 & (\sum h) & \mathcal{D}\underline{x} = x \\ \searrow & \swarrow & \downarrow \\ & \sum z \longrightarrow y & \\ = & & \\ & x \longrightarrow \sum z \longrightarrow y & \\ = & & \\ & \sum_z P(y|\mathcal{D}\underline{x} = x, z)P(z|x, \underline{s} = 1) & \\ \underline{s} = 1 & & \mathcal{D}\underline{x} = x \\ \searrow & & \downarrow \\ & \sum z \longrightarrow y & \end{array}$$

**QED**

**Claim 55** (Unconfounded Mediation, from Ref.[53])



$$P(y|\mathcal{D}\underline{d} = d, \mathcal{I}\underline{m}\underline{d} = d') = \sum_m P(y|d, m)P(m|d') \quad (22.49)$$

$$\begin{array}{ccc} \mathcal{I}\underline{d} = d' & & \mathcal{I}\underline{d} = d' \longrightarrow \sum m \\ \searrow & & \swarrow \\ \mathcal{D}\underline{d} = d \longrightarrow y & = & \mathcal{D}\underline{d} = d \longrightarrow y \end{array} \quad (22.50)$$

**proof:**

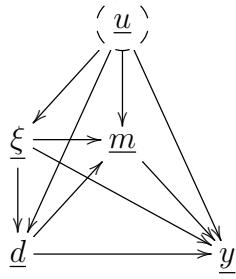
$$P(y|\mathcal{D}\underline{d} = d, \mathcal{I}\underline{d} = d') = \sum_m P(y|d, m)P(m|d')$$

$$\begin{array}{ccc} \mathcal{I}\underline{d} = d' \longrightarrow \sum m & & \\ \searrow & & \\ \mathcal{D}\underline{d} = d \longrightarrow y & & \end{array}$$

**QED**

**Claim 56** (*Mediation with universal prior  $\xi$  and universal confounder  $\underline{u}$ , from Ref.[53]*)

If  $\xi \rightarrow (\underline{u})$  then

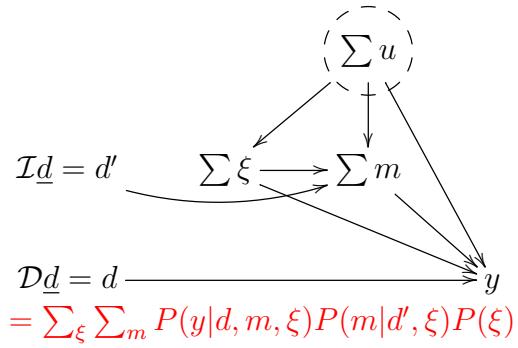


$$P(y|\mathcal{D}\underline{d} = d, \mathcal{I}\underline{m}\underline{d} = d') = \sum_{\xi} \sum_m P(y|d, m, \xi)P(m|d', \xi)P(\xi) \quad (22.51)$$

$$\begin{array}{ccc} \mathcal{I}\underline{d} = d' & & \mathcal{I}\underline{d} = d' \xrightarrow{\sum \xi} \sum m \\ \searrow & & \swarrow \\ \mathcal{D}\underline{d} = d \longrightarrow y & = & \mathcal{D}\underline{d} = d \longrightarrow y \end{array} \quad (22.52)$$

**proof:**

$$P(y|\mathcal{D}\underline{d} = d, \mathcal{I}\underline{d} = d') = \sum_{\xi,u} \sum_m P(y|d, m, \xi, u)P(m|d', \xi, u) \underbrace{P(\xi|u)P(u)}_{P(\xi,u)}$$



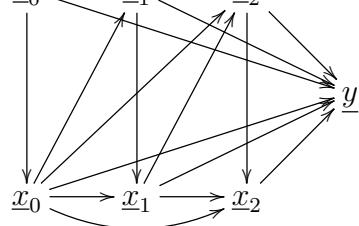
We switch from averaging over the prior of  $\xi, u$  to averaging over the prior of  $\xi$ .

$$\begin{array}{ccc} \mathcal{I}\underline{d} = d' & \sum \xi & \longrightarrow \sum m \\ & \curvearrowleft & \searrow \\ = & \mathcal{D}\underline{d} = d & \longrightarrow y \end{array}$$

QED

**Claim 57** (Sequential backdoor (SBD) adjustment formula, from Ref.[57])

If  $\underline{\underline{z}}_0 \xrightarrow{\quad} \underline{\underline{z}}_1 \xrightarrow{\quad} \underline{\underline{z}}_2$  then



$$P(y|\mathcal{D}\underline{x}^3 = x^3) = \mathcal{Q}(y|x^3) \quad (22.53)$$

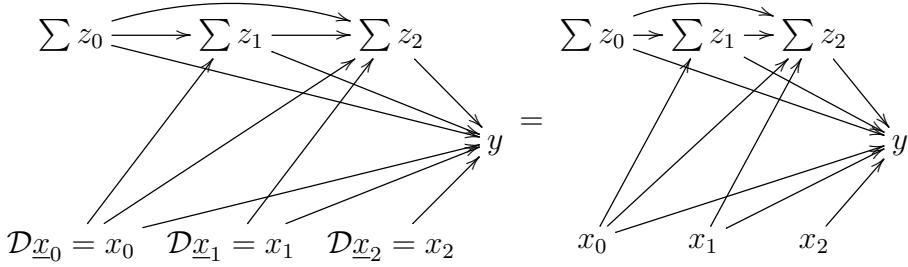
$$\sum z_0 \overbrace{\longrightarrow}^{} \sum z_1 \overbrace{\longrightarrow}^{} \sum z_2 \quad (22.54)$$

$$\mathcal{D}\underline{x}^3 = x^3 \longrightarrow y =$$

The result shown here for  $n = 3$  is true for any integer  $n \geq 1$ .

**proof:**

$$P(y|\mathcal{D}\underline{x}^3 = x^3) = \mathcal{Q}(y|x^3)$$



We can replace  $\mathcal{D}\underline{x}_i = x_i$  by  $x_i$  once all nodes in bnet are observed nodes.

**QED**

**Claim 58** (*Selection Bias (SB) Backdoor Adjustment Formula, from Ref.[3]*)

If  $\underline{s} \xrightarrow{\quad} \underline{z}^{<\underline{x}} \xrightarrow{\quad} \underline{z}^{>\underline{x}}$  where  $\underline{s} \in \{0, 1\}$  is a switch node and  $\underline{z} = (\underline{z}^{<\underline{x}}, \underline{z}^{>\underline{x}})$ , then

$$P(y|\mathcal{D}\underline{x} = x, \underline{s} = 1) = \sum_z P(y|x, z)P(z) = P(y|x) \quad (22.55)$$

$$\begin{array}{ccc} \underline{s} = 1 & & \sum z \\ \searrow & & \downarrow \\ \mathcal{D}\underline{x} = x \longrightarrow y & = & x \longrightarrow y \end{array} = x \longrightarrow y \quad (22.56)$$

**proof:**

$$P(y|\mathcal{D}\underline{x} = x, \underline{s} = 1) = \sum_z P(y|\mathcal{D}\underline{x} = x, z)P(z^{<\underline{x}}|\underline{s} = 1)P(z^{>\underline{x}}|x, z^{<\underline{x}}, \underline{s} = 1)$$

$$\begin{aligned} & \underline{s} = 1 \xrightarrow{\quad} \sum z^{<\underline{x}} \xrightarrow{\quad} \sum z^{>\underline{x}} \\ & \mathcal{D}\underline{x} = x \longrightarrow y \\ &= \sum_{z^{<\underline{x}}} P(y|\mathcal{D}\underline{x} = x, z^{<\underline{x}})P(z^{<\underline{x}}|\underline{s} = 1) \\ &= \underline{s} = 1 \longrightarrow \sum z^{<\underline{x}} \\ &= \mathcal{D}\underline{x} = x \longrightarrow y \\ &= \sum_z P(y|x, z)P(z|\underline{s} = 1) \end{aligned}$$

$$\begin{aligned}
& \underline{s} = 1 \longrightarrow \sum z & \mathcal{D} \text{ can be removed because there are} \\
& = \quad \downarrow & \text{no sums over unobserved nodes.} \\
& = x \longrightarrow y & \\
& = \sum_z P(y|x, z)P(z) & \underline{s} = 1 \text{ node can be removed} \\
& & \text{because this expression must} \\
& \sum z & \text{equal } P(y|x, \underline{s} = 1). \text{ Furthermore,} \\
& \downarrow & \underline{y} \perp \underline{s}|(\underline{x}, \underline{z}) \text{ in the hypothesis bnet.} \\
& = x \longrightarrow y & \text{Hence, this expression must also} \\
& & \text{equal } P(y|x).
\end{aligned}$$

**QED**

# Chapter 23

## D-Separation

Before reading this chapter, I recommend that you read Chapter D.

A path  $\gamma$  that isn't a loop can have 3 types of intermediate nodes  $\underline{x}$  (an intermediate node of  $\gamma$  is a node in  $\gamma$  that isn't one of the two end nodes). Suppose  $\underline{a}, \underline{b} \in \gamma$  are the two neighbors of  $\underline{x}$ . Then the 3 possible cases are:

1.  **$\underline{x}$  is a mediator node:**  $(\underline{a} \leftarrow \underline{x} \leftarrow \underline{b})$  or  $(\underline{a} \rightarrow \underline{x} \rightarrow \underline{b})$
2.  **$\underline{x}$  is a fork node:**  $(\underline{a} \leftarrow \underline{x} \rightarrow \underline{b})$
3.  **$\underline{x}$  is a collider node:**  $(\underline{a} \rightarrow \underline{x} \leftarrow \underline{b})$

We say that a non-loop path  $\gamma$  from  $\underline{a}$  to  $\underline{b}$  (i.e., with end nodes  $\underline{a}, \underline{b}$ ) is **blocked** by conditioning on a multinode  $\underline{Z}$ , if one or more of the following statements is true:

1. There is a node  $\underline{x} \in \underline{Z}$ , which is a mediator or a fork of  $\gamma$ .
2.  $\gamma$  contains a collider node  $\underline{c}$  and  $(\underline{c} \cup de(\underline{c})) \cap \underline{Z} = \emptyset$  (i.e., neither  $\underline{c}$  nor any of the descendants of  $\underline{c}$  is contained in  $\underline{Z}$ .)

This definition of a blocked path<sup>1</sup> is easy to remember if one thinks of the following analogy with pipes carrying a fluid. Think of path  $\gamma$  as if it were a pipe carrying a fluid. Think of the nodes of  $\gamma$  as junctions in the pipe. If  $\underline{Z}$  intersects  $\gamma$  at either a mediator or a fork junction, that blocks the pipe flow. A collider junction  $\underline{c}$  is like a blackhole or a huge leak. Its presence blocks passage of the fluid as long as neither  $\underline{c}$  nor any of the descendants of  $\underline{c}$  are in  $\underline{Z}$ . If, on the other hand,  $\underline{c} \in \underline{Z}$ , or  $\underline{c}' \in \underline{Z}$ , where  $\underline{c}' \in de(\underline{c})$ , then that acts as a complete (in the case of  $\underline{c} \in \underline{Z}$ ) or a partial (in the case of  $\underline{c}' \in \underline{Z}$ ) bridge across the blackhole.

See Fig.23.1 for some examples of paths that are blocked or not blocked by conditioning on a multinode  $\underline{Z}$ .

---

<sup>1</sup>Note that we speak of blocked paths or info, not of blocked nodes. Nodes are not blocked; rather they are either conditioned upon or not.

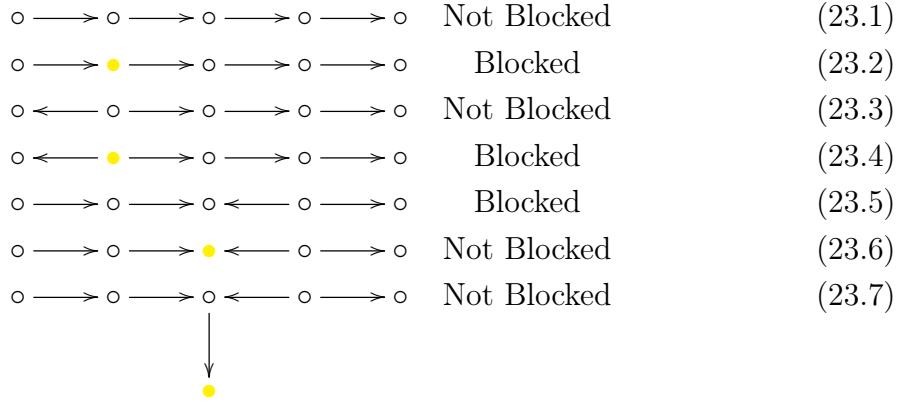


Figure 23.1: Examples of paths that are blocked or not blocked by conditioning on a multinode  $\underline{Z}.$  Nodes belonging to  $\underline{Z}.$  are colored yellow.

Given 3 disjoint multinode  $\underline{A}., \underline{B}., \underline{Z}.$  of a graph  $G$ , we write “ $\underline{A}. \perp_G \underline{B}.|\underline{Z}.$ ” or say “ $\underline{A}.$  and  $\underline{B}.$  are **d-separated** by  $\underline{Z}.$  in  $G$ ” iff there exists no path  $\gamma$  from  $\underline{a} \in \underline{A}.$  to  $\underline{b} \in \underline{B}.$  which is not blocked by conditioning on  $\underline{Z}.$ .<sup>2</sup>

The minimal Markov blanket (see Chapter 50) of a node  $\underline{a}$  is the smallest multinode  $\underline{Z}.$  such that  $\underline{a} \perp_G \underline{b}|\underline{Z}.$  for all  $\underline{b} \notin \underline{a} \cup \underline{Z}.$

We are finally ready to state the d-separation theorem, without proof.

A probability distribution  $P$  is **compatible with a DAG**  $G$  if  $P$  and  $G$  have the same random variables, and they can be combined to form a bnet without contradictions; i.e., one can calculate all the TPMs from  $P$  and multiply them together to obtain  $P$  again.

### Claim 59 (d-separation Theorem)

Suppose  $\underline{A}., \underline{B}., \underline{Z}.$  are disjoint multinode of a DAG  $G$ .

If  $\underline{A}. \perp_G \underline{B}.|\underline{Z}.$ , then  $P(\underline{B}.|\underline{A}.,\underline{Z}.) = P(\underline{B}.|\underline{Z}.)$  for all  $\underline{B}., \underline{A}., \underline{Z}.$ , for all  $P$  compatible with  $G$ .

The full converse of the theorem can also be proven, but we won't be using it in this book.

Often, the right hand side of this theorem is stated as “ $\underline{A}. \perp_P \underline{B}.|\underline{Z}.$  for all  $P$ ”. Then the theorem is stated: “If  $\underline{A}. \perp_G \underline{B}.|\underline{Z}.$ , then  $\underline{A}. \perp_P \underline{B}.|\underline{Z}.$  for all  $P$ .”

---

Note that the following are equivalent:

- $P(\underline{B}.|\underline{A}.,\underline{Z}.) = P(\underline{B}.|\underline{Z}.)$  for all  $\underline{B}., \underline{A}., \underline{Z}..$
- $\underline{A}. \perp_P \underline{B}.|\underline{Z}.$

---

<sup>2</sup> $\underline{Z}.$  are the nodes we are “conditioning on”. Unmeasured (i.e., hidden, unobserved) nodes cannot be conditioned on, because that would entail measuring them.

- $H(\underline{A}_. : \underline{B}_. | \underline{Z}_.) = 0$  (see Chapter C for definition of conditional mutual information (CMI))

---

**Extra stuff: mostly only for pure mathematicians**

Below, we will use the notation  $nde(\underline{a})$  to denote all non-descendants, including  $\underline{a}$  itself, of a node  $\underline{a}$  in a DAG  $G$ ; i.e., all nodes of  $G$  that are not in  $de(\underline{a}) \cup \underline{a}$ , where  $de(\underline{a})$  is defined in Chapter D.

Given a DAG  $G$ , define the following sets of d-separations:<sup>3</sup>

$$DS(G) = \{(\underline{A}_. \perp_G \underline{B}_. | \underline{Z}_.) : \underline{A}_., \underline{B}_., \underline{Z}_. \text{ are multinodes of } G\} . \quad (23.8)$$

$$DS_{min}(G) = \{(\underline{A}_. \perp_G nde(\underline{A}_.) | pa(\underline{A}_.)) : \underline{A}_. \text{ is a multinode of } G\} . \quad (23.9)$$

See Chapter 67 for an example where set  $DS_{min}(G)$  is calculated for a particular DAG  $G$ .

**Claim 60** *For all DAGs  $G$ ,  $DS(G) = DS_{min}(G)$ .*

Given a probability distribution  $P$ , define the following set of conditional independencies:

$$CI(P) = \{(\underline{A}_. \perp_P \underline{B}_. | \underline{Z}_.) : \underline{A}_., \underline{B}_., \underline{Z}_. \text{ are multinodes of } P\} , \quad (23.10)$$

For a DAG  $G$  and a probability distribution  $P$  compatible with  $G$ , define a map  $\phi$  by

$$\phi : DS_{min}(G) \rightarrow CI(P) \quad (23.11)$$

$$\phi : \underline{A}_. \perp_G nde(\underline{A}_.) | pa(\underline{A}_.) \mapsto \underline{A}_. \perp_P nde(\underline{A}_.) | pa(\underline{A}_.) \quad (23.12)$$

In general, this map is 1-1 but not onto.

**Claim 61** *For a bnet with a DAG  $G$  and a total probability distribution  $P$ , the map  $\phi$  is a bijection.*

$DS(G)$  does not fully specify a DAG. DAGs with the same  $DS(G)$  are said to be **d-separation equivalent**. See Chapter 67 for more info about d-separation equivalence.

---

<sup>3</sup>Note that  $(\underline{A}_. \perp_G nde(\underline{A}_.) | pa(\underline{A}_.))$  and  $(\underline{A}_. \perp_G nde(\underline{A}_.) - pa(\underline{A}_.) | pa(\underline{A}_.))$  are equivalent because  $H(\underline{a} : \underline{b}, \underline{c} | \underline{c}) = H(\underline{a} : \underline{b} | \underline{c})$ .

# Chapter 24

## D-Separation in Quantum Mechanics

See Ref.[75].

# Chapter 25

## Dynamical Bayesian Networks

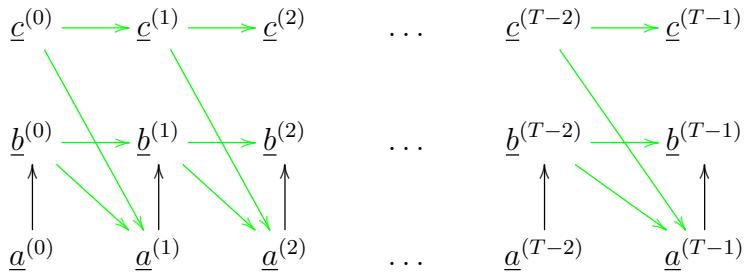


Figure 25.1: Example of a DBN. Same time-slice (in black) is repeated  $T$  times. Green arrows connect adjacent slices.

A **dynamical bnet (DBN)** is simply a Markov chain  $\underline{a}_0 \rightarrow \underline{a}_1 \rightarrow \dots \underline{a}_{T-1}$  (see Chapter 52) for which each node  $\underline{a}_i$  is called a **time-slice**. Each time-slice represents at finer resolution a sub-DAG which has the same structure (but not necessarily the same TPMs) in every time-slice.<sup>1</sup> If the TPMs are the same for all time-slices, we call it a **time-homogeneous dynamical bnet**. Fig.25.1 gives an example of a DBN. In that figure, each time-slice is represented in black, and arrows connecting adjacent time-slices are represented in green. In Fig.25.1, we've drawn the 3 nodes of each time-slice vertically, and labeled them with a superscript  $^{(t)}$ , where  $t \in \{0, 1, \dots, T-1\}$  is the time of the slice. To fully specify the DBN of Fig.25.1, we would also have to specify the TPMs

$$\begin{aligned} P(c^{(0)}), \\ P(b^{(0)}), \\ P(a^{(0)}), \\ P(c^{(1)}|c^{(0)}), \end{aligned}$$

---

<sup>1</sup>Sometimes, it is convenient to define time-slices that are influenced by the  $n$ -previous time-slices instead of just  $n = 1$ . By defining a bigger time-slice that contains  $n$  of the original time-slices, we can get bigger time-slices that only listen to the adjacent previous bigger time-slice.

$$P(b^{(1)}|b^{(0)}, a^{(1)}) \\ P(a^{(1)}|b^{(0)}, c^{(0)}), \text{ etc.}$$

Dynamical bnets are very common in AI and Data Science. Kalman filters (Chapter 44), Hidden Markov Models (Chapter 37) and Recurrent Neural Networks (Chapter 75) are famous examples of DBNs.

Bnets are acyclic; they can't have cycles (i.e, closed directed paths). Yet feedback loops are an important concept in Science. So what is the equivalent of feedback loops in the bnet world? Dynamical bnets are. Fig.25.2 represents Fig.25.1 more compactly using feedback loops. Any bnet with feedback loops can be "unrolled" into a DBN.

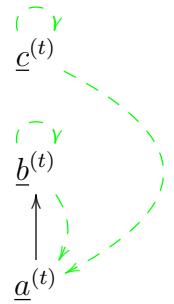


Figure 25.2: Dynamical bnet Fig.25.1 represented more compactly using feedback loops. Dashed green arrows point to the future, from nodes of the  $t$  time-slice to nodes of the  $t + 1$  time-slice.

# Chapter 26

## Expectation Maximization

This chapter is based on Refs.[110] and [168].

The Expectation Maximization (EM) algorithm is commonly used in Data Science to find the maximum over an **unknown parameter**  $\theta$  of a likelihood function

$$P(\vec{x}|\theta) = \sum_{\vec{h}} P(\vec{x}, \vec{h}|\theta), \quad (26.1)$$

where  $\vec{x}$  denotes the **observed variables**, and  $\vec{h}$  denotes the **hidden variables**. Both  $\theta$  and  $\vec{h}$  are hidden (i.e., unobserved).<sup>1</sup>

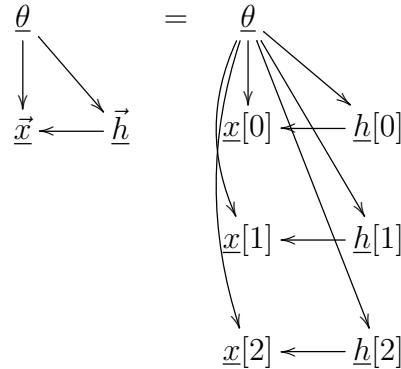


Figure 26.1: bnet for EM with  $nsam = 3$ .  $x[\sigma] = x^\sigma$  and  $h[\sigma] = h^\sigma$ .

The bnet for the EM algorithm is given by Fig.26.1 for  $nsam = 3$ . Later on in this chapter, we will give the node TPMs for this bnet for the special case in which  $P(x^\sigma | \theta)$  is a mixture (i.e., weighted sum) of Gaussians.

---

<sup>1</sup>The term “unknown parameter” is mainly of frequentist origin. For Bayesians,  $\theta$  is a random variable with a delta function prior, whereas for frequentists, it is not a random variable at all, just an unknown parameter with no randomness.

Note that if we erase the  $\underline{h}^\sigma$  nodes from Fig.26.1, we get the bnet for naive Bayes, which is used for classification into the states of  $\underline{\theta}$ . However, there is one big difference. With naive Bayes, the leaf nodes have different TPMs. Here, we will assume they are i.i.d. Naive Bayes is used for classification: i.e., given the states of the leaf nodes, we infer the state of the root node. EM is used for clustering; i.e., given many i.i.d. samples, we fit their distribution by a weighted sum of prob distributions, usually Gaussians.

Let

$L$  = likelihood function.

$nsam$  = number of samples.

$\vec{x} = (x[0], x[1], \dots, x[nsam - 1])$ ,  $x^\sigma = x[\sigma] \in S_{\underline{x}}$  for all  $\sigma$ .

$\vec{h} = (h[0], h[1], \dots, h[nsam - 1])$ ,  $h^\sigma = h[\sigma] \in S_{\underline{h}}$  for all  $\sigma$ .

We assume that the samples  $(x^\sigma, h^\sigma)$  are i.i.d. for different  $\sigma$  at fixed  $\theta$ . What this means is that there are probability distributions  $P_{\underline{x}|\underline{h},\underline{\theta}}$  and  $P_{\underline{h}|\underline{\theta}}$  such that

$$P(\vec{x}, \vec{h} | \theta) = \prod_{\sigma} [P_{\underline{x}|\underline{h},\underline{\theta}}(x^\sigma | h^\sigma, \theta) P_{\underline{h}|\underline{\theta}}(h^\sigma | \theta)] . \quad (26.2)$$

Definition of likelihood functions:

$$\underbrace{P(\vec{x} | \theta)}_{L(\theta; \vec{x})} = \sum_{\vec{h}} \underbrace{P(\vec{x}, \vec{h} | \theta)}_{L(\theta; \vec{x}, \vec{h})} \quad (26.3)$$

$\theta^*$  = maximum likelihood estimate of  $\theta$  (no prior  $P(\theta)$  assumed):

$$\theta^* = \operatorname{argmax}_{\theta} L(\theta; \vec{x}) \quad (26.4)$$

## 26.1 The EM algorithm:

### 1. Expectation step:<sup>2</sup>

$$Q(\theta | \theta^{(t)}) = E_{\vec{h} | \vec{x}, \theta^{(t)}} \ln P(\vec{x}, \vec{h} | \theta) \quad (26.5)$$

### 2. Maximization step:

$$\theta^{(t+1)} = \operatorname{argmax}_{\theta} Q(\theta | \theta^{(t)}) . \quad (26.6)$$

Claim:  $\lim_{t \rightarrow \infty} \theta^{(t)} = \theta^*$ .

Fig.26.2 portrays the recursive nature of the EM algo as a dynamical, recurrent bnet. For Fig.26.2, the TPMs, printed in blue, for the  $\underline{\theta}^{(t)}$  nodes for  $t = 1, 2, \dots$ , are as follows:

---

<sup>2</sup>Note that the right hand side of Eq.(26.5) is expressible in the form  $\sum_{\sigma} \sum_{h^\sigma} f(x^\sigma, h^\sigma)$ .

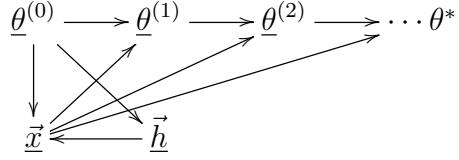


Figure 26.2: The EM algo generates a sequence of parameter estimates  $(\theta^{(t)})_{t=0,1,2,\dots}$  that converges to the optimum (i.e., best-fit) parameter  $\theta^*$ .

$$P(\theta^{(t+1)} | \vec{x}, \theta^{(t)}) = \delta(\theta^{(t+1)}, \operatorname{argmax}_{\theta} Q(\theta | \theta^{(t)})) . \quad (26.7)$$


---

### 26.1.1 Motivation

$$Q(\theta | \theta^{(t)}) = E_{\vec{h} | \vec{x}, \theta^{(t)}} \ln P(\vec{x}, \vec{h} | \theta) \quad (26.8)$$

$$= E_{\vec{h} | \vec{x}, \theta^{(t)}} [\ln P(\vec{h} | \vec{x}, \theta) + \ln P(\vec{x} | \theta)] \quad (26.9)$$

$$= -D_{KL} \left( P(\vec{h} | \vec{x}, \theta^{(t)}) \parallel P(\vec{h} | \vec{x}, \theta) \right) - H[P(\vec{h} | \vec{x}, \theta^{(t)})] + \ln P(\vec{x} | \theta) \quad (26.10)$$

When  $\theta^{(t)} = \theta$ , this becomes

$$Q(\theta | \theta) = -H[P(\vec{h} | \vec{x}, \theta)] + \ln P(\vec{x} | \theta) . \quad (26.11)$$

Hence,

$$\partial_{\theta} Q(\theta | \theta) = - \sum_{\vec{h}} \partial_{\theta} P(\vec{h} | \vec{x}, \theta) + \partial_{\theta} \ln P(\vec{x} | \theta) \quad (26.12)$$

$$= \partial_{\theta} \ln P(\vec{x} | \theta) \quad (26.13)$$

So if  $\theta^{(t)} \rightarrow \theta$  and  $Q(\theta | \theta)$  is max at  $\theta = \theta^*$ , then  $\ln P(\vec{x} | \theta)$  is max at  $\theta = \theta^*$  too.

For a more rigorous proof that  $\lim_{t \rightarrow \infty} \theta^{(t)} = \theta^*$ , see Wikipedia article Ref.[110] and references therein.

## 26.2 Minorize-Maximize (MM) algorithms

A function  $\mu(\theta | \theta^{(t)})$  is said to **minorize** a target function  $LL(\theta)$  iff for all  $\theta$  at fixed  $\theta^{(t)}$ , it satisfies the “ $\mu \leq LL$  property”

$$\mu(\theta | \theta^{(t)}) \leq LL(\theta) , \quad (26.14)$$

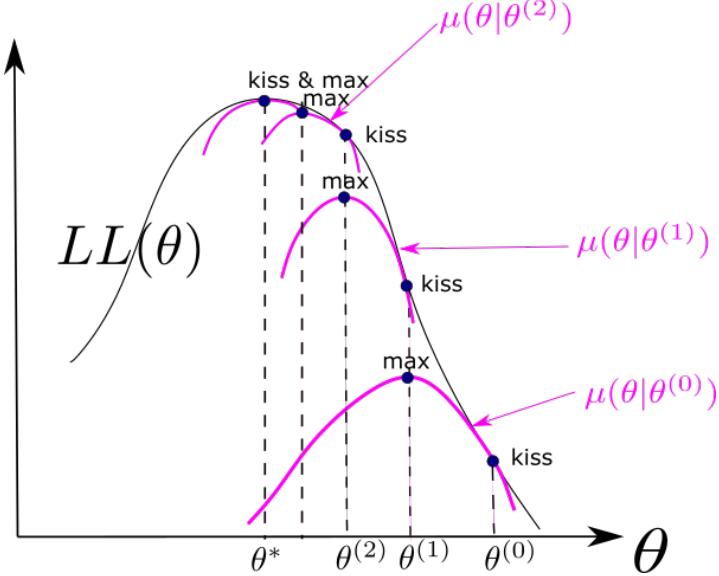


Figure 26.3: Function  $\mu(\theta|\theta^{(t)})$  minorizes the function  $LL(\theta)$ . Note that  $\mu(\theta|\theta^{(t)})$  is always below  $LL(\theta)$ . “max” indicates  $\theta^{(t+1)} = \operatorname{argmax}_{\theta} \mu(\theta|\theta^{(t)})$ . “kiss” indicates  $\mu(\theta^{(t)}|\theta^{(t)}) = LL(\theta^{(t)})$ .

and the “ $\mu = LL$  property”

$$\mu(\theta^{(t)}|\theta^{(t)}) = LL(\theta^{(t)}) . \quad (26.15)$$

We **recursively maximize a minorizing function**  $\mu(\theta|\theta^{(t)})$  if we define a sequence  $(\theta^{(t)})_{t=0,1,\dots}$  as follows:

$$\theta^{(t+1)} = \operatorname{argmax}_{\theta} \mu(\theta|\theta^{(t)}) . \quad (26.16)$$

The sequence  $(LL(\theta^{(t)}))_{t=0,1,2,\dots}$  generated by recursively maximizing a minorizing function must be nondecreasing:

$$LL(\theta^{(t+1)}) \geq \mu(\theta^{(t+1)}|\theta^{(t)}) \geq \mu(\theta^{(t)}|\theta^{(t)}) = LL(\theta^{(t)}) . \quad (26.17)$$

A **minorize-maximize (MM) algorithm** is any algo that specifies a minorizing function  $\mu(\theta|\theta^{(t)})$  for a particular target function  $LL(\theta)$ . One can also define a **majorize-minimize algo (also called MM)** by inverting the inequalities throughout.

The EM algo is an MM algo. Indeed, if we define

$$LL(\theta) = \ln P(\vec{x}|\theta) \quad (26.18)$$

and

$$\mu(\theta|\theta^{(t)}) = Q(\theta|\theta^{(t)}) + H(P(\vec{h}|\vec{x}, \theta^{(t)}), \quad (26.19)$$

then Eq.(26.10) establishes the  $\mu \leq LL$  and  $\mu = LL$  properties required of a minorizing function.

How an MM algo works is portrayed in Fig.26.3.

## 26.3 Examples

### 26.3.1 Gaussian mixture

$x^\sigma \in \mathbb{R}^d = S_{\underline{x}}$ .  $S_{\underline{h}}$  discrete and not too large.  $n_{\underline{h}} = |S_{\underline{h}}|$  is number of Gaussians that we are going to fit the samples with.

Let

$$\theta = [w_h, \mu_h, \Sigma_h]_{h \in S_{\underline{h}}}, \quad (26.20)$$

where  $[w_h]_{h \in S_{\underline{h}}}$  is a probability distribution of weights, and where  $\mu_h \in \mathbb{R}^d$  and  $\Sigma_h \in \mathbb{R}^{d \times d}$  are the mean value vector and covariance matrix of a  $d$ -dimensional Gaussian distribution.

The TPMs, printed in blue, for the bnet Fig.26.1, for the special case of a mixture of Gaussians, are as follows:

$$P(x^\sigma | h^\sigma | \theta) = \mathcal{N}_d(x^\sigma; \mu_{h^\sigma}, \Sigma_{h^\sigma}) \quad (26.21)$$

$$P(h^\sigma | \theta) = w_{h^\sigma} \quad (26.22)$$

Note that

$$P(x^\sigma | \theta) = \sum_h P(x^\sigma | h^\sigma = h, \theta) P(h^\sigma = h | \theta) \quad (26.23)$$

$$= \sum_h w_h \mathcal{N}_d(x^\sigma; \mu_h, \Sigma_h) \quad (26.24)$$

$$P(\vec{x}, \vec{h} | \theta) = \prod_\sigma [w_{h^\sigma} \mathcal{N}_d(x^\sigma; \mu_{h^\sigma}, \Sigma_{h^\sigma})] \quad (26.25)$$

$$= \prod_\sigma \prod_h [w_h \mathcal{N}_d(x^\sigma; \mu_h, \Sigma_h)]^{\mathbb{1}(h=h^\sigma)} \quad (26.26)$$

**Old Faithful:** See Wikipedia Ref.[110] for an animated gif of a classic example of using EM to fit samples with a Gaussian mixture. Unfortunately, could not include

it here because pdflatex does not support animated gifs. The gif shows samples in a 2 dimensional space (eruption time, delay time) from the Old Faithful geyser. In that example,  $d = 2$  and  $n_h = 2$ . Two clusters of points in a plane are fitted by a mixture of 2 Gaussians.

**K-means clustering** is often presented as the main competitor to EM for doing **clustering (non-supervised learning)**. In K-means clustering, the sample points are split into  $K$  mutually disjoint sets  $S_0, S_1, \dots, S_{K-1}$ . The algorithm is easy to describe:

1. Initialize by choosing at random  $K$  data points  $(\mu_k)_{k=0}^{K-1}$  called means or centroids and placing  $\mu_k$  in  $S_k$  for all  $k$ .
2. **STEP 1:** For each data point, add it to the  $S_k$  whose centroid  $\mu_k$  is closest to it.
3. **STEP 2:** Recalculate the centroids. Set  $\mu_k$  equal to the mean value of set  $S_k$ .
4. Repeat steps 1 and 2 until the centroids stop changing by much.

Step 1 is analogous to the expectation step in EM, and Step 2 to the maximization step in EM ( $\theta$  estimation versus  $\mu_k$  estimation). We won't say anything further about K-means clustering because it isn't related to bnets in any way, and this is a book about bnets. For more info about K-means clustering, see Ref.[126].

### 26.3.2 Blood Genotypes and Phenotypes

Notation:  $\vec{a} = (\underline{a}^\sigma)_{\sigma=0,1,\dots,nsam-1}$ , where  $nsam$  is the number of samples.

Suppose  $\vec{x} = (\vec{x}_0)$  (i.e., just one component)

$\vec{h} = (\vec{h}_0)$  (i.e., just one component)

$\underline{h}^\sigma \in S_h = \{AA, AO, BB, BO, OO, AB\}$  (the 6 blood genotypes)

$\underline{x}^\sigma \in S_x = \{A, B, O, AB\}$  (the 4 blood phenotypes)

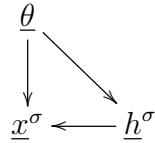


Figure 26.4: bnet for blood phenotypes  $x^\sigma$  and genotypes  $h^\sigma$ .

For the bnet Fig.26.4, the TPMs, printed in blue, are as follows:

$$P(h^\sigma | \theta) = \begin{array}{c|c} & \begin{array}{c} AA \\ AO \\ BB \\ BO \\ OO \\ AB \end{array} \\ \hline \begin{array}{c} AA \\ AO \\ BB \\ BO \\ OO \\ AB \end{array} & \begin{array}{c} p_A^2 \\ 2p_A p_O \\ p_B^2 \\ 2p_B p_O \\ p_O^2 \\ 2p_A p_B \end{array} \end{array}, \quad (26.27)$$

where  $p_A + p_B + p_O = 1$ .

$$P(x^\sigma | h^\sigma, \theta) = \begin{array}{c|cccccc} & \begin{array}{c} AA \\ AO \\ BB \\ BO \\ OO \\ AB \end{array} \\ \hline \begin{array}{c} A \\ B \\ O \\ AB \end{array} & \begin{array}{c} 1 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{array} \end{array} \quad (26.28)$$

$$\theta = (p_A, p_B) \quad (26.29)$$

Multiplying the TPMs in Eqs.(26.27 and (26.28), we get

$$P(x^\sigma | \theta) = \begin{array}{c|c} & \begin{array}{c} AA \\ AO \\ BB \\ BO \\ OO \\ AB \end{array} \\ \hline \begin{array}{c} A \\ B \\ O \\ AB \end{array} & \begin{array}{c} p_A^2 + 2p_A p_O (= \pi_A) \\ p_B^2 + 2p_B p_O (= \pi_B) \\ p_O^2 (= \pi_O) \\ 2p_A p_B (= \pi_{AB}) \end{array} \end{array} \quad (26.30)$$

Note that

$$P(\vec{x} | \theta) = \prod_\sigma P(x^\sigma | \theta) \quad (26.31)$$

$$= (\pi_A)^{N_A} (\pi_B)^{N_B} (\pi_O)^{N_O} (\pi_{AB})^{N_{AB}}, \quad (26.32)$$

where  $N_x$  for  $x \in S_{\underline{x}} = \{A, B, O, AB\}$  are the counts from the data. We can get estimates for the parameters  $p_A$  and  $p_B$  right here without doing EM. Just note that

$$\hat{\pi}_x = \frac{N_x}{N_+} \quad (26.33)$$

for  $x \in S_{\underline{x}}$ , where  $N_+ = \sum_x N_x$ . Eqs.(26.33) give 4 quadratic equations that can be solved for the parameters  $p_A, p_B$  in terms of the observed counts  $N_x$  for  $x \in S_{\underline{x}}$ .

If, instead, you want to find the optimum parameters  $p_A, p_B$  using EM, note that

$$Q(\theta|\theta^{(t)}) = \sum_{\vec{h}} P(\vec{h}|\theta^{(t)}) \ln P(\vec{x}, \vec{h}|\theta) \quad (26.34)$$

$$= \sum_{\vec{h}} \left[ \prod_{\sigma} P(h^{\sigma}|\theta^{(t)}) \right] \ln \left[ \prod_{\sigma} P(x^{\sigma}, h^{\sigma}|\theta) \right] \quad (26.35)$$

$$= \sum_{\sigma} \sum_{h^{\sigma}} P(h^{\sigma}|\theta^{(t)}) \ln P(x^{\sigma}, h^{\sigma}|\theta) \quad (26.36)$$

$$= \sum_{\sigma} \sum_{h^{\sigma}} P(h^{\sigma}|\theta^{(t)}) [\ln P(x^{\sigma}|h^{\sigma}, \theta) + \ln P(h^{\sigma}|\theta)] \quad (26.37)$$

$$= nsam \sum_{h^{\sigma}} P(h^{\sigma}|\theta^{(t)}) \ln P(h^{\sigma}|\theta) . \quad (26.38)$$

### 26.3.3 Missing Data/Imputation

The previous example on blood genotypes and phenotypes assumed no missing data in compiling the counts  $N_x$ . But what if there is missing data? Can one still apply the EM algo in that case? Yes! See Chapter 59.

# Chapter 27

## Factor Graphs

Suppose  $x^{nx} = (x_0, x_1, \dots, x_{nx-1})$ . Consider a product

$$g(x^{nx}) = \prod_{\alpha=0}^{nf-1} f_\alpha(x_{A_\alpha}) \quad (27.1)$$

of scalar functions  $f_\alpha : \underline{x}_{A_\alpha} \rightarrow \mathbb{R}$ , where  $A_\alpha \subset \{0, 1, \dots, nx - 1\}$ . For instance, consider  $g : S_{\underline{x}_0} \times S_{\underline{x}_1} \times S_{\underline{x}_2} \rightarrow \mathbb{R}$  defined by:

$$g(x_0, x_1, x_2) = f_0(x_0)f_1(x_0, x_1)f_2(x_0, x_1, x_2)f_3(x_1, x_2). \quad (27.2)$$

The **factor graph** for this function  $g$  is given by Fig.27.1.

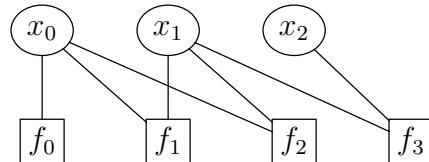


Figure 27.1: Factor graph for function  $g$  defined by Eq.(27.2).

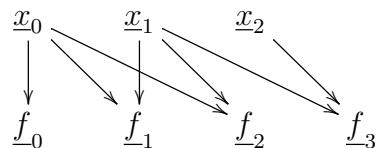


Figure 27.2: Bipartite bnet corresponding to factor graph Fig.27.1.

A **Markov Random Field (MRF)** is a statistical model whose probability distribution is of the form

$$P(x^{nx}) = \mathcal{N}(!x^{nx}) \prod_{\alpha} f_{\alpha}(x_{A_{\alpha}}) , \quad (27.3)$$

so it can be represented graphically by a factor graph. The factor functions  $f_{\alpha}$  of a factor graph are called **potentials**.

One can map any factor graph (the “source”) to a special bipartite bnet (the “image”), as follows. Replace each  $x_i$  by  $\underline{x}_i \in S_{\underline{x}_i}$  for  $i = 0, 1, \dots, nx - 1$  and each  $f_{\alpha}$  by  $\underline{f}_{\alpha}$  for  $\alpha = 0, 1, \dots, nf - 1$ . Then replace the connections (edges) of the factor graph by arrows from  $\underline{x}_i$  to  $\underline{f}_{\alpha}$ .<sup>1</sup> For example, Fig.27.2 is the image bipartite bnet of the source factor graph Fig.27.1.

Let  $\underline{x}^{nx} = (\underline{x}_0, \underline{x}_1, \dots, \underline{x}_{nx-1})$  and  $\underline{f}^{nf} = (\underline{f}_0, \underline{f}_1, \dots, \underline{f}_{nf-1})$ . Let<sup>2</sup>  $f_{\alpha} \in \{0, 1\}$  for all  $\alpha$ , and  $y_{\alpha} = f_{\alpha}(x_{nb(\underline{f}_{\alpha})})$ . Here we are using  $nb(\underline{f}_{\alpha})$  to denote the neighborhood of node  $\underline{f}_{\alpha}$  in the image bipartite bnet, and we are using  $x_S$  to denote  $(x_i)_{i \in S}$ . Without loss of generality, we will assume that  $y_{\alpha} \in [0, 1]$  for all  $\alpha$ . Then we define the TPMs, printed in blue, for the image bipartite bnet, as follows.

$$P(\underline{f}_{\alpha} | x_{nb(\underline{f}_{\alpha})}) = y_{\alpha} \delta(f_{\alpha}, 1) + [1 - y_{\alpha}] \delta(f_{\alpha}, 0) \quad (27.4)$$

for  $\alpha = 0, 1, \dots, nf - 1$  and

$$P_{\underline{x}_i}(x_i) = \text{arbitrary prior} \quad (27.5)$$

for  $i = 0, 1, \dots, nx - 1$ . Note that

$$P(\underline{f}^{nf} = 1^{nf} | \underline{x}^{nx}) = \prod_{\alpha} y_{\alpha} . \quad (27.6)$$

Fig.27.3 gives another bipartite bnet, alternative to Fig.27.2, corresponding to factor graph Fig.27.1. In this new bnet, we replaced the  $\underline{f}_{\alpha} \in \{0, 1\}$  nodes by  $y_{\alpha} \in [0, 1]$  nodes. We also defined a new leaf node  $\underline{y} \in \{0, 1\}$  with incoming arrows from all nodes  $\underline{y}_{\alpha}$ . The TPMs, printed in blue, for the  $\underline{y}_{\alpha}$  and  $\underline{y}$  nodes, are as follows.

$$P(\underline{y}_{\alpha} = y_{\alpha} | x_{nb(\underline{y}_{\alpha})}) = \delta(y_{\alpha}, f_{\alpha}(x_{nb(\underline{y}_{\alpha})})) \quad (27.7)$$

$$P(\underline{y} | \{y_{\alpha}\}_{\alpha=0}^{nf-1}) = y \prod_{\alpha} y_{\alpha} + (1 - y) \left( 1 - \prod_{\alpha} y_{\alpha} \right) \quad (27.8)$$

---

<sup>1</sup>Pointing arrows from the  $\underline{x}_i$  to the  $\underline{f}_{\alpha}$  is more causal than the opposite because the  $\underline{x}_i$  preceed the  $\underline{f}_{\alpha}$  in time.

<sup>2</sup>Note that we are using  $f_{\alpha}$  to denote both a function  $f_{\alpha}(\cdot)$  and a Boolean value. Which one we mean will be clear from context.  $f_{\alpha}$  could also be used to denote, besides a function and a Boolean value, the real number  $y_{\alpha} = f_{\alpha}(x_{nb(\underline{f}_{\alpha})})$ . However, we won't be using it that third way in this chapter.

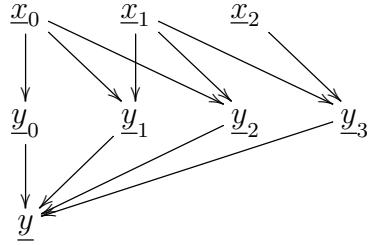


Figure 27.3: Another bipartite bnet, alternative to Fig.27.2, corresponding to factor graph Fig.27.1.

Note that

$$P(\underline{y} = 1 | \{y_\alpha\}_{\alpha=0}^{nf-1}) = \prod_{\alpha} y_\alpha \quad (27.9)$$

We've shown how to go from a factor graph to a bnet. Going from a bnet to a factor graph is also possible. Fig.27.4 gives a simple example. Bnet to factor graph conversion is used in the Junction Tree Algorithm (See Chapter 43).

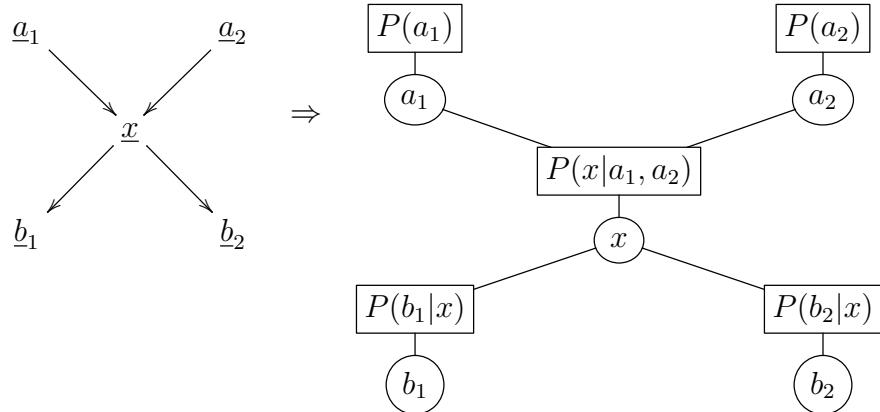


Figure 27.4: Example of converting a bnet to a factor graph.

# Chapter 28

## Frisch-Waugh-Lovell (FWL) theorem

The Frisch-Waugh-Lovell (FWL) theorem (see Ref.[112]) (mnemonic: FoWL Theorem) is a method used in Linear Regression (LR). It allows us to calculate, for LR with two features  $\underline{x}_1$  and  $\underline{x}_2$ , the regression coefficient of feature  $\underline{x}_2$  by conditioning on feature  $\underline{x}_1$ .

As in Section C.27 on LR, we will consider two cases:  $x^\sigma$  non-random, and  $x^\sigma$  random i.i.d..

### 28.1 FWL, assuming $x^\sigma$ are non-random

Suppose

$$y = X_1\beta_1 + X_2\beta_2 + \epsilon \quad (28.1)$$

where

$$\begin{aligned} y, \epsilon &\in \mathbb{R}^{nsam} \\ X_a &\in \mathbb{R}^{nsam \times k_a}, \beta_a \in \mathbb{R}^{k_a} \text{ for } a = 1, 2 \end{aligned}$$

Define the matrices  $U_1$  and  $A_1$  by

$$U_1 = X_1(X_1^T X_1)^{-1} X_1^T \quad (28.2)$$

and

$$A_1 = 1 - U_1. \quad (28.3)$$

Note that

$$U_1 X_1 = X_1, \quad A_1 X_1 = 0 \quad (28.4)$$

(mnemonic:  $A_1$  Annihilates  $X_1$ , and  $U_1$  acts like Unity on  $X_1$ ).

Applying  $A_1$  to Eq.(28.1) gives

$$A_1 y = A_1 X_2 \beta_2 + A_1 \epsilon \quad (28.5)$$

so we can estimate  $\beta_2$  by

$$\widehat{\beta}_2 = (A_1 X_2)^{-1} A_1 y . \quad (28.6)$$

## 28.2 FWL, assuming $x^\sigma$ are random

Assume for simplicity that  $k_1 = k_2 = 1$  in Eq.(28.1). Let  $\beta_1, \beta_2 \in \mathbb{R}$ . When the  $x^\sigma$  are random and i.i.d., the  $X_1, X_2$  are replaced by the random variables  $\underline{x}_1, \underline{x}_2 \in \mathbb{R}$ , and Eq.(28.1) becomes

$$\underline{y} = \beta_1 \underline{x}_1 + \beta_2 \underline{x}_2 + \underline{\epsilon}_y \quad (28.7)$$

Fig.28.1 shows two LDEN bnets in which Eq.(28.7) can arise.

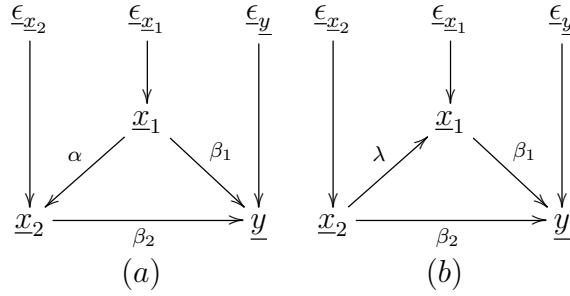


Figure 28.1: LDEN bnets for discussing the FWL theorem. (a) and (b) only differ in the direction of the arrow between  $\underline{x}_1$  and  $\underline{x}_2$ .

The structural equations, printed in blue, for the 2 bnets of Fig.28.1, are as follows:

For (a),

$$\left\{ \begin{array}{l} \underline{x}_1 = \underline{\epsilon}_{x_1} \\ \underline{x}_2 = \alpha \underline{x}_1 + \underline{\epsilon}_{x_2} \\ \boxed{\underline{y} = \beta_1 \underline{x}_1 + \beta_2 \underline{x}_2 + \underline{\epsilon}_y} \end{array} \right. \quad (28.8)$$

For (b),

$$\left\{ \begin{array}{l} \underline{x}_1 = \lambda \underline{x}_2 + \underline{\epsilon}_{x_1} \\ \underline{x}_2 = \underline{\epsilon}_{x_2} \\ \boxed{\underline{y} = \beta_1 \underline{x}_1 + \beta_2 \underline{x}_2 + \underline{\epsilon}_y} \end{array} \right. \quad (28.9)$$

What we are going to say next depends only on the boxed equation, so it applies equally to cases (a) and (b).

Assume

$$\langle \underline{\epsilon}_y \rangle = 0 \quad (28.10)$$

Note that

$$\langle \underline{x}_j, \underline{\epsilon}_{\underline{y}} \rangle = 0 \quad (28.11)$$

because the path from  $\underline{x}_j$  to  $\underline{\epsilon}_{\underline{y}}$  is blocked by a collider. Hence

$$\langle \underline{x}_2, \underline{y} \rangle^{|x_1} = \beta_2 \langle \underline{x}_2, \underline{x}_2 \rangle^{|x_1} \quad (28.12)$$

$$\beta_2 = \left[ \frac{\langle \underline{x}_2, \underline{y} \rangle}{\langle \underline{x}_2, \underline{x}_2 \rangle} \right]^{|x_1} = \left[ \frac{\partial}{\partial \underline{x}_2} \right]^{|x_1} \underline{y} \quad (28.13)$$

# Chapter 29

## Frontdoor Adjustment Formula

The frontdoor (FD) adjustment formula is proven in Chapter 21 from the rules of Do Calculus. The goal of this chapter is to give examples of the use of that theorem. We will restate the theorem in this chapter, sans proof. There is no need to understand the theorem's proof in order to use it. However, you will need to skim Chapter 21 in order to familiarize yourself with the notation used to state the theorem. This chapter also assumes that you are comfortable with the rules for checking for d-separation. Those rules are covered in Chapter 23.

Suppose that we have access to data that allows us to estimate a probability distribution  $P(x., m., y.)$ . Hence, the variables  $\underline{x}., \underline{m}., \underline{y}.$  are ALL observed (i.e., not hidden). Then we say that the frontdoor  $\underline{m}.$  satisfies the **frontdoor adjustment criterion** relative to  $(\underline{x}., \underline{y}.)$  if

1. All directed paths from  $\underline{x}.$  to  $\underline{y}.$  are intercepted by (i.e., have a node in)  $\underline{m}.$
2. All backdoor paths from  $\underline{x}.$  to  $\underline{m}.$  are blocked.
3. All backdoor paths from  $\underline{m}.$  to  $\underline{y}.$  are blocked by conditioning on  $\underline{x}..$

**Claim 62** *Frontdoor Adjustment Formula*

If  $\underline{m}.$  satisfies the frontdoor criterion relative to  $(\underline{x}., \underline{y}.)$ , and  $P(x., m.) > 0$ , then

$$P(y.|D\underline{x}. = x.) = \sum_{m.} \underbrace{\left[ \sum_{x'.} P(y.|x'., m.) P(x'.) \right]}_{P(y.|D\underline{m}. = m.)} \underbrace{P(m.|x.)}_{P(m.|D\underline{x}. = x.)} \quad (29.1)$$

$$= \sum_{x'.} \sum_{m.} \begin{array}{c} \diagdown \\ x. \longrightarrow \sum m. \longrightarrow y. \end{array} \quad (29.2)$$

where  $\sum x'.$  and  $\sum m.$  means nodes  $\underline{x}'.$  and  $\underline{m}.$  are summed over.

**proof:** See Chapter 21.

QED

## 29.1 Examples

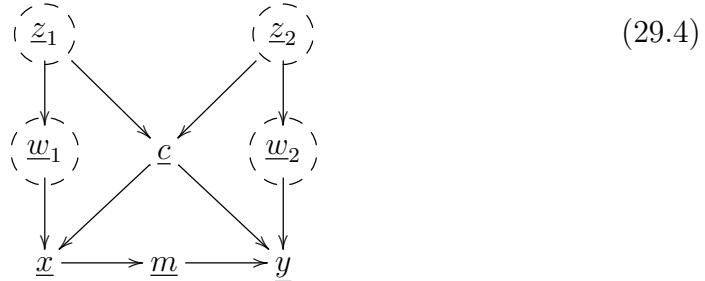
1.



If  $x_+ = \underline{x}$ ,  $m_+ = \underline{m}$  and  $y_+ = \underline{y}$ , then the FD criterion is satisfied. Can't satisfy backdoor criterion because  $\underline{c}$  unobserved so can't condition on it to block backdoor path  $\underline{x} - \underline{c} - \underline{y}$ .

---

2.



If  $x_+ = \underline{x}$ ,  $m_+ = \underline{m}$  and  $y_+ = \underline{y}$ , then the FD criterion is satisfied. Can't satisfy backdoor criterion because to block backdoor path  $\underline{x} - \underline{c} - \underline{y}$ , need to condition on  $\underline{c}$  but if this is true, then long path  $\underline{x} - \underline{w}_1 - \underline{z}_1 - \underline{c} - \underline{z}_2 - \underline{w}_2 - \underline{y}$  becomes unblocked.

# Chapter 30

## G-formula (Sequential Backdoor Adjustment Formula)



Figure 30.1: Piscina Mirabilis, ancient Roman cistern in Naples

This chapter is based on Ref.[57] by Pearl and Robins.

A **g-formula**<sup>1</sup> is any formula that defines recursively the full probability distribution of a bnet. In other words, it's a recursive definition of a Dynamical Bayesian Network.<sup>2</sup>

The goal of this chapter is to generalize the backdoor adjustment formula (see Chapter 4) from a query  $P(y|\mathcal{D}x = x)$  with a single do node to a query  $P(y|\mathcal{D}\underline{x}^n = x^n)$

---

<sup>1</sup>It's not clear from the literature what the "g" stands for. I assume it stands for "generating".

<sup>2</sup>Dynamical Bayesian Networks are discussed in Chapter 25.

with multiple do nodes. The resulting generalized adjustment formula is called a **sequential backdoor (SBD) adjustment formula** and it is associated with an **SBD g-formula**.

For  $n = 1, 2, 3 \dots$ , define

$$\mathcal{Q}(y|x^n) = \sum_{z^n} P(y|x^n, z^n) \prod_{t=0}^{n-1} P(z_t|x_{<t}, z_{<t}) \quad (30.1)$$

$$= \begin{array}{c} \sum_{z^n} z^n \\ \downarrow \\ y \\ \uparrow \\ x^n \end{array} \prod_{t=0}^{n-1} \begin{array}{c} z_{<t} \longrightarrow z_t \\ \nearrow \\ x_{<t} \end{array} \quad (30.2)$$

For  $n = 1$ ,

$$\mathcal{Q}(y|x_0) = \begin{array}{c} \sum_{z_0} z_0 \\ \downarrow \\ y \\ \uparrow \\ x_0 \end{array} = \begin{array}{c} \sum z_0 \\ \searrow \\ y \\ \nearrow \\ x_0 \end{array} . \quad (30.3)$$

For  $n = 2$ ,

$$\mathcal{Q}(y|x^2) = \begin{array}{c} \sum_{z^2} (z_0, z_1) P(z_0) z_0 \longrightarrow z_1 \\ \downarrow \\ y \\ \uparrow \\ (x_0, x_1) \end{array} \quad (30.4)$$

$$= \begin{array}{c} \sum z_0 \longrightarrow \sum z_1 \\ \nearrow \searrow \\ x_0 \quad x_1 \\ \nearrow \searrow \\ y \end{array} . \quad (30.5)$$

For  $n = 3$ ,

$$\begin{aligned} & \sum_{z^3} (z_0, z_1, z_2) P(z_0) z_0 \rightarrow z_1 (z_0, z_1) \rightarrow z_2 \\ \mathcal{Q}(y|x^3) = & \downarrow y \\ & (x_0, x_1, x_2) \end{aligned} \quad (30.6)$$

$$\begin{aligned} & \sum_{z^3} (z_0, z_1, z_2) P(z_0) z_0 \xrightarrow{\text{double}} z_1 \xrightarrow{\text{double}} z_2 \\ = & \downarrow y \\ & (x_0, x_1, x_2) \end{aligned} \quad (30.7)$$

$$\begin{aligned} & \sum z_0 \xrightarrow{\text{double}} \sum z_1 \xrightarrow{\text{double}} \sum z_2 \\ = & \downarrow y \\ & x_0 \quad x_1 \quad x_2 \end{aligned} \quad (30.8)$$

Suppose that we have access to data that allows us to estimate a probability distribution  $P(x^n, y, z^n)$ . Hence, the variables  $\underline{x}^n, \underline{y}, \underline{z}^n$  are ALL observed (i.e, not hidden). Then we say that the the multimode of "covariates"  $\underline{z}^n$  satisfies the **sequential backdoor (SBD) adjustment criterion** relative to  $(\underline{x}^n, \underline{y})$  if for all  $t \in \{0, 1, \dots, n-1\}$ ,

1.  $\underline{y} \perp \underline{x}_t \mid \underbrace{(\underline{x}_0, \underline{x}_1, \dots, \underline{x}_{t-1}, \underline{z}_0, \underline{z}_1, \dots, \underline{z}_t)}_{\text{Past of } \underline{x}_t}$  in  $\mathcal{L}_{\underline{x}_t} \mathcal{D}_{\underline{x}_{t+1}, \underline{x}_{t+2}, \dots, \underline{x}_{n-1}} G$ .
2.  $\underline{z}_t \cap de(\underline{x}_t) = \emptyset$ .

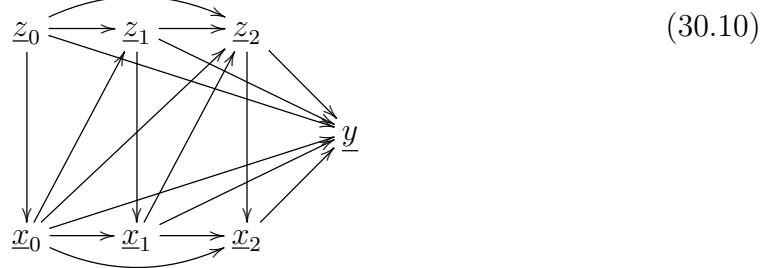
**Claim 63 (SBD Adjustment Formula)**

If  $\underline{z}^n$  satisfies the sequential backdoor criterion relative to  $(\underline{x}^n, \underline{y})$ , then

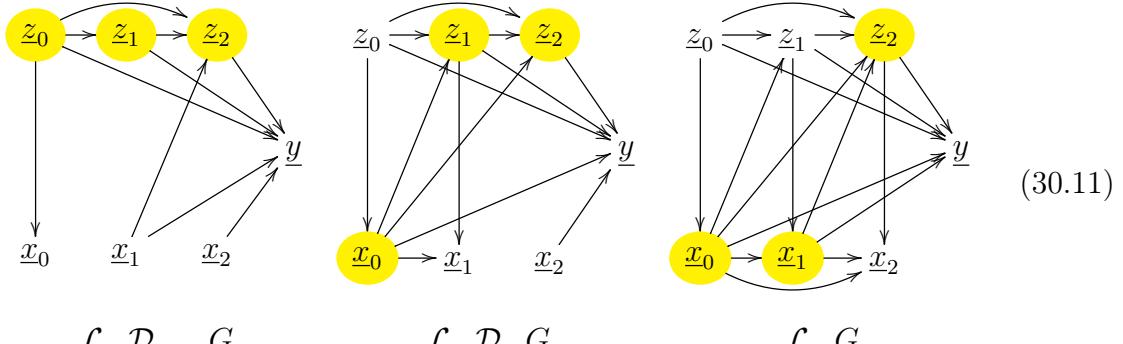
$$P(y | \mathcal{D}\underline{x}^n = x^n) = \mathcal{Q}(y|x^n), \quad (30.9)$$

where  $\mathcal{Q}(y|x^n)$  is defined by Eq.(30.2).

**proof:** If  $z^n$  satisfies the SBD criterion relative to  $(\underline{x}^n, \underline{y})$ , then  $\underline{x}^n, \underline{y}, \underline{z}^n$  might have the following structure for  $n = 3$ .



One can check using the following 3 auxiliary bnets that bnet Eq.(30.10) satisfies the SBD criterion. Note that conditioned nodes are shaded yellow.



See Claim 57 for a proof of this claim for the special case Eq.(30.10).

**QED**

# Chapter 31

## Gaussian Nodes with Linear Dependence on Parents

Bnet nodes that have a Gaussian TPM with a linear dependence on their parent nodes (GLP) are a very popular way of modeling continuous nodes of bnets. A convenient aspect of them is that their parents can be discrete or continuous nodes, and their children can be discrete or continuous nodes too. Also, they can be learned easily from the data because their parameters can be expressed in terms of two node covariances. For these reasons, they are commonly used when doing structure learning of bnets with continuous nodes (see Chapter 88).

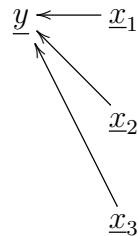


Figure 31.1: GLP node  $\underline{y}$  with 3 parent nodes  $\underline{x}^3 = (\underline{x}_1, \underline{x}_2, \underline{x}_3)$ .

Recall our notation for a Gaussian distribution:

$$\mathcal{N}(x; \mu, \sigma^2) = \frac{1}{\sigma\sqrt{2\pi}} e^{\frac{-(x-\mu)^2}{2\sigma^2}}, \quad (31.1)$$

where  $x, \mu \in \mathbb{R}$  and  $\sigma > 0$ .

A GLP node  $\underline{y}$  with  $n$  parents  $\underline{x}^n = (\underline{x}_1, \underline{x}_2, \dots, \underline{x}_n)$  has the following TPM:

$$P(y|\underline{x}^n) = \mathcal{N}(y; \beta_0 + \beta^{nT} \underline{x}^n, \sigma^2) \quad (31.2)$$

where  $\underline{y}, \beta_0 \in \mathbb{R}$  and  $\sigma^2 > 0$ , and where  $\underline{x}^n, \beta^n \in \mathbb{R}^n$  are \*\*column vectors\*\*. The  $T$  in  $\beta^{nT}$  stands for transpose. Any  $\underline{x}_i$  can have a discrete set of states as long as

they are real valued and ordinal (ordered by size). Fig.31.1 shows a diagrammatic representation of a GLP node with 3 parents.

Note that as  $\sigma \rightarrow 0$ , a GLP node becomes deterministic. In fact, it becomes a neural net node with a linear activation function.

An equivalent way of defining a GLP node  $\underline{y}$  is in terms of a random variable equation expressing  $\underline{y}$  as a hyperplane function of the parents  $\underline{x}^n$  plus a Gaussian noise variable. Define a curve-fit  $\widehat{\underline{y}}$  of a “true value”  $\underline{y}$  by

$$\widehat{\underline{y}} = \beta_0 + \beta^{nT} \underline{x}^n \quad (31.3a)$$

and

$$\underline{y} = \widehat{\underline{y}} + \underline{\epsilon} \quad (31.3b)$$

where the residual  $\underline{\epsilon}$  satisfies

$$P(\epsilon) = \mathcal{N}(\epsilon; 0, \sigma^2) \quad (31.3c)$$

and

$$\langle \underline{x}^n, \underline{\epsilon} \rangle = 0 . \quad (31.3d)$$

The notation  $\langle \underline{x}, \underline{y} \rangle$  for the covariance of random variables  $\underline{x}$  and  $\underline{y}$  is explained in Chapter C.

**Claim 64** *The parameters of a GLP node can be expressed in terms of 2-node covariances. Specifically,*

$$\beta^n = \langle \underline{x}^n, \underline{x}^{nT} \rangle^{-1} \langle \underline{y}, \underline{x}^n \rangle \quad (31.4)$$

$$\beta_0 = \langle \underline{y} \rangle - \beta^{nT} \langle \underline{x}^n \rangle \quad (31.5)$$

$$\sigma^2 = \langle \underline{y}, \underline{y} \rangle - \beta^{nT} \langle \underline{x}^n, \underline{y} \rangle \quad (31.6)$$

**proof:**

Note that  $\langle \underline{x}^n, \underline{x}^{nT} \rangle^T = \langle \underline{x}^n, \underline{x}^{nT} \rangle$  and  $\langle \underline{y}, \underline{x}^{nT} \rangle^T = \langle \underline{y}, \underline{x}^n \rangle$ .

$$\langle \underline{y}, \underline{x}^{nT} \rangle = \beta^{nT} \langle \underline{x}^n, \underline{x}^{nT} \rangle \quad (31.7)$$

$$\langle \underline{y}, \underline{x}^n \rangle = \langle \underline{x}^n, \underline{x}^{nT} \rangle \beta^n \quad (31.8)$$

$$\beta^n = \langle \underline{x}^n, \underline{x}^{nT} \rangle^{-1} \langle \underline{y}, \underline{x}^n \rangle \quad (31.9)$$

$$\langle \underline{y} \rangle = \beta_0 + \beta^{nT} \langle \underline{x}^n \rangle \quad (31.10)$$

$$\langle \underline{y}, \underline{y} \rangle = \langle \beta_0 + \beta^{nT} \underline{x}^n + \underline{\epsilon}, \underline{y} \rangle \quad (31.11)$$

$$= \beta^{nT} \langle \underline{x}^n, \underline{y} \rangle + \sigma^2 \quad (31.12)$$

**QED**

---

Let D=Discrete, GLP=Gaussian with Linear dependence in Parents

The following arrows are possible in a bnet.

- $GLP \leftarrow GLP$
- $GLP \leftarrow D$

Pass to GLP a separate set of regression coefficients  $\beta_0, \beta^n$  and variance  $\sigma^2$  for each state of D. If D is called  $\underline{d}$ , let

$$P(y|(x^n)_d, d) = \mathcal{N}(y; (\beta_0)_d + (\beta^{nT})_d(x^n)_d, \sigma_d^2) \quad (31.13)$$

for each  $d \in S_{\underline{d}}$ .

- $D \leftarrow GLP$

If D expects a continuous parent, no need to preprocess GLP output. If D expects a discrete parent, break the interval  $[a, b]$  that contains most of the range of the GLP node into sub-intervals and assign a discrete label to each subinterval.

- $D \leftarrow D$

# Chapter 32

## Generalized Linear Model (GLM)

This chapter is based on chapter 4 of Ref.[1].

### 32.1 Exponential Family of Distributions

The **Exponential Family (EF)** of probability distributions is defined by

$$P(y|\theta, \phi) = \exp\left(\frac{\theta y - b(\theta)}{a(\phi)} + c(y, \phi)\right) \quad (32.1)$$

In this chapter, we will denote averages over  $y|\theta, \phi$  by angular brackets

$$E_{y|\theta, \phi}[f(y)] = \sum_y P(y|\theta, \phi)f(y) = \langle f(y) \rangle \quad (32.2)$$

As usual in this book, let  $S_x$  denote the set of values that the random variable  $x$  can take. We will assume that  $S_y$  for EF can be either a discrete or a continuous subset of  $\mathbb{R}$ ,<sup>1</sup> but  $S_\theta$  must be continuous. When  $S_y$  is a discrete subset of  $\mathbb{R}$ ,  $P(y|\theta, \phi)$  will denote a probability distribution, whereas when  $S_y$  is continuous, it will denote a probability density.

#### Claim 65

$$\mu = \langle y \rangle = b'(\theta) \quad (32.3)$$

$$\sigma^2 = \langle y, y \rangle = a(\phi)b''(\theta) \quad (32.4)$$

**proof:**

---

<sup>1</sup>By a “continuous set” we mean a finite set of intervals each of which has non-zero length.

$$0 = \partial_\theta \int_{-\infty}^{\infty} dy P(y|\theta, \phi) \quad (32.5)$$

$$= \int_{-\infty}^{\infty} dy \frac{1}{a} [y - b'(\theta)] P(y|\theta, \phi) \quad (32.6)$$

$$= \frac{1}{a} [\langle \underline{y} \rangle - b'(\theta)] \quad (32.7)$$

$$0 = \partial_\theta^2 \int_{-\infty}^{\infty} dy P(y|\theta, \phi) \quad (32.8)$$

$$= \int_{-\infty}^{\infty} dy \left\{ \frac{-b''(\theta)}{a} + \frac{1}{a^2} [y - b'(\theta)]^2 \right\} P(y|\theta, \phi) \quad (32.9)$$

Hence,

$$\langle [y - b'(\theta)]^2 \rangle = ab''(\theta) \quad (32.10)$$

**QED**

Note that the Normal Distribution belongs to the EF. Indeed,

$$\mathcal{N}(y; \mu, \sigma^2) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{(y - \mu)^2}{2\sigma^2}\right) \quad (32.11)$$

$$= \exp\left(\frac{-y^2 + 2\mu y - \mu^2}{2\sigma^2} - \ln \sqrt{2\pi\sigma^2}\right) \quad (32.12)$$

$$= \exp\left(\frac{-\frac{1}{2}y^2 + \mu y - \frac{1}{2}\mu^2}{\sigma^2} - \ln \sqrt{2\pi\sigma^2}\right) \quad (32.13)$$

So, for the Normal Distribution,  $\theta = \mu$ ,  $a = \sigma^2$ ,  $b = \mu^2/2$ ,  $b' = \mu$ ,  $b'' = 1$ .

EF can be defined for an ensemble  $\{y_\sigma : \sigma \in \Sigma\}$  of independent (but not necessarily identically distributed) random variables  $y_\sigma$  describing individuals  $\sigma$  of a population  $\Sigma$ .

$$P(\vec{y}|\vec{\theta}, \phi) = \prod_{\sigma} \exp\left(\frac{\theta_\sigma y_\sigma - b(\theta_\sigma)}{a(\phi)} + c(y_\sigma, \phi)\right) \quad (32.14)$$

$$\mu_\sigma = \langle \underline{y}_\sigma \rangle = \partial_{\theta_\sigma} b(\theta_\sigma) \quad (32.15)$$

$$\langle \underline{y}_\sigma, \underline{y}_{\sigma'} \rangle = \delta(\sigma, \sigma') a(\phi) \partial_{\theta_\sigma}^2 b(\theta_\sigma) \quad (32.16)$$

## 32.2 GLM

The Generalized Linear Model (GLM) is a statistical model for an ensemble of independent (but not necessarily identically distributed) random variables  $\underline{y}_\sigma$ . GLM consists of 3 parts:

1. Exponential Family

Model  $\underline{y}_\sigma$  by probability distribution of exponential family (EF).

2. Linear predictor

In EF, replace  $\theta_\sigma$  by the **linear predictor**  $X_\sigma^T \beta = \sum_i X_{\sigma,i} \beta_i$ .  $X_\sigma^T \beta$  is commonly denoted by  $\eta_\sigma$ , but I will avoid that notation because I think the results are much clearer when expressed in the more explicit notation  $X_\sigma^T \beta$  instead of  $\eta_\sigma$ .

3. Link Function

$$\mu_\sigma = \langle \underline{y}_\sigma \rangle = \partial_{X_\sigma^T \beta} b \quad (32.17)$$

$$X_\sigma^T \beta = g(\mu_\sigma) = \hat{\theta}(\mu_\sigma) \quad (32.18)$$

$$\mu_\sigma = g^{-1}(X_\sigma^T \beta) = \hat{\mu}(X_\sigma^T \beta) \quad (32.19)$$

$\hat{\theta}() = g()$  is called the **link function**.

Note that in Linear Regression (LR), we consider independent (but not necessarily identically distributed) random variables  $\underline{y}_\sigma \in \mathbb{R}$  that satisfy

$$\underline{y}_\sigma = X_\sigma^T \beta + \epsilon_\sigma \quad (32.20)$$

where

$$\langle \epsilon_\sigma \rangle = 0, \quad \langle \epsilon_\sigma, \epsilon_\sigma \rangle = \delta(\sigma, \sigma') \sigma_\sigma^2 \quad (32.21)$$

Equivalently, one states that

$$\underline{y}_\sigma \sim \mathcal{N}(\mu_\sigma = X_\sigma^T \beta, \sigma_\sigma^2) \quad (32.22)$$

Hence, for LR, the link function and its inverse are the identity map.

For the Bernoulli distribution with  $y_\sigma \in \{0, 1\}$ ,

$$Ber(y_\sigma; p_\sigma) = p_\sigma^{y_\sigma} (1 - p_\sigma)^{1-y_\sigma} \quad (32.23)$$

$$= \exp(y_\sigma \ln p_\sigma + (1 - y_\sigma) \ln(1 - p_\sigma)) \quad (32.24)$$

$$= \exp \left( y_\sigma \underbrace{\ln \left( \frac{p_\sigma}{1 - p_\sigma} \right)}_{X_\sigma^T \beta} + \underbrace{\ln(1 - p_\sigma)}_{-b} \right) \quad (32.25)$$

$\mu_\sigma = p_\sigma$ , and  $X_\sigma^T \beta = \text{logit}(\mu_\sigma)$  so  $\mu_\sigma = \text{smoid}(X_\sigma^T \beta)$ .  
 $g() = \text{logit}()$  and  $g^{-1}() = \text{smoid}()$

$$a = 1 \quad (32.26)$$

$$b = -\ln(1 - \mu_\sigma) \quad (32.27)$$

$$= -\ln \left( 1 - \frac{1}{1 + e^{-X_\sigma^T \beta}} \right) \quad (32.28)$$

$$= -\ln \left( \frac{e^{-X_\sigma^T \beta}}{1 + e^{-X_\sigma^T \beta}} \right) \quad (32.29)$$

$$= \ln(1 + e^{X_\sigma^T \beta}) \quad (32.30)$$

$$\partial_{X_\sigma^T \beta} b = \frac{e^{X_\sigma^T \beta}}{1 + e^{X_\sigma^T \beta}} \quad (32.31)$$

$$= \text{smoid}(X_\sigma^T \beta) \quad (32.32)$$

$$= \mu_\sigma \quad (32.33)$$

Table 32.1 gives various probability distributions and their natural link functions, for cases where the link function is simple and easy to invert.

GLM is a generalization of LR. Recall some of the main results of LR:

$$y = X\beta + \epsilon \quad (32.34)$$

$$\langle \epsilon \rangle = 0, \quad \langle \epsilon, \epsilon^T \rangle = \sigma^2 I_N \quad (32.35)$$

where  $I_N$  is the  $N = |\Sigma|$  dimensional unit matrix.

The Maximum Likelihood Estimate (MLE) for  $\beta$  is

$$\hat{\beta} = (X^T X)^{-1} X^T y. \quad (32.36)$$

prob. distribution	link function $X_\sigma^T \beta = g(\mu_\sigma)$	$\mu_\sigma = g^{-1}(X_\sigma^T \beta)$
Normal $y_\sigma \in (-\infty, +\infty)$	$X_\sigma^T \beta = \mu_\sigma$ ( $g$ = identity map)	$\mu_\sigma = X_\sigma^T \beta$
Exponential $y_\sigma \in (0, +\infty)$	$X_\sigma^T \beta = -\frac{1}{\mu_\sigma}$	$\mu_\sigma = -\frac{1}{X_\sigma^T \beta}$
Poisson $y_\sigma \in \{0, 1, 2, \dots\}$	$X_\sigma^T \beta = \ln \mu_\sigma$	$\mu_\sigma = \exp(X_\sigma^T \beta)$
Bernoulli $y_\sigma \in \{0, 1\}$	$X_\sigma^T \beta = \text{lodds}(\mu_\sigma)$	$\mu_\sigma = \text{smoid}(X_\sigma^T \beta)$

Table 32.1: Various probability distributions and their natural link functions.

The covariance of  $\hat{\beta}$  is

$$\langle \hat{\beta}, \hat{\beta}^T \rangle = \langle X^T X)^{-1} X^T y, y^T X (X^T X)^{-1} \rangle \quad (32.37)$$

$$= \sigma^2 (X^T X)^{-1} \quad (32.38)$$

Next we will try to find analogous results for GLM. We will give (1) a numerical method for calculating an estimate  $\hat{\beta}$  and (2) an asymptotic expression for  $\langle \hat{\beta}, \hat{\beta}^T \rangle$ .

Let

$$LL = \sum_{\sigma} LL_{\sigma} \quad (32.39)$$

where

$$LL_{\sigma} = LL_{y_{\sigma} | \theta_{\sigma}} \quad (32.40)$$

$$= \frac{y_{\sigma} \theta_{\sigma} - b(\theta_{\sigma})}{a(\phi)} + c(y_{\sigma}, \phi) \quad (32.41)$$

The Newton-Raphson method for calculating an estimate  $\hat{\beta}$  is as follows. Let  $u^T = [\frac{\partial \langle LL \rangle}{\partial \beta_j}]_{j=0,1,2,\dots}$

$H = [H_{j,j'}]$ ,  $H_{j,j'} = \frac{\partial^2 \langle LL \rangle}{\partial \beta_j \partial \beta_{j'}}$ .  $H$  is called the **Hessian matrix**

For  $t = 0, 1, 2, \dots$ , consider the Taylor expansion to second order of  $\langle LL \rangle(\beta)$  about the point  $\beta = \beta^{(t)}$

$$\langle LL \rangle(\beta) \approx \langle LL \rangle(\beta^{(t)}) + u^{(t)T}(\beta - \beta^{(t)}) + \frac{1}{2}(\beta - \beta^{(t)})^T H^{(t)}(\beta - \beta^{(t)}) \quad (32.42)$$

By Section C.31, we have,

$$0 = \frac{\partial \langle LL \rangle(\beta)}{\partial \beta^T} = u^{(t)} + H^{(t)}(\beta - \beta^{(t)}) \quad (32.43)$$

This last equation suggests the recursion

$$\beta^{(t+1)} = \beta^{(t)} - (H^{(t)})^{-1}u^{(t)}. \quad (32.44)$$

Fig.32.1 gives a graphical representation of one cycle of this recursion.

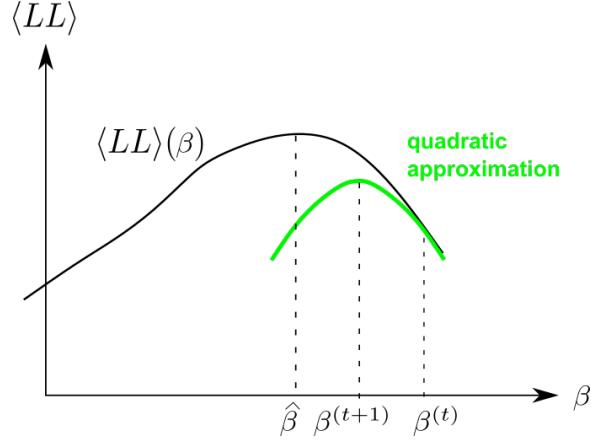


Figure 32.1: One cycle of Newton-Raphson method for calculating an estimate  $\hat{\beta}$  for the GLM.

### Claim 66

$$\frac{\partial LL_\sigma}{\partial \beta_j} = \frac{[y_\sigma - b'(X_\sigma^T \beta)]}{\langle y_\sigma, y_\sigma \rangle} \frac{\partial \hat{\mu}_\sigma}{\partial X_\sigma^T \beta} X_{\sigma,j} \quad (32.45)$$

**proof:**

$$\frac{\partial LL_\sigma}{\partial \beta_j} = \frac{\partial LL_\sigma}{\partial \theta_\sigma} \frac{\partial \theta_\sigma}{\partial \mu_\sigma} \frac{\partial \hat{\mu}_\sigma}{\partial X_\sigma^T \beta} \frac{\partial X_\sigma^T \beta}{\partial \beta_j} \quad (32.46)$$

$$\frac{\partial LL_\sigma}{\partial \theta_\sigma} = \frac{y_\sigma - b'(\theta_\sigma)}{a(\phi)} \quad (32.47)$$

$$\frac{\partial \mu_\sigma}{\partial \theta_\sigma} = b''(\theta_\sigma) = \frac{\langle y_\sigma, y_\sigma \rangle}{a(\phi)} \quad (32.48)$$

$$\frac{\partial \hat{\mu}_\sigma}{\partial X_\sigma^T \beta} = (g^{-1})'(X_\sigma^T \beta) \quad (32.49)$$

$$\frac{\partial X_\sigma^T \beta}{\partial \beta_j} = X_{\sigma,j} \quad (32.50)$$

$$\frac{\partial LL_\sigma}{\partial \beta_j} = \frac{[y_\sigma - b'(\theta_\sigma)]}{\langle y_\sigma, y_\sigma \rangle} \frac{\partial \hat{\mu}_\sigma}{\partial X_\sigma^T \beta} X_{\sigma,j} \quad (32.51)$$

**QED**

**Claim 67** (*Asymptotic expression for  $\langle \hat{\beta}, \hat{\beta}^T \rangle$  for GLM*)

$$\langle \hat{\beta}, \hat{\beta}^T \rangle \rightarrow \mathcal{I}^{-1} \quad (\text{asymptotic covariance}) \quad (32.52)$$

(Hence, more information  $\mathcal{I}$  yields a smaller variance.) where

$$\mathcal{I} = X^T W X \quad (32.53)$$

and

$$W_{\sigma,\sigma'} = \left[ \left( \frac{\partial \hat{\mu}}{\partial X_\sigma^T \beta} \right)^2 \frac{\delta(\sigma, \sigma')}{\langle y_\sigma, y_\sigma \rangle} \right]_{\beta=\hat{\beta}} \quad (32.54)$$

$\mathcal{I}$  is called the **information matrix**.

**proof:**

$$\left\langle \frac{\partial LL_\sigma}{\partial \beta_j} \frac{\partial LL_\sigma}{\partial \beta_{j'}} \right\rangle = \left\langle \frac{[y_\sigma - b'(X_\sigma^T \beta)]}{\langle y_\sigma, y_\sigma \rangle} \frac{\partial \hat{\mu}_\sigma}{\partial X_\sigma^T \beta} X_{\sigma,j} \frac{[y_\sigma - b'(X_\sigma^T \beta)]}{\langle y_\sigma, y_\sigma \rangle} \frac{\partial \hat{\mu}_\sigma}{\partial X_\sigma^T \beta} X_{\sigma,j'} \right\rangle \quad (32.55)$$

$$= \left[ \frac{\partial \hat{\mu}_\sigma}{\partial X_\sigma^T \beta} \right]^2 \frac{X_{\sigma,j} X_{\sigma,j'}}{\langle y_\sigma, y_\sigma \rangle} \quad (32.56)$$

$$\sum_\sigma \left\langle \frac{\partial LL_\sigma}{\partial \beta_j} \frac{\partial LL_\sigma}{\partial \beta_{j'}} \right\rangle = (X^T W X)_{j,j'} \quad (32.57)$$

By Section C.31, we have

$$\left\langle \frac{\partial^2 LL_\sigma}{\partial \beta_j \partial \beta_{j'}} \right\rangle = - \left\langle \frac{\partial LL_\sigma}{\partial \beta_j} \frac{\partial LL_\sigma}{\partial \beta_{j'}} \right\rangle \quad (32.58)$$

Summing both sides of the last equation over  $\sigma$ , we find

$$\left\langle \frac{\partial^2 LL}{\partial \beta_j \partial \beta_{j'}} \right\rangle = -(X^T W X)_{j,j'} \quad (32.59)$$

According to Section C.31, we have

$$\langle \hat{\beta}, \hat{\beta}^T \rangle \rightarrow (X^T W X)^{-1} \quad (32.60)$$

**QED**

# Chapter 33

## Generative Adversarial Networks (GANs)

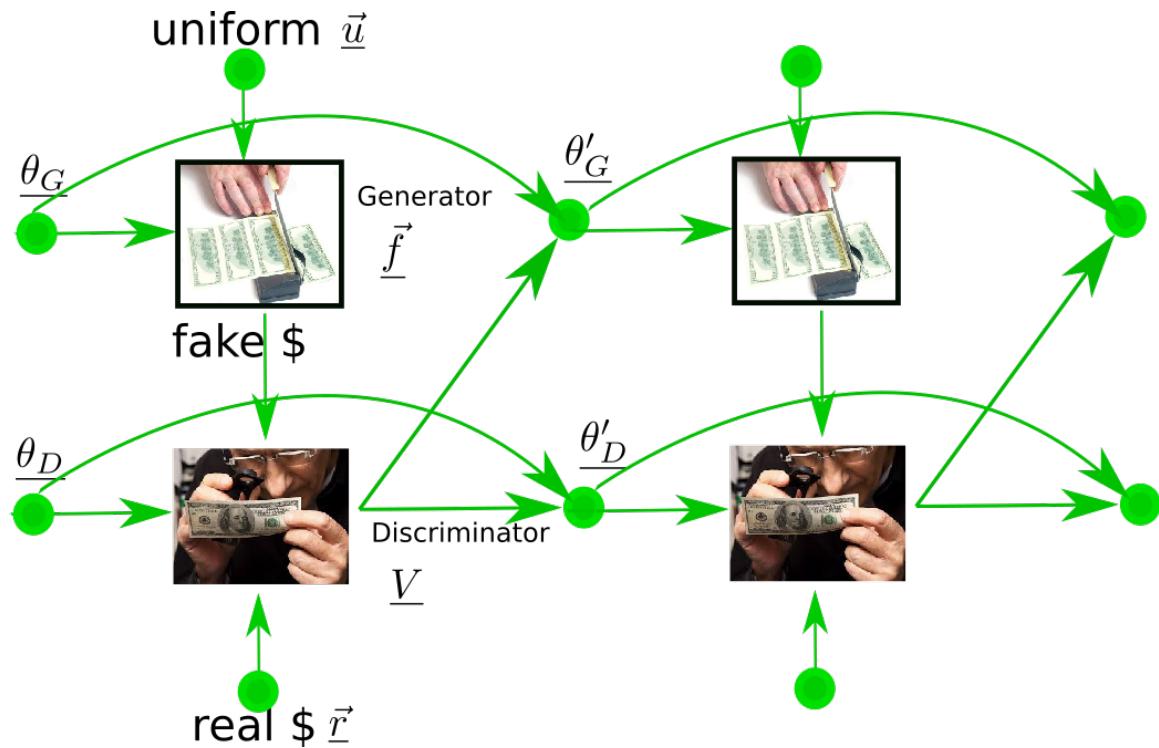


Figure 33.1: Generative Adversarial Network (GAN)

Original GAN, Ref.[18](2014).

Generator  $G$  (counterfeiter) generates samples  $\vec{f}$  of fake money and submits them to Discriminator  $D$  (Treasury agent).  $D$  also gets samples  $\vec{r}$  of real money.  $D$  submits verdict  $V \in [0, 1]$ .  $G$  depends on parameter  $\underline{\theta}_G$  and  $D$  on parameter  $\underline{\theta}_D$ . Verdict  $V$  and initial  $\underline{\theta}_G, \underline{\theta}_D$  are used to get new parameters  $\underline{\theta}'_G, \underline{\theta}'_D$ . Process is repeated.

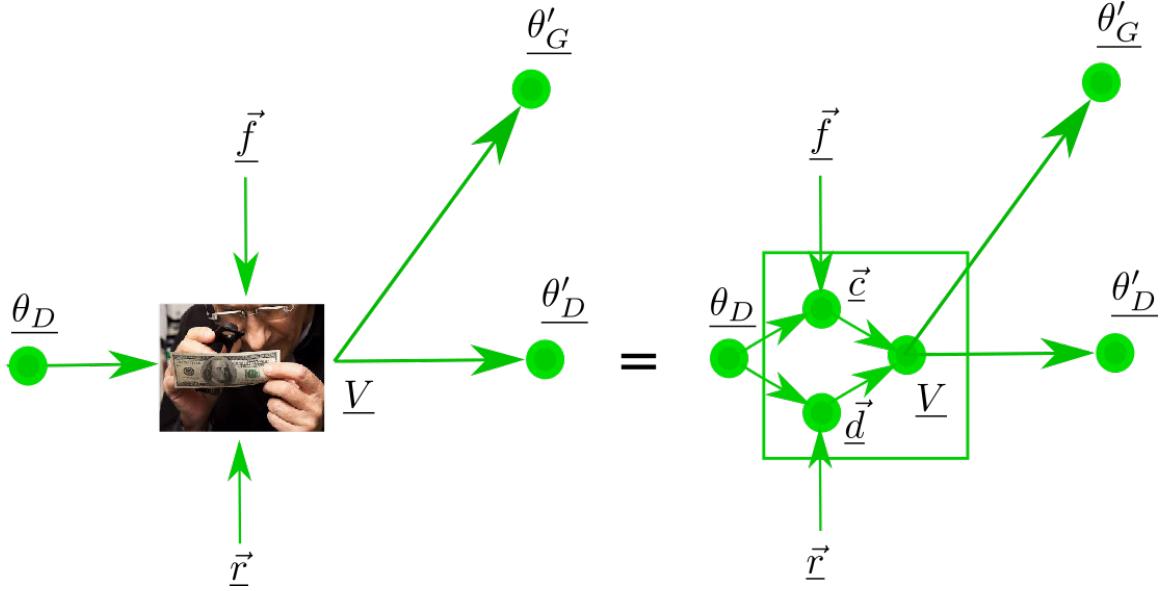


Figure 33.2: Discriminator node  $\underline{V}$  in Fig.33.1 can be split into 3 nodes  $\vec{c}$ ,  $\vec{d}$  and  $\underline{V}$ .

(Dynamical Bayesian Network) until saddle point in  $V(\theta_G, \theta_D)$  is reached.  $D$  makes  $G$  better and vice versa. Zero-sum game between  $D$  and  $G$ .

Let  $\mathcal{D}$  be the domain of  $D(\cdot, \theta_D)$ . Assume that for any  $x \in \mathcal{D}$ ,

$$0 \leq D(x, \theta_D) \leq 1 . \quad (33.1)$$

For any  $S \subset \mathcal{D}$ , define

$$\sum_{x \in S} D(x, \theta_D) = \lambda(S, \theta_D) . \quad (33.2)$$

In general,  $G(\cdot, \theta_G)$  need not be real valued.

Assume that for every  $u \in S_u$ ,  $G(u, \theta_G) = f \in S_f \subset \mathcal{D}$ . Define

$$\overline{D}(f, \theta_D) = 1 - D(f, \theta_D) . \quad (33.3)$$

Note that

$$0 \leq \overline{D}(f, \theta_D) \leq 1 . \quad (33.4)$$

Define:

$$V(\theta_G, \theta_D) = \sum_r P(r) \ln D(r, \theta_D) + \sum_u P(u) \ln \overline{D}(G(u, \theta_G), \theta_D) . \quad (33.5)$$

We want the first variation of  $V(\theta_G, \theta_D)$  to vanish.

$$\delta V(\theta_G, \theta_D) = 0 . \quad (33.6)$$

This implies

$$\partial_{\theta_G} V(\theta_G, \theta_D) = \partial_{\theta_D} V(\theta_G, \theta_D) = 0 \quad (33.7)$$

and

$$V_{opt} = \min_{\theta_G} \max_{\theta_D} V(\theta_G, \theta_D) . \quad (33.8)$$

The TPMs, printed in blue, for bnets Figs.33.1 and 33.2, are as follows:

$$P(\theta_G) = \text{ given} \quad (33.9)$$

$$P(\theta_D) = \text{ given} \quad (33.10)$$

$$P(\vec{u}) = \prod_i P(u[i]) \quad (\text{usually uniform distribution}) \quad (33.11)$$

$$P(\vec{r}) = \prod_i P(r[i]) \quad (33.12)$$

$$P(f[i] | \vec{u}, \theta_G) = \delta[f[i], G(u[i], \theta_G)] \quad (33.13)$$

$$P(c[i] | \vec{f}, \theta_D) = \delta(c[i], \overline{D}(f[i], \theta_D)) \quad (33.14)$$

$$P(d[j] | \vec{r}, \theta_D) = \delta(d[j], D(r[j], \theta_D)) \quad (33.15)$$

$$P(V|\vec{d}, \vec{c}) = \delta(V, \frac{1}{N} \ln \prod_{i,j} (c[i]d[j])) \quad (33.16)$$

where  $N = nsam(\vec{r})nsam(\vec{u})$ .

Let  $\eta_G, \eta_D > 0$ . Maximize  $V$  wrt  $\theta_D$ , and minimize it wrt  $\theta_G$ .

$$P(\theta'_G|V, \theta_G) = \delta(\theta'_G, \theta_G - \eta_G \partial_{\theta_G} V) \quad (33.17)$$

$$P(\theta'_D | V, \theta_D) = \delta(\theta'_D, \theta_D + \eta_D \partial_{\theta_D} V) \quad (33.18)$$

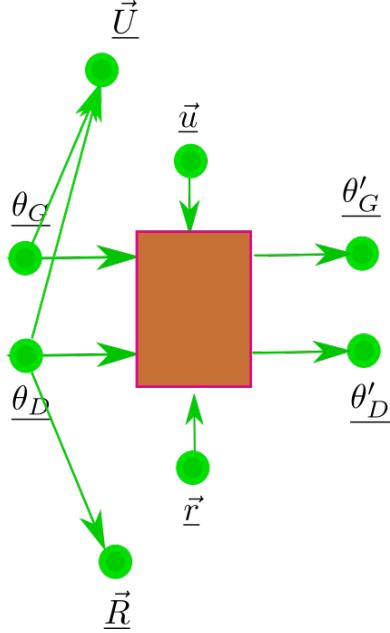


Figure 33.3: GAN, Constraining Bayesian Network

Constraining Bnet given in Fig.33.3. It adds 2 new nodes, namely  $\vec{U}$  and  $\vec{R}$ , to the bnet of Fig.33.1. The purpose of these 2 barren (childrenless) nodes is to constrain certain functions to be probability distributions.

The TPMs, printed in blue, for the 2 new nodes, are as follows.

$$P(U[i] | \theta_G) = \frac{\overline{D}(G(U[i], \theta_G), \theta_D)}{\bar{\lambda}(\theta_G, \theta_D)} \quad (33.19)$$

where  $S_{\underline{U}[i]} = S_u$  and  $\bar{\lambda}(\theta_G, \theta_D) = \sum_u \overline{D}(G(u, \theta_G), \theta_D)$ .

$$P(R[i] | \theta_G, \theta_D) = \frac{D(R[i], \theta_D)}{\lambda(\theta_D)} \quad (33.20)$$

where  $S_{\underline{R}[i]} = S_r$  and  $\lambda(\theta_D) = \sum_r D(r, \theta_D)$ .

$$P(V | \vec{u}, \vec{r}) = \delta(V, \frac{1}{N} \ln \prod_{i,j} (P(R[i] = r[i] | \theta_G, \theta_D) P(\underline{U}[i] = u[j] | \theta_G))) \quad (33.21)$$

where  $N = nsam(\vec{r})nsam(\vec{u})$ .

$L$  = likelihood

$$L = P(\vec{r}, \vec{u} | \theta_G, \theta_D) \quad (33.22)$$

$$= \prod_{i,j} \left[ \frac{D(r[i], \theta_D)}{\lambda(\theta_D)} \frac{\overline{D}(G(u[j], \theta_G), \theta_D))}{\overline{\lambda}(\theta_G, \theta_D)} \right] \quad (33.23)$$

$$\ln L = N[V(\theta_G, \theta_D) - \ln \lambda(\theta_D) - \ln \overline{\lambda}(\theta_G, \theta_D)] \quad (33.24)$$

# Chapter 34

## Goodness of Causal Fit

See my paper and software Ref.[72].

# Chapter 35

## Gradient Descent

**Gradient Descent** (GD) is when we have a sequence of points  $w_k \in \mathbb{R}^n$  and a convex loss function  $\mathcal{L} : \mathbb{R}^n \rightarrow \mathbb{R}$  such that

$$w_{k+1} = w_k - \alpha \nabla_w \mathcal{L}(w_k) \quad (35.1)$$

for some “learning rate”  $\alpha > 0$ . Since the function  $\mathcal{L}(w)$  is convex, it has a minimum  $w^*$  and  $w_k \rightarrow w^*$  as  $k \rightarrow \infty$ .

In Machine Learning (ML), it is usually the case that

$$\mathcal{L}(w) = \sum_{\sigma=1}^{nsam} \hat{\mathcal{L}}(\hat{y}^\sigma(x^\sigma, w), y^\sigma) \quad (35.2)$$

where the sum is over  $nsam$  samples. Normally,  $nsam$  would be all the samples in a dataset. In ML,  $nsam$  is often very large, and  $\nabla_w \hat{\mathcal{L}}$  cannot be calculated analytically so it must be calculated numerically<sup>1</sup>, individually for each of the  $nsam$  samples. In such cases, a Monte Carlo method called **Stochastic Gradient Descent** (SGD) is often used. SGD just means choosing at random a small subset of the  $nsam$  samples (“mini-batch”), and approximating  $\nabla_w \mathcal{L}(w)$  by an average of the gradients for the mini-batch.

This description of GD is fairly complete, so why this chapter? In this chapter, we will give a dynamical bnet (see Chapter 25) illustrating how GD is used in ML.

Samples  $(x^\sigma, y^\sigma) \in S_x \times S_y$  are given.  $nsam(\vec{x}) = nsam(\vec{y})$ .

Estimator function  $\hat{y}(x; w)$  for  $x \in S_x$  and  $w \in \mathbb{R}$  is given.

Let

$$P_{\underline{x}, \underline{y}}(x, y) = \frac{1}{nsam(\vec{x})} \sum_{\sigma} \mathbb{1}(x = x^\sigma, y = y^\sigma). \quad (35.3)$$

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<sup>1</sup>Gradients can be calculated numerically by the method of back-propagation, which is explained in Chapter 5.

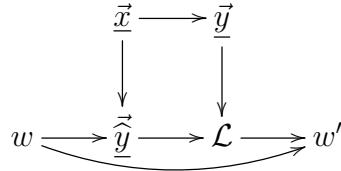


Figure 35.1: Basic gradient descent bnet.

Let

$$\mathcal{L}(\vec{x}, \vec{y}, w) = \frac{1}{nsam(\vec{y})} \sum_{\sigma} |y^{\sigma} - \hat{y}(x^{\sigma}; w)|^2 \quad (35.4)$$

$\mathcal{L}$  is called the **mean square error**.

Best fit is parameters  $w^*$  such that

$$w^* = \underset{w}{\operatorname{argmin}} \mathcal{L}(\vec{x}, \vec{y}, w) . \quad (35.5)$$

The TPMs, printed in blue, for the basic curve fitting bnet Fig.35.1, are as follows.

$$P(w) = \text{given} . \quad (35.6)$$

The first time it is used,  $w$  is arbitrary. After the first time, it is determined by previous stage.

$$P(\vec{x}) = \prod_{\sigma} P_{\underline{x}}(x^{\sigma}) \quad (35.7)$$

$$P(\vec{y}|\vec{x}) = \prod_{\sigma} P_{\underline{y}|\underline{x}}(y^{\sigma} | x^{\sigma}) \quad (35.8)$$

$$P(\hat{y}^{\sigma}|w, \vec{x}) = \delta(\hat{y}^{\sigma}, \hat{y}(x^{\sigma}; w)) \quad (35.9)$$

$$P(\mathcal{L}|\vec{y}, \vec{y}) = \delta(\mathcal{L}, \frac{1}{nsam(\vec{y})} \sum_{\sigma} |y^{\sigma} - \hat{y}^{\sigma}|^2) . \quad (35.10)$$

$$P(w'|w, \mathcal{L}) = \delta(w', w - \alpha \partial_w \mathcal{L}) \quad (35.11)$$

$\alpha > 0$  is called **the descent rate or learning rate**. If  $\Delta w = w' - w = -\alpha \frac{\partial \mathcal{L}}{\partial w}$ , then  $\Delta \mathcal{L} = \frac{-1}{\alpha} (\Delta w)^2 < 0$  so this will minimize the error  $\mathcal{L}$ . This is an example of GD.

# Chapter 36

## Granger Causality

This chapter is based on the Wikipedia article Ref.[118] and Scholarpedia article Ref.[61] on Granger causality and on the book Ref.[20] on time series analysis by Hamilton.

This chapter assumes the reader has read Chapter 93 on the stationary time series  $ARMA(p, q)$  and  $VAR(p)$ .

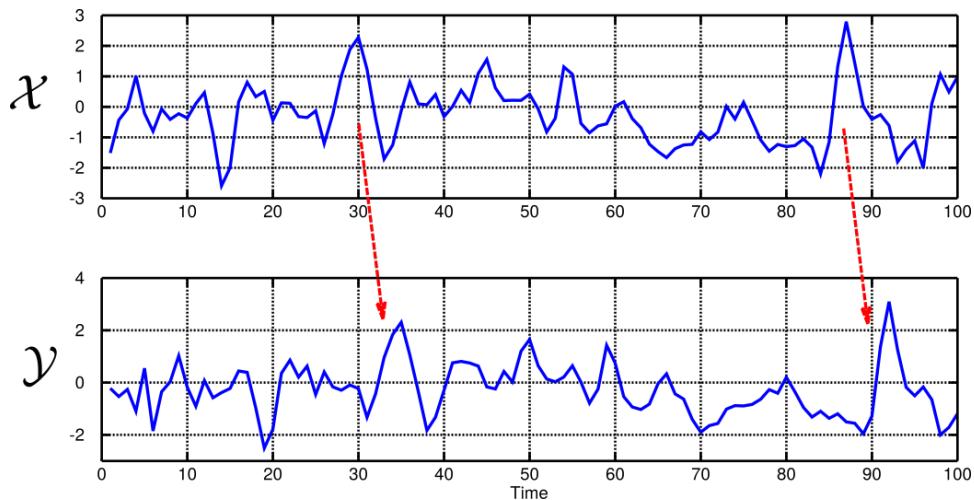


Figure 36.1: When t-series  $\mathcal{X}$  Granger-causes t-series  $\mathcal{Y}$ , the patterns in  $\mathcal{X}$  are approximately repeated in  $\mathcal{Y}$  after some time lag (two examples are indicated with arrows). Thus, past values of  $\mathcal{X}$  can be used for the prediction of future values of  $\mathcal{Y}$ . (image and caption from Ref.[118])

Let  $\underline{x}_t = [x_t^A]_{\forall A} \in \mathbb{R}^{nr_1 \times 1}$  and  $\underline{y}_t = [y_t^B]_{\forall B} \in \mathbb{R}^{nr_2 \times 1}$ . Thus,  $\underline{x}_t$  for each  $t$  is a column vector with  $nr_1$  rows, and  $\underline{y}_t$  for each  $t$  is a column vector with  $nr_2$  rows. Let  $nr_1 + nr_2 = nr$ , the total number of rows. Consider a vector t-series  $\{\underline{x}_t, \underline{y}_t\}_{\forall t}$  of type  $VAR(p)$ , as defined by Eq.(93.183). To simplify the notation of Eq.(93.183), we are replacing  $x^1$  by  $x$ ,  $x^2$  by  $y$ ,  $n^1$  by  $n$ , and  $n^2$  by  $w$ .

$$\begin{bmatrix} \underline{x}_t^A \\ \underline{y}_t^B \end{bmatrix} = \sum_{j=1}^p \begin{bmatrix} \alpha_j^{\underline{x}|x;A,A'} & \alpha_j^{\underline{x}|y;A,B'} \\ \alpha_j^{\underline{y}|x;B,A'} & \alpha_j^{\underline{y}|y;B,B'} \end{bmatrix} \begin{bmatrix} \underline{x}_{t-j}^{A'} \\ \underline{y}_{t-j}^{B'} \end{bmatrix} + \begin{bmatrix} \underline{n}_t^A \\ \underline{w}_t^B \end{bmatrix} \quad (36.1)$$

Hence,

$$E_{|\vec{x}_{<t}, \vec{y}_{<t}} \left[ \underline{y}_t^B \right] = \sum_{j=1}^p \alpha_j^{\underline{y}|x;B,A'} \underline{x}_{t-j}^{A'} + \sum_{j=1}^p \alpha_j^{\underline{y}|y;B,B'} \underline{y}_{t-j}^{B'} \quad (36.2)$$

Let  $\mathcal{X} = \{\vec{x}_t\}_{\forall t}$  and  $\mathcal{Y} = \{\vec{y}_t\}_{\forall t}$ .

We say  $\mathcal{X}$  **does not G-cause** (or **does not G-forecast**)  $\mathcal{Y}$ , and symbolize this by  $\mathcal{X} \dashv_G \mathcal{Y}$ , if

$$\alpha_j^{\underline{y}|x;B,A'} = 0 \quad \forall (j, B, A') \quad (36.3)$$

or, equivalently,

$$E_{|\vec{x}_{<t}, \vec{y}_{<t}} \left[ \underline{y}_t^B \right] = E_{|\vec{y}_{<t}} \left[ \underline{y}_t^B \right] \quad \forall (B, t) \quad (36.4)$$

We say  $\mathcal{X}$  **G-causes** (or **G-forecasts**)  $\mathcal{Y}$  and symbolize this by  $\mathcal{X} \xrightarrow[G]{ } \mathcal{Y}$ , if  $\mathcal{X} \dashv_G \mathcal{Y}$  is false.

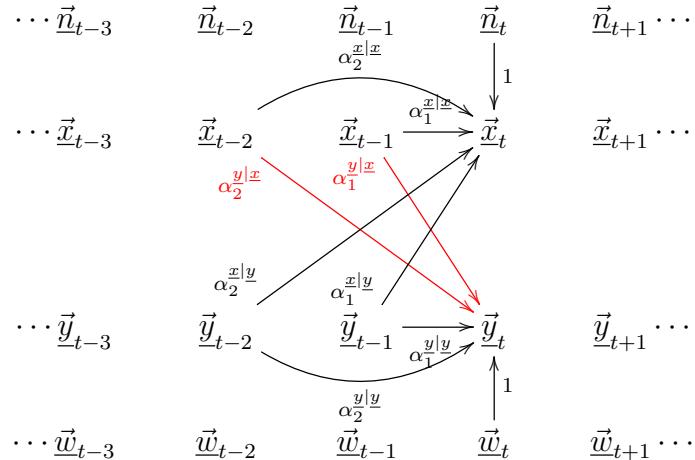


Figure 36.2: Bnet for  $VAR(2)$ . For clarity, we only show the arrows entering nodes  $\vec{x}_t$  and  $\vec{y}_t$ . Remove red arrows if  $\mathcal{X}$  does not G-cause  $\mathcal{Y}$ , and keep them if it does.

Eq.(36) describing a bipartite  $VAR(p)$  t-series can be represented by the bnet Fig.36.2. The TPMs, printed in blue, for the two nodes  $\vec{x}_t$  and  $\vec{y}_t$ , are as follows:

$$P(\vec{x}_t | \vec{x}_{[t-p,t-1]}, \vec{y}_{[t-p,t-1]}, \vec{n}_t) = \prod_A \mathbb{1} \left( \vec{x}_t^A = \sum_{j=1}^p \alpha_j^{x|A,A'} \vec{x}_{t-j}^{A'} + \sum_{j=1}^p \alpha_j^{x|B,B'} \vec{y}_{t-j}^{B'} + n_t^A \right) \quad (36.5)$$

$$P(\vec{y}_t | \vec{x}_{[t-p,t-1]}, \vec{y}_{[t-p,t-1]}, \vec{w}_t) = \prod_B \mathbb{1} \left( \vec{y}_t^B = \underbrace{\sum_{j=1}^p \alpha_j^{y|x;B,A'} \vec{x}_{t-j}^{A'}}_{0?} + \sum_{j=1}^p \alpha_j^{y|B,B'} \vec{y}_{t-j}^{B'} + w_t^B \right) \quad (36.6)$$

### Testing for GC

- Consider the datasets

$$\mathcal{D}_{\underline{x}} = \{(t, \vec{x}_{[t-p,t-1]}, \vec{y}_{[t-p,t-1]}, \boxed{\vec{x}_t}) : t\} \quad (36.7)$$

$$\mathcal{D}_{\underline{y}} = \{(t, \vec{x}_{[t-p,t-1]}, \vec{y}_{[t-p,t-1]}, \boxed{\vec{y}_t}) : t\} \quad (36.8)$$

One can do Linear Regression on  $\mathcal{D}_{\underline{x}}$  with x-variables  $(\vec{x}_{[t-p,t-1]}, \vec{y}_{[t-p,t-1]})$ , y-variable  $\vec{x}_t$ , and regression coefficients  $\alpha_{[1,p]}^{x|x}$ ,  $\alpha_{[1,p]}^{x|y}$ . One can also do Linear Regression on  $\mathcal{D}_{\underline{y}}$  with x-variables  $(\vec{x}_{[t-p,t-1]}, \vec{y}_{[t-p,t-1]})$ , y-variable  $\vec{y}_t$ , and regression coefficients  $\alpha_{[1,p]}^{y|x}$ ,  $\alpha_{[1,p]}^{y|y}$ . The LR software yields confidence intervals for the regression coefficients.

- One can do hypothesis testing using the Likelihood Ratio Test<sup>1</sup>

Null hypothesis  $H_0 : \mathcal{X} \xrightarrow[G]{-} \mathcal{Y}$ , Alternative hypothesis  $H_1 : \mathcal{X} \xrightarrow[G]{} \mathcal{Y}$

- Test for both  $\mathcal{X} \xrightarrow[G]{} \mathcal{Y}$  and  $\mathcal{Y} \xrightarrow[G]{} \mathcal{X}$ .

### Limitations

It has been remarked that G-causality is not true causality because, even though an event A must precede an event B in order to cause it, that does not necessarily mean that A causes B. I think the problem with G-causality is that it uses a bnet that is a good fit for the dataset, but not necessarily also a good *causal* fit for the experiment. One can measure the goodness of causal fit of a bnet by doing do-intervention experiments (See Chapter 34).

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<sup>1</sup>The Likelihood Ratio Test is discussed in Section C.23.

# Chapter 37

## Hidden Markov Model

A dynamical Bayesian network (DBN) (see Chapter 25) is a generalization of a Hidden Markov Model (HMM), which in turn is a generalization of a Kalman Filter (KF) (see Chapter 44).

See Wikipedia article Ref.[119] to learn about the history and many uses of HMMs. This chapter is based on Refs.[44], [119], [165], [90].

In this chapter, we use the following conventions.

Random variables are underlined and their values are not. For example,  $\underline{a} = a$  means the random variable  $\underline{a}$  takes the value  $a$ . A diagram with all its nodes underlined represents a Bayesian Network (bnet), whereas the same diagram with the letters not underlined represents a specific **instantiation** of that bnet. For example  $\underline{a} \rightarrow \underline{b} \rightarrow \underline{c}$  represents the bnet with full probability distribution  $P(c|b)P(b|a)P(a)$ , whereas  $a \rightarrow b \rightarrow c$  represents  $P(c|b)P(b|a)$ . Note that, for convenience, we define  $a \rightarrow b \rightarrow c$  to exclude the priors of root nodes such as  $P(a)$ .

If  $\underline{a}$  is a root node, then  $\sum a$  signifies a weighted sum  $\sum_a P(a)$ . For example,

$$\sum a \rightarrow b \rightarrow c = \sum_a P(c|b)P(b|a)P(a) \quad (37.1)$$

If  $\underline{a}$  is not a root node, then  $\sum a$  signifies a simple unweighted sum  $\sum_a$ . For example,

$$x \rightarrow \sum a \rightarrow y = \sum_a P(y|a)P(a|x) \quad (37.2)$$

Two bnets are equated if their full probability distributions (i.e., their full instantiations) are equal numerically. For example,

$$\underline{a} \rightarrow \underline{b} \rightarrow \underline{c} = P(c|b)P(b|a)P(a) = \underline{a} \leftarrow \underline{b} \leftarrow \underline{c} \quad (37.3)$$

Unobserved (a.k.a. hidden, latent) nodes are indicated in a bnet by enclosing their label in a dashed circle. For example,  $(\bar{u})$ . Alternatively, they are indicated by using dashed arrows for all arrows emanating from the unobserved node.

Suppose

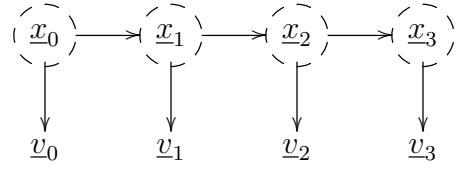


Figure 37.1: HMM bnet with  $n = 4$ .

$v^n = (\underline{v}_0, \underline{v}_1, \dots, \underline{v}_{n-1})$  are  $n$  visible nodes that are measured, and  $x^n = (\underline{x}_0, \underline{x}_1, \dots, \underline{x}_{n-1})$  are the  $n$  hidden, unmeasurable state nodes of a system that is being monitored.

For the bnet of Fig.37.1, one has

$$P(x^n, v^n) = \prod_{t=0}^{n-1} P(x_t | x_{t-1}) P(v_t | x_t), \quad (37.4)$$

where  $x_{-1} = \emptyset$ .

We assume that this bnet is stationary. The following notation emphasizes that fact:

$\pi(x)$  = prior probability

$$\pi(x) = P(\underline{x}_0 = x) \quad (37.5)$$

$A(x|x')$  = transition matrix

$$A(x|x') = P(\underline{x}_t = x | \underline{x}_{t-1} = x') \quad (37.6)$$

$B(v|x)$  = emission probability

$$B(v|x) = P(\underline{v}_t = v | \underline{x}_t = x) \quad (37.7)$$

Let  $x_{<t} = (x_0, x_1, \dots, x_{t-1})$ .

For  $t = 0, 1, \dots, n-1$ , define

$\mathcal{F}_t(x_t)$ =future measurements probability

$$\mathcal{F}_t(x_t) = P(v_{>t} | x_t) \quad (37.8)$$

$$= x_t \longrightarrow \sum x_{>t} \quad (37.9)$$

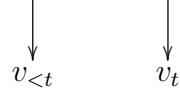
$\downarrow$

$v_{>t}$

$\overline{\mathcal{F}}_t(x_t)$ = past and present measurements probability

$$\bar{\mathcal{F}}_t(x_t) = P(v_{<t}, v_t, x_t) \quad (37.10)$$

$$= \sum x_{<t} \longrightarrow x_t \quad (37.11)$$



$\lambda_t(x_t)$  = present measurement probability, (a.k.a. emission probability  $B(v_t|x_t)$ ).  $\lambda_t(x_t)$  is the likelihood of  $x_t$ .

$$\lambda_t(x_t) = P(v_t|x_t) \quad (37.12)$$

$$= x_t \quad (37.13)$$



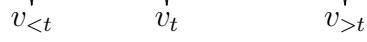
$$v_t$$

### 37.1 Calculating $P(x_t, v^n)$ and $P(x_t, x_{t+1}, v^n)$

**Claim 68** For  $t \geq 0$ ,

$$P(x_t, v^n) = \bar{\mathcal{F}}_t(x_t) \mathcal{F}_t(x_t) \quad (37.14)$$

$$= \sum x_{<t} \longrightarrow x_t \quad x_t \longrightarrow \sum x_{>t} . \quad (37.15)$$



For  $t > 0$ ,

$$P(x_{t-1}, x_t, v^n) = \bar{\mathcal{F}}_{t-1}(x_{t-1}) P(x_t|x_{t-1}) \lambda_t(x_t) \mathcal{F}_t(x_t) \quad (37.16)$$

$$= \sum x_{<t-1} \longrightarrow x_{t-1} \quad x_{t-1} \longrightarrow x_t \quad x_t \longrightarrow \sum x_{>t} \quad (37.17)$$



**proof:**

$$P(x_t, v^n) = \sum_{x_{<i}} \sum_{x_{>i}} P(x^n, v^n) \quad (37.18)$$

$$= \sum_{x_{<i}} \sum_{x_{>i}} P(x^n, v^n | x_t) P(x_t) \quad (37.19)$$

$$= \sum_{x_{<i}} \sum_{x_{>i}} P(x_{<i}, v_{<i}, v_t | x_t) P(x_{>t}, v_{>i} | x_t) P(x_t) \quad (37.20)$$

$$= P(v_{<i}, v_t | x_t) P(v_{>i} | x_t) P(x_t) \quad (37.21)$$

$$= \overline{\mathcal{F}}_t(x_t) \mathcal{F}_t(x_t) \quad (37.22)$$

$$P(x_{t-1}, x_t, v^n) = \sum_{x_{<t-1}} \sum_{x_{>t}} P(x^n, v^n) \quad (37.23)$$

$$= \sum_{x_{<t-1}} \sum_{x_{>t}} P(x^n, v^n | x_{t-1}, x_t) P(x_{t-1}, x_t) \quad (37.24)$$

$$= \sum_{x_{<t-1}} \sum_{x_{>t}} P(x_{<t-1}, v_{<t-1}, v_{t-1} | x_{t-1}) P(v_t | x_t) P(x_{t-1}, x_t) P(x_{>i}, v_{>i} | x_t) \quad (37.25)$$

$$= P(v_{<t-1}, v_{t-1} | x_{t-1}) P(v_t | x_t) P(x_{t-1}, x_t) P(v_{>i} | x_t) \quad (37.26)$$

$$= \overline{\mathcal{F}}_{t-1}(x_{t-1}) \lambda_t(x_t) P(x_t | x_{t-1}) \mathcal{F}_t(x_t) \quad (37.27)$$

QED

## 37.2 Calculating $\mathcal{F}_t$ and $\overline{\mathcal{F}}_t$

**Claim 69** For  $t > 0$ ,  $\mathcal{F}_t$  and  $\overline{\mathcal{F}}_t$  can be calculated recursively as follows:

$$\overline{\mathcal{F}}_t(x_t) = \sum_{x_{t-1}} \overline{\mathcal{F}}_{t-1}(x_{t-1}) P(x_t | x_{t-1}) \lambda_t(x_t) \quad (37.28)$$

$$= \sum_{x_{t-1}} \sum_{x_{<t-1}} x_{<t-1} \longrightarrow x_{t-1} \quad x_{t-1} \longrightarrow x_t \quad x_t \\ \downarrow \qquad \qquad \qquad \downarrow \qquad \qquad \qquad \downarrow \\ v_{<t-1} \qquad \qquad \qquad v_{t-1} \qquad \qquad \qquad v_t \quad (37.29)$$

and

$$\mathcal{F}_{t-1}(x_{t-1}) = \sum_{x_t} P(x_t|x_{t-1})\lambda_t(x_t)\mathcal{F}_t(x_t) \quad (37.30)$$

$$= \sum_{x_t} x_{t-1} \longrightarrow x_t \quad x_t \quad x_t \longrightarrow \sum x_{>t} \quad (37.31)$$

$\downarrow \quad \quad \quad \downarrow$

$v_t \quad \quad \quad v_{>t}$

**proof:**

$$\bar{\mathcal{F}}_t(x_t)\mathcal{F}_t(x_t) = P(x_t, v^n) \quad (37.32)$$

$$= \sum_{x_{t-1}} P(x_{t-1}, x_t, v^n) \quad (37.33)$$

$$= \sum_{x_{t-1}} \bar{\mathcal{F}}_{t-1}(x_{t-1})\lambda_t(x_t)P(x_t|x_{t-1})\mathcal{F}_t(x_t) \quad (37.34)$$

$$\bar{\mathcal{F}}_{t-1}(x_{t-1})\mathcal{F}_{t-1}(x_{t-1}) = P(x_{t-1}, v^n) \quad (37.35)$$

$$= \sum_{x_t} P(x_{t-1}, x_t, v^n) \quad (37.36)$$

$$= \sum_{x_t} \bar{\mathcal{F}}_{t-1}(x_{t-1})\lambda_t(x_t)P(x_t|x_{t-1})\mathcal{F}_t(x_t) \quad (37.37)$$

**QED**

### 37.3 Calculating $P(x^n|v^n)$

**Claim 70**

$$P(x_t|x_{t-1}, v^n) = \frac{P(x_t|x_{t-1})\lambda_t(x_t)\mathcal{F}_t(x_t)}{\mathcal{F}_{t-1}(x_{t-1})} \quad (37.38)$$

$$= \frac{x_{t-1} \longrightarrow x_t \quad x_t \quad x_t \longrightarrow \sum x_{>t}}{x_{t-1} \longrightarrow \sum x_t \longrightarrow \sum x_{>t}} \quad (37.39)$$

$\downarrow \quad \quad \quad \downarrow$

$v_t \quad \quad \quad v_{>t}$

Note that actually,  $P(x_t|x_{t-1}, v^n) = P(x_t|x_{t-1}, v_{\geq t})$  by d-separation, but we won't use this fact.

$$P(x_{t-1}|x_t, v^n) = \frac{\bar{\mathcal{F}}_{t-1}(x_{t-1})P(x_t|x_{t-1})\lambda_t(x_t)}{\bar{\mathcal{F}}_t(x_t)} \quad (37.40)$$

$$= \frac{\sum x_{<t-1} \longrightarrow x_{t-1} \quad x_{t-1} \longrightarrow x_t \quad x_t}{\sum x_{<t-1} \longrightarrow \sum x_{t-1} \longrightarrow x_t} \quad (37.41)$$

Note that actually  $P(x_{t-1}|x_t, v^n) = P(x_{t-1}|x_t, v_{\leq t-1})$  by d-separation, but we won't use this fact.

**proof:**

$$P(x_t|x_{t-1}, v^n) = \frac{P(x_{t-1}, x_t, v^n)}{P(x_{t-1}, v^n)} \quad (37.42)$$

$$= \frac{\bar{\mathcal{F}}_{t-1}(x_{t-1})\lambda_t(x_t)P(x_t|x_{t-1})\mathcal{F}_t(x_t)}{\bar{\mathcal{F}}_{t-1}(x_{t-1})\mathcal{F}_{t-1}(x_{t-1})} \quad (37.43)$$

Analogous proof for Eq.(37.41).

**QED**

$$P(x^n|v^n) = \prod_{t=1,\dots,n-1,n} P(x_t|x_{t-1}, v^n) \quad (\text{forward propagation}) \quad (37.44)$$

$$= \prod_{t=n+1,n,\dots,3,2} P(x_{t-1}|x_t, v^n) \quad (\text{backward propagation}) \quad (37.45)$$

## 37.4 Calculating $P(v^n|A, B, \pi)$

$P(v^n|A, B, \pi)$  can be calculated

- from  $\bar{\mathcal{F}}_{n-1}(x_{n-1})$  (past of  $x_{n-1}$ )

$$P(v^n|A, B, \pi) = \sum_{x_{n-1}} \underbrace{P(v_{<n-1}, v_{n-1}, x_{n-1})}_{\bar{\mathcal{F}}_{n-1}(x_{n-1})} \quad (37.46)$$

$$= \sum x_{<n-1} \longrightarrow \sum x_{n-1} \quad (37.47)$$

- from  $\mathcal{F}_0(x_0)$  (future of  $\underline{x}_0$ )

$$P(v^n|A, B, \pi) = \sum_{x_0} P(x_0) P(v_0|x_0) \underbrace{P(v_{>0}|x_0)}_{\mathcal{F}_0(x_0)} \quad (37.48)$$

$$= \sum_{x_0} x_0 \longrightarrow \sum_{x_{>0}} x_{>0} \quad (37.49)$$

$\downarrow$                      $\downarrow$   
 $v_0$                      $v_{>0}$

- from  $\bar{\mathcal{F}}_t(x_t)$  and  $\mathcal{F}_t(x_t)$  for some  $t$  (past and future of  $\underline{x}_t$ )

$$P(v^n|A, B, \pi) = \sum_{x_t} \underbrace{P(v_{<t}, v_t, x_t)}_{\bar{\mathcal{F}}_t(x_t)} \underbrace{P(v_{>t}|x_t)}_{\mathcal{F}_t(x_t)} \quad (37.50)$$

$$= \sum_{x_{<t}} x_{<t} \longrightarrow \sum_{x_t} x_t \longrightarrow \sum_{x_{>t}} x_{>t} . \quad (37.51)$$

$\downarrow$                      $\downarrow$                      $\downarrow$   
 $v_{<t}$                      $v_t$                      $v_{>t}$

## 37.5 Calculating $\hat{x}^n$ (Viterbi algorithm)

$x^n$  is not visible, only  $v^n$  is. Here is how to find an estimate  $\hat{x}^n$  of  $x^n$ .

Define

$$\bar{\mathcal{F}}_t^{max}(x_t) = \max_{x_{<t}} P(v_{<t}, v_t, x_{<t}, x_t) \quad (37.52)$$

$$= \max x_{<t} \longrightarrow x_t \quad (37.53)$$

$\downarrow$                      $\downarrow$   
 $v_{<t}$                      $v_t$

$$\hat{x}_{t-1}(x_t) = \operatorname{argmax}_{x_{t-1}} \bar{\mathcal{F}}_{t-1}^{max}(x_{t-1}) P(x_t|x_{t-1}) \lambda_t(x_t) \quad (37.54)$$

$$= \max x_{<t-1} \longrightarrow \operatorname{argmax} x_{t-1} \longrightarrow x_t \quad (37.55)$$

$\downarrow$                      $\downarrow$                      $\downarrow$   
 $v_{<t-1}$                      $v_{t-1}$                      $v_t$

For  $t > 0$ ,  $\bar{\mathcal{F}}_t^{max}$  and  $\hat{x}_{t-1}(x_t)$  can be calculated recursively as follows:

$$\overline{\mathcal{F}}_t^{max}(x_t) = \max_{x_{t-1}} \overline{\mathcal{F}}_{t-1}^{max}(x_{t-1}) P(x_t|x_{t-1}) \lambda_t(x_t) \quad (37.56)$$

$$= \max_{x_{t-1}} \max x_{<t-1} \longrightarrow x_{t-1} \quad x_{t-1} \longrightarrow x_t \quad x_t \\ \downarrow \qquad \qquad \qquad \downarrow \qquad \qquad \qquad \downarrow \\ v_{<t-1} \qquad \qquad \qquad v_{t-1} \qquad \qquad \qquad v_t \quad (37.57)$$

$$\hat{x}_{t-1}(x_t) = \operatorname{argmax}_{x_{t-1}} \overline{\mathcal{F}}_{t-1}^{max}(x_{t-1}) P(x_t|x_{t-1}) \lambda_t(x_t) \quad (37.58)$$

$$= \operatorname{argmax}_{x_{t-1}} \max x_{<t-1} \longrightarrow x_{t-1} \quad x_{t-1} \longrightarrow x_t \quad x_t \\ \downarrow \qquad \qquad \qquad \downarrow \qquad \qquad \qquad \downarrow \\ v_{<t-1} \qquad \qquad \qquad v_{t-1} \qquad \qquad \qquad v_t \quad (37.59)$$

**Claim 71** (*Viterbi Algorithm*)

If

$$\hat{x}^n = \operatorname{argmax}_{x^n} P(x^n|v^n), \quad (37.60)$$

then the components of  $\hat{x}^n$  can be calculated recursively from the last one  $\hat{x}_{n-1}$  to the first one  $\hat{x}_0$ , as follows. Let

$$\hat{x}_{n-1} = \operatorname{argmax}_{x_{n-1}} \overline{\mathcal{F}}_{n-1}^{max}(x_{n-1}) \quad (37.61)$$

$$= \max x_{<n-1} \longrightarrow \operatorname{argmax} x_{n-1} \quad (37.62)$$

$$\downarrow \qquad \qquad \qquad \downarrow \\ v_{<n-1} \qquad \qquad \qquad v_{n-1}$$

and for  $t < n - 1$ , use

$$\hat{x}_{t-1} = \hat{x}_{t-1}(\hat{x}_t) \quad (37.63)$$

$$= \max x_{<t-1} \longrightarrow \operatorname{argmax} x_{t-1} \longrightarrow \hat{x}_t \quad (37.64)$$

$$\downarrow \qquad \qquad \qquad \downarrow \qquad \qquad \qquad \downarrow \\ v_{<t-1} \qquad \qquad \qquad v_{t-1} \qquad \qquad \qquad v_t$$

**proof:**

**QED**

## 37.6 Calculating $\hat{A}$ , $\hat{B}$ , $\hat{\pi}$ (Baum-Welch algorithm)

Let  $\theta = (A, B, \pi)$ .  $\theta$  is a set of hidden parameters. Here is how to find an estimate  $\hat{\theta}$  of  $\theta$ .

If  $x^n$  and  $v^n$  were visible, we could use

$$\hat{\pi}(x) = \mathbb{1}(\underline{x}_0 = x) \quad (37.65)$$

$$\hat{A}(x'|x) = \frac{\sum_{t=0}^{n-2} \mathbb{1}(\underline{x}_t = x, \underline{x}_{t+1} = x')}{\sum_x \text{numerator}} \quad (37.66)$$

$$\hat{B}(v|x) = \frac{\sum_{t=0}^{n-1} \mathbb{1}(\underline{v}_t = v, \underline{x}_t = x)}{\sum_v \text{numerator}} \quad (37.67)$$

But  $x^n$  is not visible. So how can we estimate  $\theta$  under those circumstances?

Define

$$\gamma_t(x_t) = P(x_t|v^n) \quad (37.68)$$

$$= \frac{P(x_t, v^n)}{P(v^n)} \quad (37.69)$$

$$= \frac{\mathcal{F}_t(x_t)\mathcal{F}_t(x_t)}{\sum_{x_t} \text{numerator}} \quad (37.70)$$

$$= \frac{\sum x_{<t} \longrightarrow x_t \quad x_t \longrightarrow \sum x_{>t}}{\sum_{x_t} \text{numerator}} \quad (37.71)$$

$$\xi_t(x_t, x_{t+1}) = \frac{P(x_t, x_{t+1}, v^n)}{\sum_{x_t} \sum_{x_{t+1}} \text{numerator}} \quad (37.72)$$

$$= \frac{\mathcal{F}_{t-1}(x_{t-1})P(x_t|x_{t-1})\lambda_t(x_t)\mathcal{F}_t(x_t)}{\sum_{x_t} \sum_{x_{t+1}} \text{numerator}} \quad (37.73)$$

$$= \frac{\sum x_{<t-1} \longrightarrow x_{t-1} \quad x_{t-1} \longrightarrow x_t \quad x_t \longrightarrow \sum x_{>t}}{\sum_{x_t} \sum_{x_{t+1}} \text{numerator}} \quad (37.74)$$

**Claim 72** (*Baum-Welch algorithm*)

If

$$\widehat{\theta} = \operatorname{argmax}_{\theta} P(v^n | \theta) , \quad (37.75)$$

then we can find  $\widehat{\theta}$  using the following formulae:

$$\widehat{\pi}(x) = \overbrace{\gamma_0(x)}^{\sim P(x)} \quad (37.76)$$

$$\widehat{A}(x'|x) = \frac{\sum_{t=0}^{n-2} \overbrace{\xi_t(x, x')}^{\sim P(x, x')}}{\sum_{t=0}^{n-2} \underbrace{\gamma_t(x)}_{P(x)}} \quad (37.77)$$

$$\widehat{B}(v|x) = \frac{\sum_{t=0}^{n-1} \overbrace{\mathbb{1}(\underline{v}_t = v)}^{\sim P(v|x)} \overbrace{\gamma_t(x)}^{\sim P(x)}}{\sum_{t=0}^{n-1} \underbrace{\gamma_t(x)}_{\sim P(x)}} \quad (37.78)$$

proof:

QED

# Chapter 38

## Identification of do queries via LDEN diagrams

The most general way to decide whether a do query for a particular DAG is identifiable, is by using Pearl's Do Calculus rules (see Chapter 21). However, those rules are fairly complicated and therefore difficult to automate.

We contend that by analyzing any DAG *symbolically* using SCuMpy (see Ref.[77]), one can decide rigorously whether a do query for that DAG is identifiable or not. Hence, SCuMpy allows us, *if we have a single specific DAG in mind*, to bypass and supplant, in an automated fashion, the Do Calculus rules.

SCuMpy uses LDEN diagrams (a.k.a. linear SCM, see Chapter 48) whereas the Do Calculus rules are for general bnets. However, the answer to the question of whether a do query is identifiable for a particular DAG, only depends on the DAG, so it is independent of whether the DAG came from an LDEN diagram, or from the more general corresponding bnet.

In this chapter, we will briefly summarize the results presented in the Jupyter notebook entitled "unconfounded-children" in SCuMpy (Ref.[77]). See that notebook for more details.

Consider the LDEN diagram of Fig.38.1. This DAG does not satisfy either the backdoor or frontdoor criteria, but the query  $P(y|do(x))$  is still known to be identifiable for this DAG.

For the LDEN diagram of Fig.38.1, SCuMpy gives the following covariance between nodes  $\underline{x}$  and  $\underline{y}$ :

$$\langle \underline{x}, \underline{y} \rangle = \begin{cases} \alpha_{\underline{x}|h_1} \sigma_{\epsilon_{h_1}}^2 \left( \alpha_{m_1|x} \alpha_{x|h_1} \alpha_{y|m_1} + \alpha_{m_2|x} \alpha_{x|h_1} \alpha_{y|m_2} + \alpha_{y|h_1} \right) \\ + \sigma_{\epsilon_{\underline{x}}}^2 \left( \alpha_{m_1|\underline{x}} \alpha_{y|m_1} + \alpha_{m_2|\underline{x}} \alpha_{y|m_2} \right) \end{cases} \quad (38.1)$$

Suppose we amputate, from the LDEN diagram of Fig.38.1, all arrows entering node  $\underline{x}$  (for this example, that means amputating the arrow  $h_1 \rightarrow \underline{x}$ ). Such an amputation is demanded by the definition of the do query  $P(y|do(x))$ . Then SCuMpy gives instead:

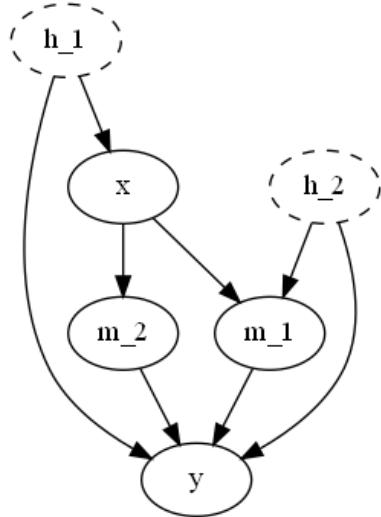


Figure 38.1: LDEN diagram for which the query  $P(y|do(x))$  is known to be identifiable. External root nodes  $\underline{\epsilon}_a$  pointing into each node  $\underline{a}$ , are left implicit. The path coefficients (a.k.a arrow gains) are not shown either. For any two nodes  $\underline{a}, \underline{b}$ , these gains are denoted by  $\alpha_{\underline{b}|\underline{a}}$  for an arrow  $\underline{a} \rightarrow \underline{b}$ .

$$\langle \underline{x}, \underline{y} \rangle = \sigma_{\underline{\epsilon}_{\underline{x}}}^2 \left( \alpha_{\underline{m}_1|\underline{x}} \alpha_{\underline{y}|\underline{m}_1} + \alpha_{\underline{m}_2|\underline{x}} \alpha_{\underline{y}|\underline{m}_2} \right) \quad (38.2)$$

so

$$\frac{\partial \underline{x}}{\partial \underline{y}} = \frac{\langle \underline{x}, \underline{y} \rangle}{\langle \underline{x}, \underline{x} \rangle} = \alpha_{\underline{m}_1|\underline{x}} \alpha_{\underline{y}|\underline{m}_1} + \alpha_{\underline{m}_2|\underline{x}} \alpha_{\underline{y}|\underline{m}_2} \quad (38.3)$$

Note that upon amputating the arrows entering  $\underline{x}$ , the covariance  $\langle \underline{x}, \underline{y} \rangle$  becomes independent of the hidden (i.e., unobserved) variables  $\underline{h}_1, \underline{h}_2$ . Thus, the do query  $P(y|do(x))$  is identifiable, because it doesn't depend on unobserved quantities.

# Chapter 39

## Influence Diagrams & Utility Nodes

Influence diagrams are just arbitrary bnets enhanced with a new kind of node called an utility node. The rest of this brief chapter will be devoted to discussing utility nodes.

Suppose  $U(x)$  is a deterministic function  $U : S_x \rightarrow \mathbb{R}$  called the **utility function**. Then the **expected utility** is defined as

$$E_U[U] = \sum_U P(U)U \quad (39.1)$$

$$= \sum_x \sum_U \underbrace{P(U|x)}_{\delta[U, U(x)]} P(x)U \quad (39.2)$$

$$= \sum_x P(x)U(x) . \quad (39.3)$$

An **utility node** can be understood as a node composed of 3 simpler bnet nodes. This is illustrated in Fig.39.1.

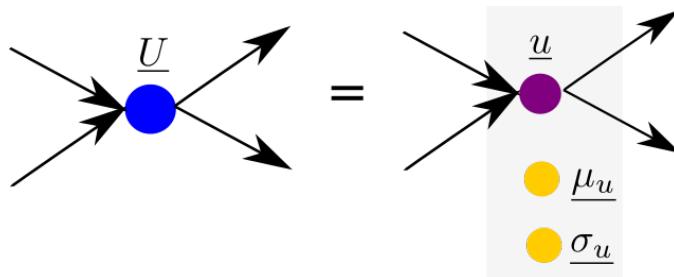


Figure 39.1: An utility node can be understood as a node composed of 3 simpler bnet nodes.

The TPMs, printed in blue, for the bnet Fig.39.1, are as follows:

$$P(U|pa(U)) = \delta[U, U(pa(U))] , \quad (39.4)$$

where if  $U : S_{\underline{x}} \rightarrow \mathbb{R}$ , then  $\underline{x} = pa(\underline{U})$ .

$$P(u|pa(U)) = \delta[u, U(pa(U))] \quad (39.5)$$

Node  $\underline{\mu}_u$  calculates the expected value (mean value) of  $\underline{u}$ :

$$P(\underline{\mu}_u) = \delta(\underline{\mu}_u, E_{\underline{u}}[\underline{u}]) \quad (39.6)$$

Node  $\underline{\sigma}_u$  calculates the standard deviation of  $\underline{u}$ :

$$P(\underline{\sigma}_u) = \delta(\underline{\sigma}_u, \sqrt{E_{\underline{u}}[(\underline{u} - E_{\underline{u}}[\underline{u}])^2]}) \quad (39.7)$$

Note that in order to calculate expected values, it is necessary that  $\underline{U}, \underline{u} \in \mathbb{R}$ . Note that nodes  $\underline{u}, \underline{\mu}_u, \underline{\sigma}_u$  must all 3 have access to the TPM  $P(U|pa(U))$  of node  $\underline{U}$ . In fact, in order to calculate  $E_{\underline{u}}[\cdot]$ , it is necessary for nodes  $\underline{\mu}_u$  and  $\underline{\sigma}_u$  to have access not just to  $P(U|pa(U))$  but also to  $P(pa(U))$ .

See Fig.39.2. An influence diagram may have multiple utility nodes ( $\underline{U}_1$  and  $\underline{U}_2$  in Fig.39.2). Then one can define a merging utility node  $\underline{U}$  that sums the values of all the other utility nodes.

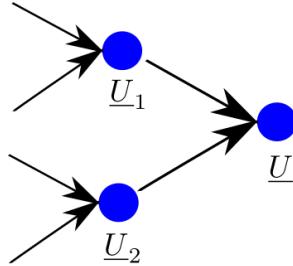


Figure 39.2: An influence diagram may have multiple utility nodes, say  $\underline{U}_1$  and  $\underline{U}_2$ . Then one can define an utility node  $\underline{U} = \underline{U}_1 + \underline{U}_2$ .

For the node  $\underline{U}$  of Fig.39.2,

$$P(U|U_1, U_2) = \delta(U, U_1 + U_2) \quad (39.8)$$

# Chapter 40

## Instrumental Inequality and beyond

This chapter is based on Refs. [13] and [48].

Instrumental Variables (IVs) are discussed in Chapter 41. This chapter will discuss the original Instrumental inequality (I-inequality) discovered by Pearl, and other related inequalities. The I-inequality arises in bnets that use an IV. The I-inequality bounds the effect that an IV  $\underline{z}$  can have on the outcome  $\underline{y}$  of a treatment  $\underline{d} \rightarrow \underline{y}$ . Since there is a path  $\underline{z} \rightarrow \underline{d} \rightarrow \underline{y}$ , the treatment dose  $\underline{d}$  acts as a mediator between the IV  $\underline{z}$  and the treatment outcome  $\underline{y}$ . The I-inequality is reminiscent of the data processing inequality  $H(\underline{z} : \underline{y}) \leq H(\underline{d} : \underline{y})$  which is valid for a simple Markov chain bnet  $\underline{z} \rightarrow \underline{d} \rightarrow \underline{y}$ . The data processing inequality is saying that the endpoint  $\underline{y}$  receives more information from  $\underline{d}$  than from  $\underline{z}$ . This is reasonable, since  $\underline{y}$  is “closer” to  $\underline{d}$  than to  $\underline{z}$ .

### 40.1 I-inequality

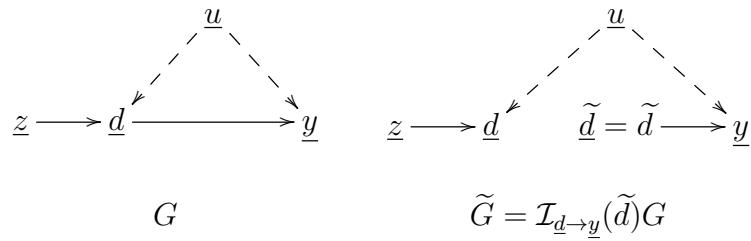


Figure 40.1: In bnet  $G$ , an IV  $\underline{z}$  acts on a treatment  $\underline{d} \rightarrow \underline{y}$ . Bnet  $\widetilde{G}$  is obtained by applying an imagine operator to arrow  $\underline{d} \rightarrow \underline{y}$  of bnet  $G$ .

**Claim 73** *The TPMs for the bnet  $G$  in Fig.40.1 satisfy*

$$\max_d \sum_y \max_z P(d, y|z) \leq 1 \quad (40.1)$$

**proof:**

Below, any probability that alludes to a value  $\tilde{d}$  refers to bnet  $\tilde{G}$ . Otherwise, if it doesn't allude to  $\tilde{d}$ , then it refers to  $G$  (or to  $\tilde{G}$ , since the TPMs of  $\tilde{G}$  are defined from those of  $G$  in a consistent manner.)

$G$  satisfies

$$P(d, y|z) = \sum_u P(u)P(y|u, d)P(d|u, z), \quad (40.2)$$

and  $\tilde{G}$  satisfies

$$P(d, y|z, \tilde{d}) = \sum_u P(u)P(y|u, \tilde{d})P(d|u, z). \quad (40.3)$$

Note that Eqs.(40.2) and (40.3) imply that

$$P(d, y|z, d) = P(d, y|z) \quad (40.4)$$

and that

$$P(\tilde{d}, y|z, \tilde{d}) \leq \sum_d P(d, y|z, \tilde{d}) = P(y|\tilde{d}). \quad (40.5)$$

Thus,

$$\max_{\tilde{d}} \sum_y \max_z P(\tilde{d}, y|z, \tilde{d}) \leq \max_{\tilde{d}} \sum_y \max_z P(y|\tilde{d}) \quad (40.6)$$

$$\leq \max_{\tilde{d}} \sum_y P(y|\tilde{d}) \quad (40.7)$$

$$\leq \max_{\tilde{d}} 1 \quad (40.8)$$

$$\leq 1 \quad (40.9)$$

**QED**

As pointed out in Ref.[13] from which I learned the above proof, the above proof is highly generalizable.

Fig.40.2 gives a graphical representation of the boxed Eq.(40.5) which is crucial to the proof.

And here is a meta-description of the steps in the proof:

1. Use imagine operator to create a non-negative matrix  $M_{d, \tilde{d}}$ .
2. Use fact that row or column sum of  $M_{d, \tilde{d}}$  is larger than diagonal element in sum:  
 $\sum_d M_{d, \tilde{d}} \geq M_{\tilde{d}, \tilde{d}}$ .

$$\sum_u \begin{array}{c} u \\ \swarrow \quad \searrow \\ \underline{z} \longrightarrow \underline{d} = \tilde{\underline{d}} \end{array} \quad \leq \quad \sum_d \sum_u \begin{array}{c} u \\ \swarrow \quad \searrow \\ \underline{z} \longrightarrow \underline{d} \quad \tilde{\underline{d}} = \tilde{\underline{d}} \longrightarrow \underline{y} \end{array} \quad = \quad .$$

Figure 40.2: Graphical representation of the boxed equation Eq.(40.5).

#### 40.1.1 I-inequality for binary $\underline{z}, \underline{d}, \underline{y}$

It is enlightening to write down the I-inequality for the special case that  $\underline{z}, \underline{d}, \underline{y}$  are binary.

$$P(d=1, y|z) = \begin{matrix} z = 0 & z = 1 \\ y = 0 & \begin{array}{|c|c|} \hline A & B \\ \hline C & D \\ \hline \end{array} \\ y = 1 & \end{matrix}$$

$$A + D \leq 1$$

$$B + C \leq 1$$

Figure 40.3: I-inequality for binary  $\underline{z}, \underline{d}, \underline{y}$ . The same picture except with  $d = 0$  is also true.

In the binary case, the I-inequality implies 4 different inequalities. These are as follows. One gets two inequalities by setting  $d = 1$  in the next 2 equations.

$$\sum_{y=0}^1 \sum_{z=0}^1 \mathbb{1}(y=z) P(d, y|z) , \quad (40.10a)$$

$$\sum_{y=0}^1 \sum_{z=0}^1 \mathbb{1}(y \neq z) P(d, y|z) . \quad (40.10b)$$

One gets an additional 2 inequalities by setting  $d = 0$  in Eqs.(40.10). These 4 inequalities are illustrated in Fig.40.3.

What do they mean? That at fixed  $\underline{d}$ , the correlation between  $\underline{z}$  and  $\underline{y}$  is limited.

## 40.2 Bounds on Effect of IV on treatment outcome $\mathbf{y}$

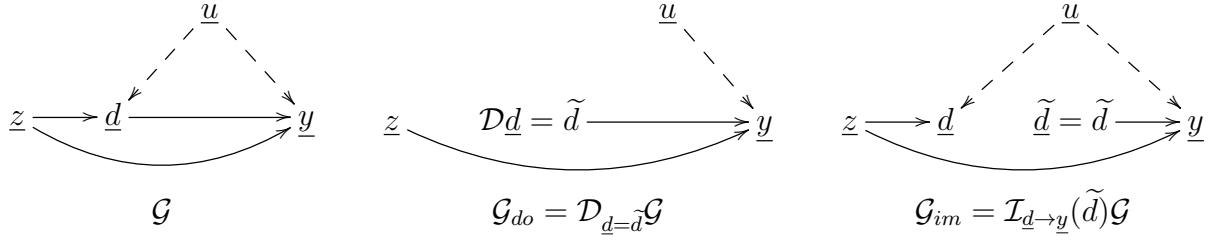


Figure 40.4: Bnet  $\mathcal{G}$  is obtained from the bnet  $G$  in Fig.40.1 by adding to  $G$  an arrow from the IV  $\underline{z}$  to the treatment outcome  $\underline{y}$ . Bnet  $\mathcal{G}_{do}$  is obtained by applying a do operator to node  $\underline{d}$  of  $\mathcal{G}$ . Bnet  $\mathcal{G}_{im}$  is obtained by applying an imagine operator to arrow  $\underline{d} \rightarrow \underline{y}$  of  $\mathcal{G}$ .

In this section, we will assume that random variables  $\underline{z}, \underline{d}, \underline{y}$  are binary. Just as with the binary case of the I-inequality, we will find an inequality for each value of  $\underline{d} \in \{0, 1\}$ .

Below, we will use the following 3 shorthand notations:

$$P_{y|z}(d) = P(d, y|z) , \quad (40.11)$$

$$P_{|z}(d) = \sum_y P(d, y|z) , \quad (40.12)$$

and

$$\pi_{|z}(d) = 1 - P_{|z}(d) . \quad (40.13)$$

For the bnet  $\mathcal{G}_{do}$  in Fig.40.4, define the IV effect at fixed  $\mathcal{D}\underline{d} = \tilde{d}$  by

$$IVE(\tilde{d}) = P(y = 1|z = 1, \mathcal{D}\underline{d} = \tilde{d}) - P(y = 1|z = 0, \mathcal{D}\underline{d} = \tilde{d}) . \quad (40.14)$$

**Claim 74** *The TPMs for the bnet  $\mathcal{G}_{do}$  in Fig.40.4 satisfy*

$$\pi_{|0}(d) \leq [IVE(d) - \{P_{1|1}(d) - P_{1|0}(d)\}] \leq \pi_{|1}(d) \quad (40.15)$$

**proof:**

$$P(y|z, \mathcal{D}\underline{d} = \tilde{d}) = \sum_u P(u)P(y|u, z, \tilde{d}) \quad (40.16)$$

$$= \sum_u P(u) \sum_d P(d, y|u, z, \tilde{d}) \quad (40.17)$$

$$\geq \sum_u P(u)P(\tilde{d}, y|u, z, \tilde{d}) \quad (40.18)$$

$$= \sum_u P(u)P(\tilde{d}, y|u, z) \quad (40.19)$$

$$= P_{y|z}(\tilde{d}) \quad (40.20)$$

Next note that  $P(d, y|z, \tilde{d}) \geq 0$ , and  $\sum_{d,y} P(d, y|z, \tilde{d}) = 1$ . If we write a table for  $P(d, y|z, \tilde{d})$  at fixed  $z, \tilde{d}$  with row and column indices  $(d, y)$ , then a partial sum of the entries of that table must be  $\leq 1$ :

$$\sum_{d \neq \tilde{d}} P(d, y|z, \tilde{d}) + \underbrace{\sum_{y'} P(\tilde{d}, y'|z, \tilde{d})}_{P_{|z}(\tilde{d})} \leq 1 . \quad (40.21)$$

Using the definitions of  $P_{|z}$  and  $\pi_{|z}$ , we can rewrite the last equation as

$$\sum_{d \neq \tilde{d}} P(d, y|z, \tilde{d}) \leq \pi_{|z}(\tilde{d}) . \quad (40.22)$$

Next note that

$$P(y|z, \mathcal{D}\underline{d} = \tilde{d}) = \sum_u P(u)P(y|u, z, \tilde{d}) \quad (40.23)$$

$$= \sum_u P(u) \sum_d P(d, y|u, z, \tilde{d}) \quad (40.24)$$

$$= P(\tilde{d}, y|z, \tilde{d}) + \sum_{d \neq \tilde{d}} P(d, y|z, \tilde{d}) \quad (40.25)$$

$$= P_{y|z}(\tilde{d}) + \sum_{d \neq \tilde{d}} P(d, y|z, \tilde{d}) \quad (40.26)$$

$$\leq P_{y|z}(\tilde{d}) + \pi_{|z}(\tilde{d}) . \quad (40.27)$$

Hence,

$$P_{y|z}(\tilde{d}) \leq P(y|z, \mathcal{D}\underline{d} = \tilde{d}) \leq P_{y|z}(\tilde{d}) + \pi_{|z} \quad (40.28)$$

$$P_{1|1}(\tilde{d}) \leq P(y=1|z=1, \mathcal{D}\underline{d} = \tilde{d}) \leq P_{1|1}(\tilde{d}) + \pi_{|1} \quad (40.29)$$

$$-P_{1|0}(\tilde{d}) - \pi_{|0} \leq -P(y=1|z=0, \mathcal{D}\underline{d} = \tilde{d}) \leq -P_{1|0}(\tilde{d}) \quad (40.30)$$

**QED**

# Chapter 41

## Instrumental Variables

This chapter is based on Refs.[12] and [122].

The theory of potential outcomes (PO) discussed in Chapter 72 assumes that confounders can be ignored by conditioning on them. However, there are cases when that is not possible, as when there are some unmeasured (i.e., unobserved, hidden) confounder nodes in the bnet, because one can only condition on observed random variables, by definition. So what if confounders can't be ignored? Are we then precluded from using PO theory? Not necessarily. It might still be possible to use PO theory if one can find a suitable instrumental variable (IV) for the problem.

IVs were actually invented by Sewall Wright and his father Philip Wright long before PO theory was invented by Rubin. The reason why IVs save PO theory is greatly clarified by using Pearl causal DAGs and his d-separation theorem (see Chapter 23).

Most of the discussion in this chapter is limited to LDEN (linear deterministic bnets with external noise). These are discussed in Chapter 48. However, as will become obvious to the reader, IVs are also applicable and useful in general bnet modeling.

### 41.1 $\delta$ with unmeasured confounder

In this section, we explain, using LDENs, why unmeasured confounders prejudice PO  $\delta$  calculations.

Consider the LDEN bnet of Fig.41.1. For some  $\delta, \mu \in \mathbb{R}$ , we have

$$\underline{y} = \delta \underline{d} + \mu \underline{u} + \underline{\epsilon}_y . \quad (41.1)$$

Note that

$$\left\langle \underline{d}, \underline{\epsilon}_y \right\rangle = 0 \quad (41.2)$$

because the path from  $\underline{d}$  to  $\underline{\epsilon}_y$  is blocked by a collider. Note also that  $\langle \underline{d}, \underline{u} \rangle \neq 0$  because there is an unblocked path between  $\underline{d}$  and  $\underline{u}$ . Hence

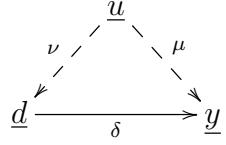


Figure 41.1: An LDEN bnet. The direct path  $\underline{d} \rightarrow \underline{y}$  is confounded by a hidden variable  $\underline{u}$ . External root nodes  $\epsilon_d, \epsilon_u, \epsilon_y$  are left implicit.

$$\langle \underline{d}, \underline{y} \rangle = \delta \langle \underline{d}, \underline{d} \rangle + \mu \langle \underline{d}, \underline{u} \rangle . \quad (41.3)$$

If  $\langle \underline{d}, \underline{u} \rangle$  were always zero, or if we could measure  $\langle \underline{d}, \underline{u} \rangle$  (we can't because  $\underline{u}$  is unobserved), we could solve for  $\delta$ , but that is unfortunately not the case.

## 41.2 $\delta$ (with unmeasured confounder) can be inferred via IV

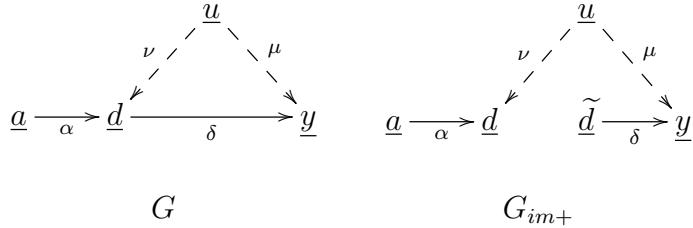


Figure 41.2: Two LDEN bnets. The direct path  $\underline{d} \rightarrow \underline{y}$  is confounded by a hidden variable  $\underline{u}$ , but by using the IV  $\underline{a}$ , we are still able to identify (i.e., calculate)  $\delta$ . External root nodes  $\epsilon_a, \epsilon_d, \epsilon_u, \epsilon_y$  are left implicit.

Now consider the two LDEN bnets shown in Fig.41.2. Note that there are no arrows  $\underline{a} \rightarrow \underline{y}$  or  $\underline{a} \rightarrow \underline{u}$ . Note that node  $\underline{d}$  is a collider in the path  $\underline{a} - \underline{d} - \underline{u} - \underline{y}$ . Therefore, the only unblocked path from  $\underline{a}$  to  $\underline{y}$  in  $G$  is  $\underline{a} \rightarrow \underline{d} \rightarrow \underline{y}$  and that path has been removed in  $G_{im+}$ . These observations are encapsulated in the following statements.

$$\underline{d} \perp_G \underline{y} = \text{false}, \quad \underline{a} \perp_G \underline{y} = \text{false} . \quad (41.4)$$

$$\underline{d} \perp_{G_{im+}} \underline{y} = \text{false}, \quad \underline{a} \perp_{G_{im+}} \underline{y} = \text{true} . \quad (41.5)$$

For  $G$ , the following is true.

$$\begin{cases} \underline{y} = \delta \underline{d} + \mu \underline{u} + \epsilon_{\underline{y}} \\ \underline{d} = \alpha \underline{a} + \nu \underline{u} + \epsilon_{\underline{d}} \end{cases} \quad (41.6)$$

Note that

$$\langle \underline{a}, \underline{u} \rangle = \langle \underline{a}, \epsilon_{\underline{y}} \rangle = \langle \underline{a}, \epsilon_{\underline{d}} \rangle = 0 \quad (41.7)$$

because in all cases, paths between the two nodes in the covariance are blocked by a collider. Therefore

$$\langle \underline{a}, \underline{y} \rangle = \delta \langle \underline{a}, \underline{d} \rangle \quad (41.8)$$

and

$$\langle \underline{a}, \underline{d} \rangle = \alpha \langle \underline{a}, \underline{a} \rangle . \quad (41.9)$$

Note that  $\langle \underline{a}, \underline{y} \rangle = \delta = 0$  for  $G_{im+}$  but not for  $G$ , so we are speaking about  $G$  from here on. It follows that<sup>1</sup>

$$\alpha = \frac{\langle \underline{a}, \underline{d} \rangle}{\langle \underline{a}, \underline{a} \rangle} = \frac{\partial \underline{d}}{\partial \underline{a}} \quad (41.10)$$

and

$$\delta = \frac{\langle \underline{a}, \underline{y} \rangle}{\langle \underline{a}, \underline{d} \rangle} \quad (41.11)$$

$$= \frac{\langle \underline{a}, \underline{y} \rangle \langle \underline{a}, \underline{a} \rangle}{\langle \underline{a}, \underline{a} \rangle \langle \underline{a}, \underline{d} \rangle} \quad (41.12)$$

$$= \frac{\frac{\partial \underline{y}}{\partial \underline{a}}}{\frac{\partial \underline{d}}{\partial \underline{a}}} \quad (\neq \frac{\partial \underline{y}}{\partial \underline{d}}) \quad (41.13)$$

$$= \frac{\partial \underline{y}}{\partial (\alpha \underline{a})} . \quad (41.14)$$

Eq.(41.13) is illustrated in Fig.41.3.

### 41.3 More general bnets with IVs

Figs.41.4 and 41.5 are examples of other bnets for which the effect  $\delta$  is identifiable thanks to the IV  $\underline{a}$ .

---

<sup>1</sup>As usual in this book, we define  $\frac{\partial \underline{y}}{\partial \underline{x}} = \frac{\langle \underline{x}, \underline{y} \rangle}{\langle \underline{x}, \underline{x} \rangle}$  for any random variables  $\underline{x}, \underline{y}$ .

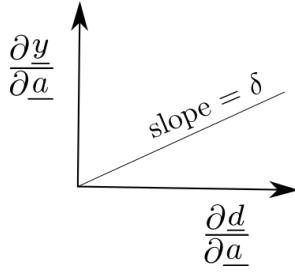


Figure 41.3: Effect  $\delta$  as slope of line.

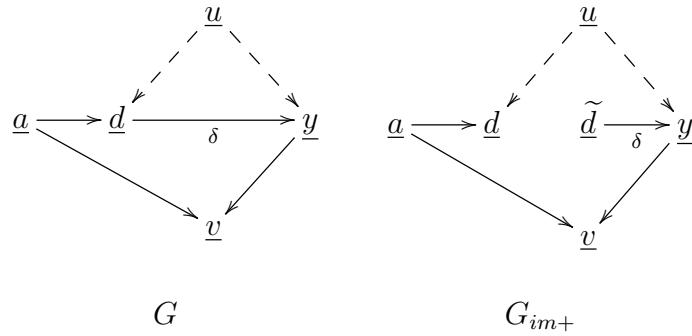


Figure 41.4: The 2 paths in  $G_{im+}$  from IV variable  $\underline{a}$  to  $\underline{y}$  are blocked by not conditioning on colliders  $\underline{v}$  and  $\underline{d}$ . Thus,  $\underline{d} \perp_{G_{im+}} \underline{y} = \text{false}$ ,  $\underline{a} \perp_{G_{im+}} \underline{y} = \text{true}$ .

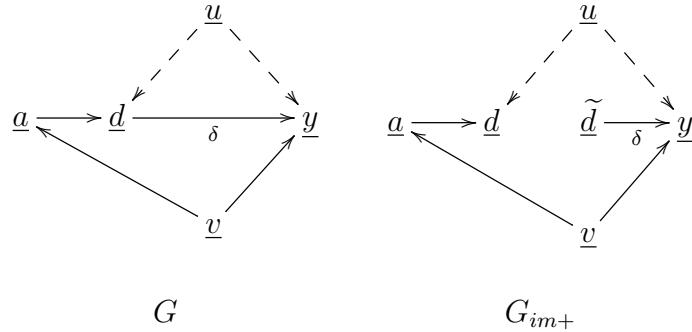


Figure 41.5: There are 2 paths in  $G_{im+}$  from IV variable  $\underline{a}$  to  $\underline{y}$ . One is blocked by not conditioning on the collider  $\underline{d}$  and the other can be blocked by conditioning on  $\underline{v}$ . Thus,  $\underline{d} \perp_{G_{im+}} \underline{y} | \underline{v} = \text{false}$ ,  $\underline{a} \perp_{G_{im+}} \underline{y} | \underline{v} = \text{true}$ .

## 41.4 Instrumental Inequality

Pearl's instrumental inequality and related inequalities are discussed in Chapter 40.

# Chapter 42

## Jackknife Resampling

This chapter is based on Ref. [124].

Before reading this chapter, we recommend that you read the section entitled "Demystifying Population and Sample Variances", in Chapter C.

Jackknife Resampling (JR) is a way of generating from an original list of  $n$  samples, a new list of  $n$  synthetic (i.e., man made, not occurring physically in Nature) samples obtained by deleting one of the samples from the original list and averaging over the rest.

Let  $\Sigma = \{0, 1, 2, \dots, n - 1\}$ . Let us consider the list of samples

$$\vec{x} = (x^\sigma)_{\sigma \in \Sigma}, \quad (42.1)$$

where the  $x^\sigma$  are assumed to be i.i.d. with

$$E[\underline{x}^\sigma] = \mu \quad (42.2)$$

and

$$\left\langle \underline{x}^\sigma, \underline{x}^{\sigma'} \right\rangle = V_1 \delta(\sigma, \sigma') . \quad (42.3)$$

If we define  $\mu$  and  $V_1$  estimators by

$$\hat{\mu} = \frac{1}{n} \sum_{\sigma} x^\sigma \quad (42.4a)$$

$$\hat{V}_1 = \frac{1}{n-1} \sum_{\sigma} (x^\sigma - \hat{\mu})^2 , \quad (42.4b)$$

then one can show that:

$$E[\hat{\mu}] = \mu , \quad E[\hat{V}_1] = V_1 \quad (42.5)$$

so both of these estimators are unbiased.

Now define lists of samples with one of the items in  $\vec{x}$  deleted:

$$\vec{x}_\xi = (x^\sigma)_{\sigma \in \Sigma - \{\xi\}} . \quad (42.6)$$

Suppose we are given functions of  $\vec{x}$  and  $\vec{x}_\xi$

$$A = A^n(\vec{x}) , \quad (42.7)$$

$$A_\xi = A^{n-1}(\vec{x}_\xi) . \quad (42.8)$$

Then define a list  $\vec{A}$  by

$$\vec{A} = (A_\xi)_{\xi \in \Sigma} . \quad (42.9)$$

One can also define a list  $\vec{B}$  by:

$$\vec{B} = (B_\xi)_{\xi \in \Sigma} \quad (42.10)$$

where

$$B_\xi = nA - (n-1)A_\xi \quad (42.11)$$

$$= A_\xi - n[A_\xi - A] . \quad (42.12)$$

Later on, we will see why the list  $\vec{B}$  just defined is of interest.

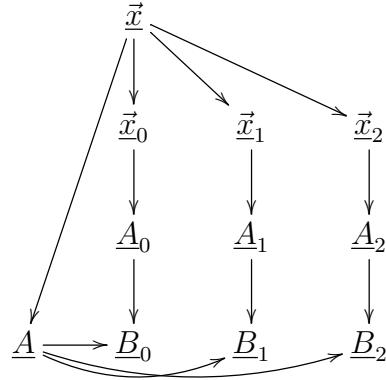


Figure 42.1: Bnet for jackknife resampling (JR).

Fig.42.1 is a bnet that encapsulates JR. The TPMs, printed in blue, for that bnet, are as follows:

$$P(\vec{x}_\xi | \vec{x}) = \mathbb{1}(\vec{x}_\xi = \text{defined by Eq.(42.6)}) \quad (42.13)$$

$$P(A_\xi | \vec{x}_\xi) = \mathbb{1}(A_\xi = \text{defined by Eq.(42.8)}) \quad (42.14)$$

$$P(B_\xi | \vec{A}_\xi, A) = \mathbb{1}(\quad B_\xi = \text{ defined by Eq.(42.12)} \quad ) \quad (42.15)$$

## 42.1 Case $A = A^n(\vec{x}) = \frac{1}{n} \sum_{\sigma} x^{\sigma}$

Suppose

$$A = \underbrace{\frac{1}{n} \sum_{\sigma} x^{\sigma}}_{E_{\sigma}[x^{\sigma}]} \quad (42.16)$$

and

$$A_\xi = \underbrace{\frac{1}{n-1} \sum_{\sigma \in \Sigma - \{\xi\}} x^{\sigma}}_{E_{\sigma|\xi}[x^{\sigma}] \text{ where } P(\sigma|\xi) = \frac{1}{n-1}} . \quad (42.17)$$

Then

$$\frac{1}{n} \sum_{\xi} A_\xi = E_{\xi} E_{\sigma|\xi}[x^{\sigma}] = E_{\sigma}[x^{\sigma}] = A \quad (42.18)$$

**Claim 75**

$$E[\underline{A}_{\xi}] = \mu \quad (42.19)$$

$$\langle \underline{A}_{\xi}, \underline{A}_{\xi'} \rangle = V_1 \left[ \frac{n-2-\delta(\xi, \xi')}{n-1} \right] \quad (42.20)$$

**proof:**

$$E[\underline{A}_{\xi}] = \frac{1}{n-1} \sum_{\sigma} \mathbb{1}(\xi \neq \sigma) E[x^{\sigma}] = \mu \quad (42.21)$$

$$\langle \underline{A}_{\xi}, \underline{A}_{\xi'} \rangle = \frac{1}{n-1} \sum_{\sigma} \sum_{\sigma'} [1 - \delta(\sigma, \xi)][1 - \delta(\sigma', \xi')] \langle x^{\sigma}, x^{\sigma'} \rangle \quad (42.22)$$

$$= \frac{V_1}{n-1} \sum_{\sigma} \sum_{\sigma'} [1 - \delta_{\xi}^{\sigma} - \delta_{\xi'}^{\sigma'} + \delta_{\xi}^{\sigma} \delta_{\xi'}^{\sigma'}] \delta_{\sigma'}^{\sigma} \quad (42.23)$$

$$= \frac{V_1}{n-1} [n-2 + \delta_{\xi'}^{\xi}] \quad (42.24)$$

QED

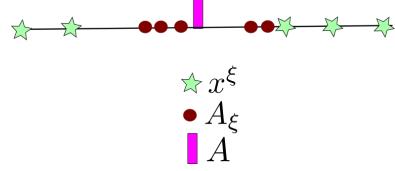


Figure 42.2: For each point  $x^\xi$ , there is a corresponding point  $A_\xi$  which is  $n - 1$  times closer to the average  $A$  than  $x^\xi$  is.

### Claim 76

$$A_\xi - A = \frac{A - x^\xi}{n - 1} \quad (42.25)$$

Hence, the distance of a point  $x^\xi$  to the mean value  $A$  is  $n - 1$  times as large as the distance of  $A_\xi$  to  $A$ . (see Fig.42.2)

**proof:**

$$A_\xi - A = \frac{1}{n - 1} \left( \sum_{\sigma} x^\sigma - x^\xi \right) - \frac{1}{n} \sum_{\sigma} x^\sigma \quad (42.26)$$

$$= x^\xi \left( \frac{-1}{n - 1} \right) + \sum_{\sigma} x^\sigma \underbrace{\left( \frac{1}{n - 1} - \frac{1}{n} \right)}_{\frac{1}{n(n-1)}} \quad (42.27)$$

$$= \frac{A - x^\xi}{n - 1} \quad (42.28)$$

**QED**

Note that

$$(n - 1) \sum_{\xi} (A_\xi - E_{\xi}[A_\xi])^2 = \hat{V}_1 \quad (42.29)$$

by Eq.(42.25). Hence, we can estimate  $V_1$  from  $\vec{A}$  instead of  $\vec{x}$ .

Note that

$$B_\xi = nA - (n - 1)A_\xi \quad (42.30)$$

$$= \sum_{\sigma} x^\sigma - \sum_{\sigma \neq \xi} x^\sigma = x^\xi \quad (42.31)$$

Since  $B_\xi = x^\xi$ , they have identical statistics. In particular, one can use for  $B_\xi$  the same  $\mu$  and  $V_1$  estimators that we defined in Eqs.(42.4) for  $x^\sigma$ .

# Chapter 43

## Junction Tree Algorithm

The Junction Tree (JT) algorithm is an algo for evaluating exact marginals of a bnet, including cases in which some nodes are fixed to a single state. (fixed nodes are called the a priori evidence.)

The JT algo starts by clustering the loops of a bnet into bigger nodes so as to transform the bnet into a polytree bnet. Then it applies Pearl Belief Propagation (see Chapter 56) to the ensuing polytree. The first breakthrough paper to achieve this agenda in full was Ref.[32] by Lauritzen, and Spiegelhalter in 1988. See the Wikipedia article Ref.[125] for more info and references on the JT algorithm.

I won't describe the JT algo any further here, because it would take too long for this brief book to give a complete treatment of it, including the mathematical proofs. If all you want to do is to code the JT algo, without delving into the mathematical theorems and proofs behind it, I strongly recommend Ref.[26]. Ref.[26] is an excellent cookbook for programmers of the JT algo. My open source program QuantumFog (see Ref.[76]) implements the JT algo in Python, following the recipe of Ref.[26].

# Chapter 44

## Kalman Filter

This chapter is based on Ref.[127], except we've replaced the variables  $F_t, w_t, v_t$  in that reference by  $A_t, \xi_t, \zeta_t$ , respectively.

A Kalman Filter (KF) is a special case of a Hidden Markov Model. HMMs are discussed in Chapter 37.

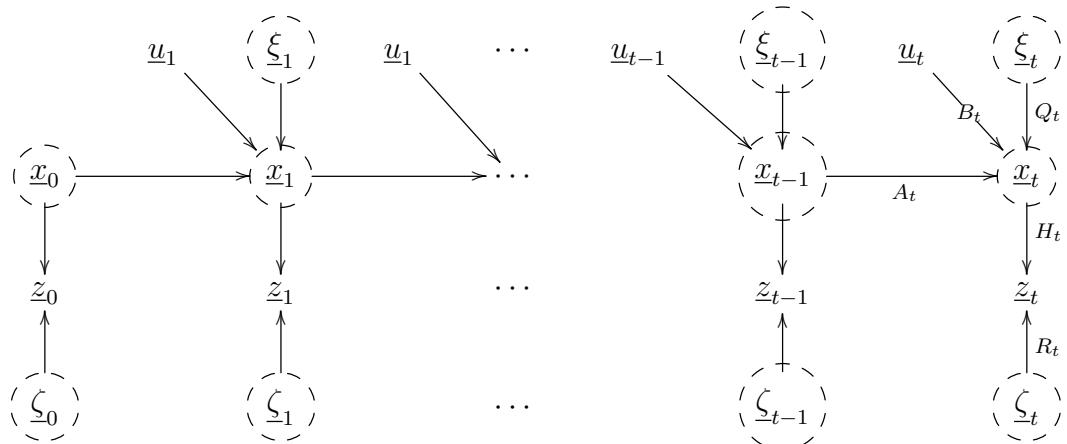


Figure 44.1: Kalman Filter (KF) bnet.

Let

$t = 0, 1, 2, \dots, T - 1$  be the time.

$\underline{\xi}_t \in \mathbb{R}^{nx}, \underline{\zeta}_t \in \mathbb{R}^{nz}$  be random variables that represent hidden (unobserved) external Gaussian white noise.

$\underline{x}_t \in \mathbb{R}^{nx}$  be random variables that represent the hidden (unobserved) true state of the system.

$\underline{u}_t \in \mathbb{R}^{nu}, \underline{z}_t \in \mathbb{R}^{nz}$  be random variables that represent the measured (observed) state of the system.

The TPMs, printed in blue, for the KF bnet Fig.44.1, are as follows:

$$P(\xi_t) = \mathcal{N}(\xi_t; 0, Q_t), \quad (44.1)$$

where  $Q_t$  is given.

$$P(x_t|x_{t-1}, u_t, \xi_t) = \mathbb{1}(x_t = A_t x_{t-1} + B_t u_t + \xi_t), \quad (44.2)$$

where  $A_t, B_t u_t$  are given.  $P(x_t|x_{t-1}, u_t, \xi_t)$  becomes  $P(x_t)$  for  $t = 0$ .

$$P(\zeta_t) = \mathcal{N}(\zeta_t; 0, R_t), \quad (44.3)$$

where  $R_t$  is given.

$$P(z_t|x_t, \zeta_t) = \mathbb{1}(z_t = H_t x_t + \zeta_t), \quad (44.4)$$

where  $H_t$  is given.

## 44.1 Prediction Problem

Find  $\hat{x}_t$  (the best possible estimate of  $x_t$ ) and  $P_t$  (the state of the filter at time  $t$ ) in terms of

1.  $\hat{x}_{t-1}$  and  $P_{t-1}$ .
2. the 5 matrices  $\mathcal{M}_t = (A_t, B_t, H_t, Q_t, R_t)$
3. the observed values of  $z_t$  and  $u_t$ .

See Fig.44.2. For that figure,

$$P(\hat{x}_t, P_t | \hat{x}_{t-1}, P_{t-1}, \mathcal{M}_t, z_t, u_t) = \delta(\hat{x}_t, ?) \delta(P_t, ?). \quad (44.5)$$

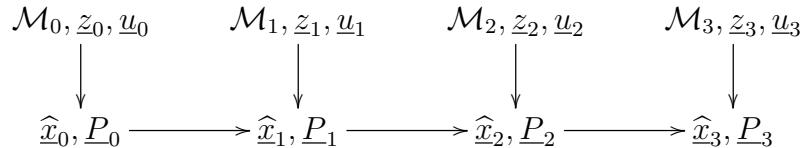


Figure 44.2: Evolution of  $\hat{x}_t, P_t$  for a KF.

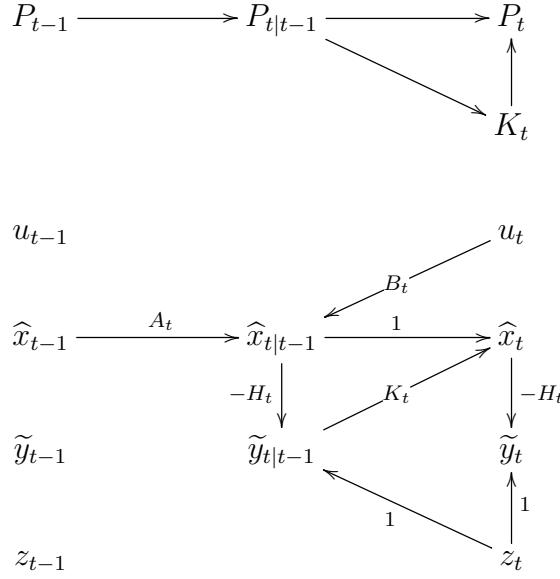


Figure 44.3: Bnet representation of the algebraic solution of the prediction problem for a KF.

## 44.2 Solution

The algebraic solution of the prediction problem for a KF is as follows. See Fig.44.3 for a bnet representation of this algebraic solution.

Define  $\eta_{t|t} = \eta_t$  for  $\eta = \hat{x}, P$ .

- **Initial Conditions**  $\hat{x}_0, P_0$

- **A priori estimates**

a priori state estimate

$$\hat{x}_{t|t-1} = \underbrace{A_t \hat{x}_{t-1} + B_t u_t}_{x_t - \xi_t} \quad (44.6)$$

a priori covariance estimate

$$P_{t|t-1} = A_t P_{t-1} A_t^T + Q_t \quad (44.7)$$

- **A posteriori estimates**

Optimal Kalman gain  $K_t$

$$S_t = H_t P_{t|t-1} H_t^T + R_t \quad (44.8)$$

$$K_t = P_{t|t-1} H_t^T S_t^{-1} \quad (44.9)$$

$$= P_{t|t-1} H_t^T [H_t P_{t|t-1} H_t^T + R_t]^{-1} \quad (44.10)$$

a posteriori state estimate

$$\tilde{y}_{t|t-1} = z_t - H_t \hat{x}_{t|t-1} \quad (44.11)$$

$$\hat{x}_t = \hat{x}_{t|t-1} + K_t \tilde{y}_{t|t-1} \quad (44.12)$$

$$= (1 - K_t H_t) \hat{x}_{t|t-1} + K_t \underbrace{z_t}_{H_t x_t + \zeta_t} \quad (\text{interpolation formula}) \quad (44.13)$$

$$\tilde{y}_t = z_t - H_t \hat{x}_t \quad (44.14)$$

a posteriori covariance estimate

$$P_t = (I - K_t H_t) P_{t|t-1} \quad (44.15)$$

### 44.3 Simple Example

$r_t$  position,  $v_t$  velocity,  $a_t$  acceleration of point particle.

$$x_t = Ax_{t-1} + Bu_t + \xi_t \quad (44.16)$$

$$x_t = \begin{bmatrix} r_t \\ v_t \end{bmatrix}, \quad u_t = a_t \quad (44.17)$$

$$A = \begin{bmatrix} 1 & \Delta t \\ 0 & 1 \end{bmatrix}, \quad B = \begin{bmatrix} \frac{1}{2}(\Delta t)^2 \\ \Delta t \end{bmatrix} \quad (44.18)$$

$$z_t = Hx_t + \zeta_t \quad (44.19)$$

$$H = \begin{bmatrix} 1 & 0 \end{bmatrix} \quad (44.20)$$

## 44.4 Invariants

Note that

$$x_t - \hat{x}_{t|t-1} = \xi_t \quad (44.21)$$

$$x_t - \hat{x}_t = (1 - K_t H_t)(x_t - \hat{x}_{t|t-1}) - K_t \zeta_t \quad (44.22)$$

$$= (1 - K_t H_t)\xi_t - K_t \zeta_t \quad (44.23)$$

$$\tilde{y}_{t|t-1} = \underbrace{z_t}_{H_t x_t + \zeta_t} - H_t \hat{x}_{t|t-1} \quad (44.24)$$

$$= H_t \xi_t + \zeta_t \quad (44.25)$$

$$\tilde{y}_t = \underbrace{z_t}_{H_t x_t + \zeta_t} - H_t \hat{x}_t \quad (44.26)$$

$$= H_t(x_t - \hat{x}_t) + \zeta_t \quad (44.27)$$

$$= H_t(1 - K_t H_t)\xi_t + (1 - H_t K_t)\zeta_t \quad (44.28)$$

$(x_t - \hat{x}_{t|t-1})$ ,  $(x_t - \hat{x}_t)$ ,  $\tilde{y}_{t|t-1}$  and  $\tilde{y}_t$  are called **residuals**. Since  $\xi_t$  and  $\zeta_t$  have zero mean value,

$$E[x_t - \hat{x}_t] = E[x_t - \hat{x}_{t|t-1}] = 0 \quad (44.29)$$

$$E[\tilde{y}_t] = E[\tilde{y}_{t|t-1}] = 0 \quad (44.30)$$

These zero mean value identities are called **invariants**.

## 44.5 Derivation of Solution

First, some notational conventions. Let

$$Cov(\underline{a})_{i,j} = \langle \underline{a}_i, \underline{a}_j \rangle \quad (44.31)$$

$$Cov(\underline{a}) = \langle \underline{a}, \underline{a}^T \rangle = \langle \underline{a}, tp. \rangle \quad (44.32)$$

$$[A, B]_+ = AB + B^T A^T \quad (44.33)$$

$$A + tp. = A + A^T \quad (44.34)$$

*tp.* stands for transpose.

Now define

$$P_t = Cov(\underline{x}_t - \hat{\underline{x}}_t) \quad (44.35)$$

$$P_{t|t-1} = Cov(\underline{x}_t - \hat{\underline{x}}_{t|t-1}) \quad (44.36)$$

$$S_t = Cov(\tilde{y}_{t|t-1}) \quad (44.37)$$

It follows that

$$P_t = \langle \underline{x}_t - \hat{\underline{x}}_t, tp. \rangle \quad (44.38)$$

$$= \left\langle (1 - K_t H_t)(\underline{x}_t - \hat{\underline{x}}_{t|t-1}) - K_t \underline{\zeta}_t, tp. \right\rangle \quad (\text{by Eq.(44.23)}) \quad (44.39)$$

$$= \left\langle (1 - K_t H_t)(\underline{x}_t - \hat{\underline{x}}_{t|t-1}), tp. \right\rangle + \left\langle K_t \underline{\zeta}_t, tp. \right\rangle \quad (\underline{\zeta}_t \text{ uncorrelated with } (\underline{x}_t - \hat{\underline{x}}_{t|t-1})) \quad (44.40)$$

$$= (1 - K_t H_t) \underbrace{\langle \underline{x}_t - \hat{\underline{x}}_{t|t-1}, tp. \rangle}_{P_{t|t-1}} (1 - K_t H_t)^T + K_t \underbrace{\langle \underline{\zeta}_t, tp. \rangle}_{R_t} K_t^T \quad (44.41)$$

$$= P_{t|t-1} - [K_t H_t, P_{t|t-1}]_+ + K_t \underbrace{(H_t P_{t|t-1} H_t^T + R_t)}_{S_t} K_t^T \quad (44.42)$$

Next we find the optimal Kalman gain  $K_t$  by minimizing with respect to  $K_t$  the following mean squared error.

$$\mathcal{E} = \sum_i E[(\underline{x}_t - \hat{\underline{x}}_t)_i^2] \quad (44.43)$$

$$= \text{tr} E[(\underline{x}_t - \hat{\underline{x}}_t)(\underline{x}_t - \hat{\underline{x}}_t)^T] \quad (44.44)$$

$$= \text{tr} P_t \quad (44.45)$$

$$= \text{tr}(P_{t|t-1} - [K_t H_t, P_{t|t-1}]_+ + K_t S_t K_t^T) \quad (44.46)$$

If we set to zero the variation of  $\mathcal{E}$  when  $K_t$  varies, we get

$$0 = \delta \mathcal{E} = \text{tr} [(-P_{t|t-1} H_t^T + K_t S_t) \delta K_t^T] + tp. \quad (44.47)$$

Hence

$$-P_{t|t-1} H_t^T + K_t S_t = 0 \quad (44.48)$$

$$K_t = P_{t|t-1} H_t^T S_t^{-1} \quad (44.49)$$

# Chapter 45

## LATE (Local Average Treatment Effect)

This chapter is based on Refs.[41, 14].

The **Local Average Treatment Effect (LATE)** is the same as the ATE estimand<sup>1</sup>, but it only counts “compliers” (i.e., individuals that comply with the treatment they’ve been assigned). LATE assumes the same bnet that we considered when we discussed Instrumental Variables (IV)<sup>2</sup>

$\sigma$	$a^\sigma$	$d^\sigma(a^\sigma = 0)$	$d^\sigma(a^\sigma = 1)$	$y^\sigma(d^\sigma = 0)$	$y^\sigma(d^\sigma = 1)$
1	0	1			0
2	0	0		1	
3	0	1			1
4	0	0		0	
5	0	0		1	
6	1		1		0
7	1		0	0	
8	1		1		0
9	1		0	1	
10	1		1		1

Table 45.1: Hypothetical dataset for LATE problem. Pink cells indicate missing data.

Table 45.1 shows a hypothetical dataset for the LATE problem.

Consider the bnets  $G$  and  $G_+$  of Fig.45.1.<sup>3</sup>

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<sup>1</sup>ATE is defined in the Potential Outcomes chapter, i.e., Chapter 72.

<sup>2</sup>Instrumental Variables are discussed in Chapters 41 and 40.

<sup>3</sup>If there were an arrow  $\underline{a} \rightarrow \underline{y}$  in bnet  $G$ , then we could also apply the imagine operator  $\mathcal{I}_{\underline{a} \rightarrow \underline{y}}$  to  $G$ . This would lead to nodes  $[\underline{y}(a', d')]_{a'=0}^1 |_{d'=0}^1$ . Since there is no arrow  $\underline{a} \rightarrow \underline{y}$ , we would have  $y(a, d) = y(d)$  for all  $a, d$ , i.e.,  $y$  does not depend directly on the instrument  $a$ . This independence of  $y(a, d)$  on  $a$  is called the **excludability assumption**. One could say the excludability assumption is built into our bnet  $G_+$ .

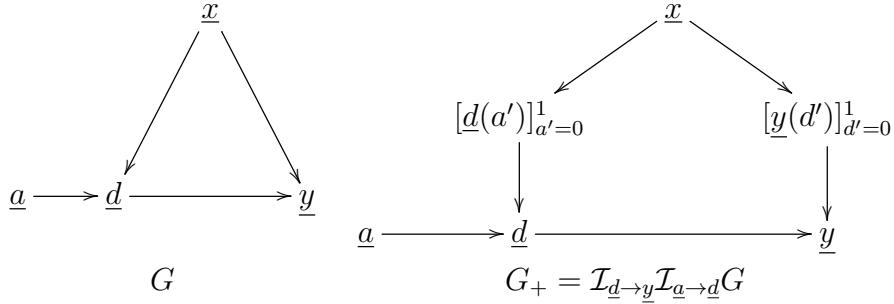


Figure 45.1: Bnet  $G_+$  is bnet  $G$  after application of 2 imagine operators. Imagine operators are discussed in Chapter 12.

Let

$\underline{a} \in \{0, 1\}$ , instrumental variable, initially assigned dose

$\underline{d} \in \{0, 1\}$ , actual treatment dose

$\underline{y} \in \{0, 1\}$ , treatment outcome

The definition of the imagine operators used in  $G_+$  stipulates that nodes  $y$  and  $\underline{d}$  in  $G_+$  must be have the following deterministic TPMs (printed in blue below).

$$P(d|\underline{a}, [d(a')]_{a'=0}^1) = \mathbb{1}(d = \underbrace{ad(1) + (1-a)d(0)}_{=\sum_{a'=0}^1 \delta(a,a')d(a')} = d(a)) \quad (45.1)$$

$$P(y|d, [y(d')]_{d'=0}^1) = \mathbb{1}(y = y(d)) \quad (45.2)$$

	$d^\sigma(0)$	$d^\sigma(1)$
never-takers	0	0
compliers	0	1
defiers	1	0
always-takers	1	1

Table 45.2: Possible compliance behaviors for individual  $\sigma$ .

Table 45.2 gives a name to the 4 possible compliance behaviors that might be exhibited by an individual  $\sigma$  of a dataset. Below, we will use  $\mathcal{C}$  to denote the conditions that define a **complier**:

$$\mathcal{C} = \{\underline{d}(0) = 0, \underline{d}(1) = 1\} \quad (45.3)$$

**Monotonicity** is said to hold if

$$d^\sigma(1) \geq d^\sigma(0) \quad (45.4)$$

Note that monotonicity rules out defiers (i.e.,  $d^\sigma(1) = 0$ ,  $d^\sigma(0) = 1$ ), but allows the other 3 compliance behaviors.

It is convenient to define the following expected values:

$$\mathcal{D}_{|a} = \sum_d d P(d|a) = E_{|a}[d] \quad (45.5)$$

$$\mathcal{Y}_{|d,a} = \sum_y y P(y|d, a) = E_{|d,a}[y] \quad (45.6)$$

$$\mathcal{Y}_{|\underline{d}=d} = \sum_y y P(y|d) = E_{|d}[y] \quad (45.7)$$

$$\mathcal{Y}_{|\underline{a}=a} = \sum_y y P(y|a) = E_{|a}[y] \quad (45.8)$$

Assume that  $\mathcal{D}_{|1} \neq \mathcal{D}_{|0}$ . Then LATE is defined by

$$\boxed{LATE = \frac{\mathcal{Y}_{|\underline{a}=1} - \mathcal{Y}_{|\underline{a}=0}}{\mathcal{D}_{|1} - \mathcal{D}_{|0}}} \quad (45.9)$$

**Claim 77** *If monotonicity is satisfied, then*

$$P(\mathcal{C}) = \mathcal{D}_{|1} - \mathcal{D}_{|0} \quad (45.10)$$

**proof:**

$$\mathcal{D}_{|1} - \mathcal{D}_{|0} = \sum_{d(0), d(1)} P(d(0), d(1)) [d(1) - d(0)] \quad (45.11)$$

$$= \begin{cases} P(d(0) = 0, d(1) = 0) \underbrace{[d(1) - d(0)]}_0 \\ + P(d(0) = 0, d(1) = 1) \underbrace{[d(1) - d(0)]}_1 \\ + \underbrace{P(d(0) = 1, d(1) = 0)}_{=0 \text{ by monotonicity}} [d(1) - d(0)] \\ + P(d(0) = 1, d(1) = 1) \underbrace{[d(1) - d(0)]}_0 \end{cases} \quad (45.12)$$

$$= P(\mathcal{C}) \quad (45.13)$$

**QED**

**Claim 78** Recall

$$ATE = E[\underline{y}(1) - \underline{y}(0)] \quad (45.14)$$

If monotonicity is satisfied, then

$$LATE = E_{|\mathcal{C}}[\underline{y}(1) - \underline{y}(0)] \quad (45.15)$$

**proof:**

$$\mathcal{Y}_{|\underline{a}=1} - \mathcal{Y}_{|\underline{a}=0} = E_{|\underline{a}=1}[\underline{y}] - E_{|\underline{a}=0}[\underline{y}] \quad (45.16)$$

$$= \sum_x \sum_{y(0), y(1)} \sum_{d(0), d(1)} \left\{ \begin{array}{l} [y(d(1)) - y(d(0))] \\ *P(y(0), y(1)|x) \\ *P(d(0), d(1)|x) \\ *P(x) \end{array} \right\} \quad (45.17)$$

$$= \sum_{y(0), y(1)} \sum_{d(0), d(1)} [y(d(1)) - y(d(0))] \left\{ \begin{array}{l} P(y(0), y(1)|d(0), d(1)) \\ *P(d(0), d(1)) \end{array} \right\} \quad (45.18)$$

$$= \sum_{y(0), y(1)} \left\{ \begin{array}{l} \underbrace{[y(0) - y(0)]}_0 \left\{ \begin{array}{l} P(y(0), y(1)|d(0) = 0, d(1) = 0) \\ *P(d(0) = 0, d(1) = 0) \end{array} \right\} \\ + [y(1) - y(0)] \left\{ \begin{array}{l} P(y(0), y(1)|d(0) = 0, d(1) = 1) \\ *P(d(0) = 0, d(1) = 1) \end{array} \right\} \\ + [y(0) - y(1)] \left\{ \begin{array}{l} P(y(0), y(1)|d(0) = 0, d(1) = 0) \\ *P(\underbrace{d(0) = 1, d(1) = 0}_{=0 \text{ monotonicity}}) \end{array} \right\} \\ + \underbrace{[y(1) - y(1)]}_0 \left\{ \begin{array}{l} P(y(0), y(1)|d(0) = 1, d(1) = 1) \\ *P(d(0) = 1, d(1) = 1) \end{array} \right\} \end{array} \right\} \quad (45.19)$$

$$= P(\mathcal{C}) \sum_{y(0), y(1)} [y(1) - y(0)] P(y(0), y(1)|\mathcal{C}) \quad (45.20)$$

$$= P(\mathcal{C}) E_{|\mathcal{C}}[\underline{y}(1) - \underline{y}(0)] \quad (45.21)$$

**QED**

It is instructive to evaluate LATE for the special case in which  $G$  of Fig.45.1 is an LDEN (Linear Deterministic with External Noise) bnet.<sup>4</sup>

Consider Fig.45.2. From that figure

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<sup>4</sup>LDEN bnets are discussed in Chapter 48.

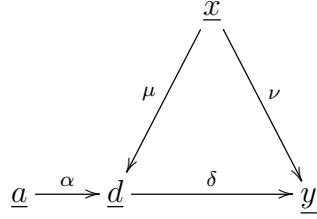


Figure 45.2: LDEN bnet for LATE. External root nodes  $\underline{\epsilon}_a, \underline{\epsilon}_d, \underline{\epsilon}_x, \underline{\epsilon}_y$  are left implicit.

$$\underline{d} = \alpha \underline{a} + \mu \underline{x} + \underline{\epsilon}_d \quad (45.22)$$

$$\underline{y} = \delta \underline{d} + \nu \underline{x} + \underline{\epsilon}_y \quad (45.23)$$

**Claim 79** For the LDEN bnet of Fig.45.2,

$$LATE = \delta = \frac{\frac{\partial \underline{y}}{\partial \underline{d}}}{\frac{\partial \underline{d}}{\partial \underline{a}}} \quad (45.24)$$

**proof:**

Note that

$$\langle \underline{a}, \underline{x} \rangle = \langle \underline{a}, \underline{\epsilon}_d \rangle = \langle \underline{a}, \underline{\epsilon}_y \rangle = 0 \quad (45.25)$$

because in all cases, the path between the two nodes of the covariance is blocked by a collider. Thus

$$\langle \underline{a}, \underline{d} \rangle = \alpha \langle \underline{a}, \underline{a} \rangle \quad (45.26)$$

$$\langle \underline{a}, \underline{y} \rangle = \delta \langle \underline{a}, \underline{d} \rangle \quad (45.27)$$

Hence,

$$\alpha = \frac{\langle \underline{a}, \underline{d} \rangle}{\langle \underline{a}, \underline{a} \rangle} = \frac{\partial \underline{d}}{\partial \underline{a}} \quad (45.28)$$

and

$$\delta = \frac{\langle \underline{a}, \underline{y} \rangle}{\langle \underline{a}, \underline{d} \rangle} = \frac{\langle \underline{a}, \underline{y} \rangle}{\langle \underline{a}, \underline{a} \rangle} \frac{\langle \underline{a}, \underline{a} \rangle}{\langle \underline{a}, \underline{d} \rangle} = \frac{\frac{\partial \underline{y}}{\partial \underline{a}}}{\frac{\partial \underline{d}}{\partial \underline{a}}} \quad (45.29)$$

$$E_{\underline{a}=1}[\underline{y}] - E_{\underline{a}=0}[\underline{y}] = E_{\underline{a}=1}[\delta \underline{d} + \nu \underline{x}] - E_{\underline{a}=0}[\delta \underline{d} + \nu \underline{x}] \quad (45.30)$$

$$= \delta(E_{\underline{a}=1}[\underline{d}] - E_{\underline{a}=0}[\underline{d}]) + \nu \underbrace{(E_{\underline{a}=1}[\underline{x}] - E_{\underline{a}=0}[\underline{x}])}_0 \quad (45.31)$$

**QED**

# Chapter 46

## LDEN with feedback loops

This chapter assumes that the reader has read Chapter 48 on LDEN (linear deterministic with external noise) diagrams and Section C.46 on the Z-transform. The algorithm described in this chapter was first published here, and is implemented in my software SCuMpy (see Ref.[77]).

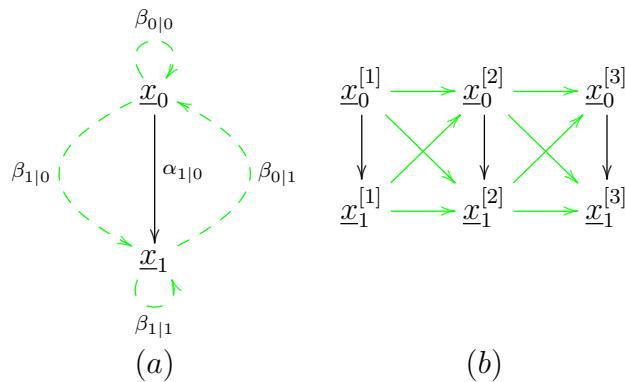


Figure 46.1: LDEN diagrams with two  $\underline{x}_j$  nodes (exogenous nodes  $\underline{u}_j$  not shown). Figure (a) shows a single time-slice with feedback loops. Figure (b) is an “unrolled” version of figure (a) showing 3 time-slices. LDEN diagrams with feedback loops are a special case of Dynamic Bayesian networks (DBN) (see Chapter 25)

Consider Fig.46.1 of an LDEN diagram with feedback loops. It represents the following two “structural equations”:

$$\underline{x}_0^{[n+1]} = \underbrace{\sum_{j=0}^1 \beta_{0|j} \underline{x}_j^{[n]}}_{\text{from past}} + \underline{u}_0^{[n+1]} \quad (46.1)$$

$$\underline{x}_1^{[n+1]} = \underbrace{\sum_{j=0}^1 \beta_{1|j} \underline{x}_j^{[n]}}_{\text{from past}} + \alpha_{1|0} \underline{x}_0^{[n+1]} + \underline{u}_1^{[n+1]} \quad (46.2)$$

for  $n = 0, 1, 2, \dots$  with  $\underline{x}_j^{[0]} = \underline{u}_j^{[0]} = 0$  for all  $j$ .

From the results of Section C.46, we conclude that

$$\mathcal{Z}(\underline{x}_j^{[n+1]}) = z \left( \tilde{\underline{x}}_j(z) - z \underline{x}_j^{[0]} \right) = z \tilde{\underline{x}}_j(z) \quad (46.3)$$

$$\mathcal{Z}(\underline{u}_j^{[n+1]}) = z \tilde{\underline{u}}_j(z) \quad (46.4)$$

Therefore, in  $z$ -space, the two structural equations are as follows:

$$z \tilde{\underline{x}}_0(z) = \sum_{j=0}^1 \beta_{0|j} \tilde{\underline{x}}_j(z) + z \tilde{\underline{u}}_0(z) \quad (46.5)$$

$$z \tilde{\underline{x}}_1(z) = \sum_{j=0}^1 \beta_{1|j} \tilde{\underline{x}}_j(z) + \alpha_{1|0} z \tilde{\underline{x}}_0(z) + z \tilde{\underline{u}}_1(z) \quad (46.6)$$

We can express these two  $z$ -space structural equations in matrix form. Let

$$\tilde{\underline{x}} = \begin{bmatrix} \tilde{\underline{x}}_0 \\ \tilde{\underline{x}}_1 \end{bmatrix}, \quad \tilde{\underline{u}} = \begin{bmatrix} \tilde{\underline{u}}_0 \\ \tilde{\underline{u}}_1 \end{bmatrix}, \quad A = \begin{bmatrix} 0 & 0 \\ \alpha_{1|0} & 0 \end{bmatrix}, \quad B = \begin{bmatrix} \beta_{0|0} & \beta_{0|1} \\ \beta_{1|0} & \beta_{1|1} \end{bmatrix} \quad (46.7)$$

$$\mathbb{1}_A = 1 - A \quad (46.8)$$

$$M(z) \tilde{\underline{x}}(z) = \tilde{\underline{u}}(z) \quad (46.9)$$

Then the two  $z$ -space structural equations reduce to the single matrix equation:

$$M(z) \tilde{\underline{x}}(z) = \tilde{\underline{u}}(z) \quad (46.10)$$

If the DAG for a single time-slice has  $N > 2$  nodes, then this matrix equation is still valid. In that case,  $A$  and  $B$  must be  $N \times N$  matrices. The graph for a single time slice is acyclic (i.e., a DAG), so we can order its nodes topologically. This just means that  $\underline{x}_i$  is a child of  $\underline{x}_j$  if  $i > j$ . If the nodes are indexed topologically, then  $\alpha_{i|j} = 0$

for  $i \leq j$ , so matrix  $A$  is strictly lower diagonal. Henceforth, everything we say will be valid for an arbitrary number  $N \geq 2$  of nodes.

For  $\underline{a} = \underline{x}, \underline{u}$ , let

$$[C_{\underline{a}}^{[n]}]_{i,j} = \langle \underline{a}_i^{[n]}, \underline{a}_j^{[n]} \rangle, \quad [C_{\underline{a}}^{[n,n+1]}]_{i,j} = \langle \underline{a}_i^{[n]}, \underline{a}_j^{[n+1]} \rangle \quad (46.11)$$

and

$$[C_{\tilde{\underline{a}}}^{z_1, z_2}]_{i,j} = \langle \tilde{\underline{a}}_i(z_1), \tilde{\underline{a}}_j(z_2) \rangle, \quad (46.12)$$

Let

$\mathcal{C}$  = single time covariance matrices  $[C_{\underline{x}}^{[n]}]_{i,j} = \langle \underline{x}_i^{[n]}, \underline{x}_j^{[n]} \rangle$  and  $[C_{\underline{x}}^{[n+1]}]_{i,j} = \langle \underline{x}_i^{[n+1]}, \underline{x}_j^{[n+1]} \rangle$ , and two-times covariance matrix  $[C_{\underline{x}}^{[n,n+1]}]_{i,j} = \langle \underline{x}_i^{[n]}, \underline{x}_j^{[n+1]} \rangle$ .

$A$  = strictly lower triangular matrix with entries  $\alpha_{i|j}$  = gain of arrow  $x_j^{[n]} \rightarrow x_i^{[n]}$

$B$  = matrix with entries  $\beta_{i|j}$  = gain of arrow  $x_j^{[n]} \rightarrow x_i^{[n+1]}$

The rest of this chapter will be dedicated to accomplishing the following 2 tasks:

1. Express  $\mathcal{C}$  in terms of  $A$  and  $B$
2. Express  $A$  and  $B$  in terms of  $\mathcal{C}$

Due to the linearity of the model, we will find that these two tasks can be accomplished exactly, in closed form.

**Claim 80**  $C_{\underline{x}}^{[n]} = \langle \underline{x}^{[n]}, \underline{x}^{[n]T} \rangle$  satisfies

$$C_{\underline{x}}^{[n]} = G^{n-1} C_{\underline{x}}^{[1]} (G^T)^{n-1} \quad (46.13)$$

for  $n = 1, 2, 3, \dots$ , where the “growth matrix”  $G$  is given by

$$G = \mathbb{1}_A^{-1} B \quad (46.14)$$

and the “initial covariance matrix”  $C_{\underline{x}}^{[1]} = \langle \underline{x}^{[1]}, \underline{x}^{[1]T} \rangle$  by

$$C_{\underline{x}}^{[1]} = \mathbb{1}_A^{-1} \text{diag}(\sigma_{u_i}^2) (\mathbb{1}_A^{-1})^T \quad (46.15)$$

Once we know the single time covariance matrix  $\langle \underline{x}^{[n]}, \underline{x}^{[n]T} \rangle$ , the 2 times covariance matrix  $\langle \underline{x}^{[n]}, \underline{x}^{[n+1]T} \rangle$  can be found using the equation

$$\langle \underline{x}^{[n]}, \underline{x}^{[n+1]T} \rangle = \langle \underline{x}^{[n]}, \underline{x}^{[n]T} \rangle G^T \quad (46.16)$$

**proof:**

Recall from Section C.46 that  
Z-transform of same-time product

$$x_1^{[n]} x_2^{[n]} = \mathcal{Z}^{-1} \left[ \frac{1}{2\pi i} \oint_C \frac{dw}{w} \tilde{x}_1(w) \tilde{x}_2 \left( \frac{z}{w} \right) \right] \quad (46.17)$$

It follows that

$$\underbrace{\langle \underline{x}^{[n]}, \underline{x}^{[n]T} \rangle}_{C_{\underline{x}}^{[n]}} = \mathcal{Z}^{-1} \left[ \frac{1}{2\pi i} \oint_C \frac{dw}{w} \underbrace{\langle \tilde{\underline{x}}(w), \tilde{\underline{x}}^T \left( \frac{z}{w} \right) \rangle}_{C_{\tilde{\underline{x}}}^{w,z/w}} \right] \quad (46.18)$$

where

$$C_{\tilde{\underline{x}}}^{w,z/w} = M^{-1}(w) C_{\tilde{\underline{u}}}^{w,z/w} (M^{-1})^T(z/w) \quad (46.19)$$

so therefore

$$C_{\underline{x}}^{[n]} = \mathcal{Z}^{-1} \left[ \frac{1}{2\pi i} \oint_C \frac{dw}{w} M^{-1}(w) C_{\tilde{\underline{u}}}^{w,z/w} (M^{-1})^T(z/w) \right] \quad (46.20)$$

At this juncture, we would like to find an expression for  $C_{\tilde{\underline{u}}}^{w,z/w}$  to plug into Eq.(46.20). This shaded frame is dedicated to finding such an expression.

For all  $i$ ,  $\underline{u}_i^{[0]} = 0$ . Keep in mind that  $\mathbf{H}_0^{[n]} = 1$  at  $n = 0$ , so we must have

$$\langle \underline{u}_i^{[n]}, \underline{u}_j^{[n]} \rangle = \delta(i, j) \sigma_{\underline{u}_i}^2 \mathbf{H}_1^{[n]} \quad (46.21)$$

Recall from Section C.46 that:

Z-transform of Heavyside unit step function:

$$\mathcal{Z} \left[ a^n \mathbf{H}_0^{[n]} \right] = \frac{1}{1 - a/z} = \frac{z}{z - a} \quad \text{for } |z| > |a| \quad (46.22)$$

Z-transform of discrete Kronecker delta function:

$$\mathcal{Z}[\delta_{n_0}^{[n]}] = z^{-n_0} \quad (46.23)$$

Unit step function as a sum of delta functions:

$$H_0^{[n]} = \sum_{k=0}^{\infty} \delta_k^{[n]} \quad (46.24)$$

It follows that

$$\mathbf{H}_1^{[n]} = \mathbf{H}_0^{[n]} - \delta_0^{[n]} \quad (46.25)$$

$$\mathcal{Z}[\mathbf{H}_1^{[n]}] = \mathcal{Z}[\mathbf{H}_0^{[n]}] - \mathcal{Z}[\delta_0^{[n]}] \quad (46.26)$$

$$= \frac{z}{z-1} - 1 \quad (46.27)$$

$$= \frac{1}{z-1} \quad (46.28)$$

Therefore,

$$\mathcal{Z}[\langle \underline{u}_i^{[n]}, \underline{u}_j^{[n]} \rangle] = \delta(i, j) \sigma_{\underline{u}_i}^2 \frac{1}{z-1} \quad (46.29)$$

We can satisfy Eq.(46.29) and the following equation

$$\mathcal{Z}[\langle \underline{u}_i^{[n]}, \underline{u}_j^{[n]} \rangle] = \frac{1}{2\pi i} \oint_C \frac{dw}{w} \left\langle \tilde{\underline{u}}_i(w), \tilde{\underline{u}}_j \left( \frac{z}{w} \right) \right\rangle \quad (46.30)$$

if we set

$$\langle \tilde{\underline{u}}_i(w), \tilde{\underline{u}}_j(z/w) \rangle = \delta(i, j) \sigma_{\underline{u}_i}^2 \frac{1}{z-1} \approx \delta(i, j) \sigma_{\underline{u}_i}^2 \frac{1}{z} \quad (46.31)$$

I believe that approximating  $1/(z-1)$  by  $1/z$  leads to a very small change in the subsequent results of this chapter. This approximation merely shifts a pole from  $z = 1$  to  $z = 0$ , and we will only use this expression to do complex contour integrals over a circle in the complex plane with radius  $|z| \gg 1$ .

Plugging Eq.(46.31) into Eq.(46.20) now yields

$$C_{\underline{x}}^{[n]} = \mathcal{Z}^{-1} \left[ \frac{1}{2\pi i} \oint_C \frac{dw}{w} M^{-1}(w) \frac{\text{diag}(\sigma_{\underline{u}_i}^2)}{z} (M^{-1})^T(z/w) \right] \quad (46.32)$$

where

$$M^{-1}(w) = (\mathbb{1}_A - B/w)^{-1} \quad (46.33)$$

$$= (\mathbb{1}_A w - B)^{-1} w \quad (46.34)$$

$$= (w - \mathbb{1}_A^{-1} B)^{-1} w \mathbb{1}_A^{-1} \quad (46.35)$$

$$= \frac{w}{w - \mathbb{1}_A^{-1} B} \mathbb{1}_A^{-1} \quad (46.36)$$

and

$$(M^{-1})^T(z/w) = (\mathbb{1}_A^{-1})^T \frac{z/w}{z/w - B^T(\mathbb{1}_A^{-1})^T} \quad (46.37)$$

$$= (\mathbb{1}_A^{-1})^T \frac{z}{z - B^T(\mathbb{1}_A^{-1})^T w} \quad (46.38)$$

Next, we will avail ourselves of 2 more results from Section C.46:  
Inverse Z-transform:

$$\underbrace{\mathcal{Z}^{-1}[\tilde{x}(z)]}_{x^{[n]}} = \frac{1}{2\pi i} \oint_C dz \tilde{x}(z) z^{n-1} \quad (46.39)$$

Time delay:

$$x^{[n-1]} = \mathcal{Z}^{-1} \left[ \frac{1}{z} \tilde{x}(z) \right] \quad (46.40)$$

Using Eq.(46.22) and Eq.(46.40), we get

$$\mathcal{Z}_z^{-1} \left[ \frac{1}{z} (M^{-1})^T(z/w) \right] = (\mathbb{1}_A^{-1})^T [B^T(\mathbb{1}_A^{-1})^T w]^{n-1} \quad (46.41)$$

$$C_{\underline{x}}^{[n]} = \frac{1}{2\pi i} \oint_C \frac{dw}{w} M^{-1}(w) \text{diag}(\sigma_{\underline{u}_i}^2) \mathcal{Z}_z^{-1} \left[ \frac{1}{z} (M^{-1})^T(z/w) \right] \quad (46.42)$$

$$= \left[ \frac{1}{2\pi i} \oint_C dw \frac{w^{n-1}}{w - \mathbb{1}_A^{-1} B} \right] \mathbb{1}_A^{-1} \text{diag}(\sigma_{\underline{u}_i}^2) (\mathbb{1}_A^{-1})^T [B^T(\mathbb{1}_A^{-1})^T]^{n-1} \quad (46.43)$$

$$= \mathcal{Z}_w^{-1} \left[ \frac{1}{w - \mathbb{1}_A^{-1} B} \right] \mathbb{1}_A^{-1} \text{diag}(\sigma_{\underline{u}_i}^2) (\mathbb{1}_A^{-1})^T [B^T(\mathbb{1}_A^{-1})^T]^{n-1} \quad (\text{by Eq.(46.39)}) \quad (46.44)$$

$$= [\mathbb{1}_A^{-1} B]^{n-1} \mathbb{1}_A^{-1} \text{diag}(\sigma_{\underline{u}_i}^2) (\mathbb{1}_A^{-1})^T [B^T(\mathbb{1}_A^{-1})^T]^{n-1} \quad (\text{by Eqs.(46.22)(46.40)}) \quad (46.45)$$

Eq.(46.16) is the same as Eq.(46.49), and the latter is proven below.

**QED**

The structural equations in  $n$  (i.e., time) space, and in matrix form, can be expressed as:

$$\underline{x}^{[n+1]} = B\underline{x}^{[n]} + A\underline{x}^{[n+1]} + \underline{u}^{[n+1]} \quad (46.46)$$

Applying  $\langle \cdot, \underline{x}^{[n]T} \rangle$  from the right to Eq.(46.46), we get

$$(1 - A) \langle \underline{x}^{[n+1]}, \underline{x}^{[n]T} \rangle = B \langle \underline{x}^{[n]}, \underline{x}^{[n]T} \rangle + \langle \underline{u}^{[n+1]}, \underline{x}^{[n]T} \rangle \quad (46.47)$$

Note that

$$\langle \underline{u}^{[n+1]}, \underline{x}^{[n]T} \rangle = 0 \quad (46.48)$$

by causality, because the  $\underline{x}^{[n]}$  can't be affected by the noise in the future. Therefore

$$\mathbb{1}_A \langle \underline{x}^{[n]}, \underline{x}^{[n+1]T} \rangle^T = B \langle \underline{x}^{[n]}, \underline{x}^{[n]T} \rangle \quad (46.49)$$

Applying  $\langle \cdot, \underline{x}^{[n+1]T} \rangle$  from the right to Eq.(46.46), we get

$$\langle \underline{x}^{[n+1]}, \underline{x}^{[n+1]T} \rangle = B \langle \underline{x}^{[n]}, \underline{x}^{[n+1]T} \rangle + A \langle \underline{x}^{[n+1]}, \underline{x}^{[n+1]T} \rangle + \langle \underline{u}^{[n+1]}, \underline{x}^{[n+1]T} \rangle \quad (46.50)$$

For any matrix  $A$ , define  $SL(A)$  to be the strictly lower triangular matrix obtained from matrix  $A$  by setting to zero all entries on the main diagonal of  $A$  and above it. Note that

$$SL(\langle \underline{u}^{[n+1]}, \underline{x}^{[n+1]T} \rangle) = 0 \quad (46.51)$$

by causality, because the nodes are assumed to be topologically ordered (when the feedback arrows are removed), and the future noise  $\underline{u}_i^{[n+1]}$  cannot be correlated with  $\underline{x}_j^{[n+1]}$  where  $i > j$ . Thus,

$$SL \left( \langle \underline{x}^{[n+1]}, \underline{x}^{[n+1]T} \rangle - \underbrace{B \langle \underline{x}^{[n]}, \underline{x}^{[n+1]T} \rangle}_K \right) = SL \left( A \langle \underline{x}^{[n+1]}, \underline{x}^{[n+1]T} \rangle \right) \quad (46.52)$$

$A$  and  $B$  satisfy a system of 2 linear equations (the two boxed equations above, Eq.(46.49) and Eq.(46.52)) with two unknowns  $A, B$ . To solve that system of 2 equations in  $(A, B)$ , we can:

1. First solve Eq.(46.52)) for  $A$  in terms of  $B$  and  $\mathcal{C}$ , thus obtaining  $A(B, \mathcal{C})$ . To do this step, we can use the same method that was used in Chapter 48, for LDEN without feedback loops, to solve for  $A$  when  $K = 0$ .

Caveat: Eq.(46.52)) for  $A$  has the same number of equations as unknowns as long as, for all  $i > j$ ,  $\alpha_{i|j} \neq 0$ . If some of those  $\alpha_{i|j}$  are zero, then we get an overdetermined system of linear equations. To solve that problem, for every  $i, j$  such that  $i > j$  and  $\alpha_{i|j} = 0$ , replace that unknown by  $\langle \underline{x}_i^{[n]}, \underline{x}_j^{[n]} \rangle$ .

2. Then we can substitute  $A(B, \mathcal{C})$  into the remaining equation Eq.(46.49) to obtain  $B(\mathcal{C})$ .

Caveat: Eq.(46.49)) for  $B$  has the same number of equations as unknowns as long as all  $\beta_{i|j} \neq 0$  for all  $i, j$ . If some of those  $\beta_{i|j}$  are zero, then we get an overdetermined system of linear equations. To solve that problem, for every  $i, j$  such that  $\beta_{i|j} = 0$ , replace that unknown by  $\langle \underline{x}_j^{[n]}, \underline{x}_i^{[n+1]} \rangle$ .

3. Finally, we can substitute  $B(\mathcal{C})$  into  $A(B, \mathcal{C})$  to get  $A(B(\mathcal{C}), \mathcal{C})$ .

# Chapter 47

## Linear and Logistic Regression

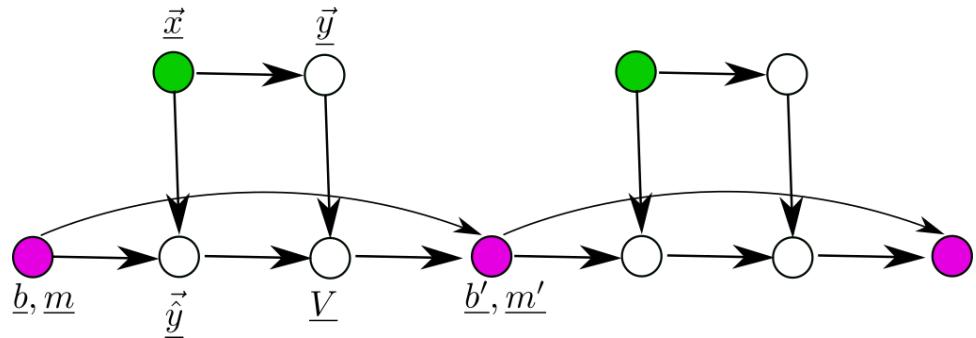


Figure 47.1: Linear Regression

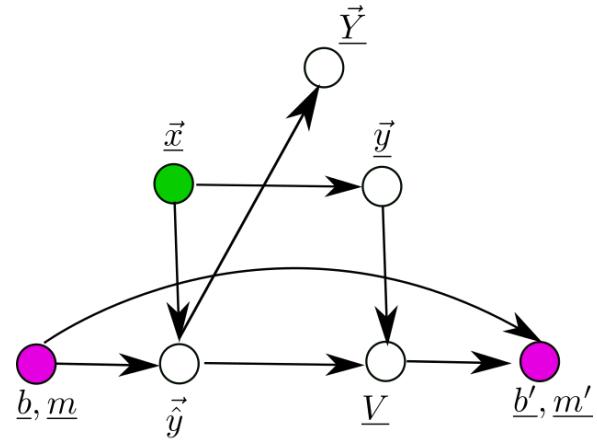


Figure 47.2: Bnet of Fig.47.1 with new  $\vec{Y}$  node.

Estimators  $\hat{y}$  for linear and logistic regression.

- **Linear Regression:**  $y \in \mathbb{R}$ . Note  $\hat{y} \in \mathbb{R}$ .  $(x, \hat{y}(x))$  is the graph of a straight

line with y-intercept  $b$  and slope  $m$ .

$$\hat{y}(x; b, m) = b + mx \quad (47.1)$$

- **Logistic Regression:**  $y \in \{0, 1\}$ . Note  $\hat{y} \in [0, 1]$ .  $(x, \hat{y}(x))$  is the graph of a sigmoid. Often in literature,  $b, m$  are replaced by  $\beta_0, \beta_1$ .

$$\hat{y}(x; b, m) = \text{smoid}(b + mx) \quad (47.2)$$

Define

$$V(b, m) = \sum_{x,y} P(x, y) |y - \hat{y}(x; b, m)|^2. \quad (47.3)$$

We want to minimize  $V(b, m)$  (called a cost or loss function) wrt  $b$  and  $m$ .

The TPMs, printed in blue, for the Bnet Fig.47.1, are as follows.

$$P(b, m) = \text{given} \quad (47.4)$$

The first time it is used,  $(b, m)$  is arbitrary. After the first time, it is determined by previous stage.

Let

$$P_{\underline{x}, \underline{y}}(x, y) = \frac{1}{nsam(\vec{x})} \sum_{\sigma} \mathbb{1}(x = x^{\sigma}, y = y^{\sigma}). \quad (47.5)$$

$$P(\vec{x}) = \prod_{\sigma} P(x^{\sigma}) \quad (47.6)$$

$$P(\vec{y}|\vec{x}) = \prod_{\sigma} P(y^{\sigma} | x^{\sigma}) \quad (47.7)$$

$$P(\vec{\hat{y}}|\vec{x}, b, m) = \prod_{\sigma} \delta(\hat{y}^{\sigma}, \hat{y}(x^{\sigma}, b, m)) \quad (47.8)$$

$$P(V|\vec{\hat{y}}, \vec{y}) = \delta(V, \frac{1}{nsam(\vec{x})} \sum_{\sigma} |y^{\sigma} - \hat{y}^{\sigma}|^2) \quad (47.9)$$

Let  $\eta_b, \eta_m > 0$ . For  $x = b, m$ , if  $x' - x = \Delta x = -\eta \frac{\partial V}{\partial x}$ , then  $\Delta V \approx \frac{-1}{\eta} (\Delta x)^2 \leq 0$  for  $\eta > 0$ . This is called “gradient descent”.

$$P(b'|V, b) = \delta(b', b - \eta_b \partial_b V) \quad (47.10)$$

$$P(m'|V, m) = \delta(m', m - \eta_m \partial_m V) \quad (47.11)$$

## 47.1 Generalization to $x$ with multiple components (features)

Suppose that for each sample  $\sigma$ , instead of  $x^\sigma$  being a scalar, it has  $n$  components called features:

$$x^\sigma = (x_0^\sigma, x_1^\sigma, x_2^\sigma, \dots, x_{n-1}^\sigma) . \quad (47.12)$$

Slope  $m$  is replaced by weights

$$w = (w_0, w_1, w_2, \dots, w_{n-1}) , \quad (47.13)$$

and the product of 2 scalars  $mx^\sigma$  is replaced by the inner vector product  $w^T x^\sigma$ .

## 47.2 Alternative $V(b, m)$ for logistic regression

For logistic regression, since  $y^\sigma \in \{0, 1\}$  and  $\hat{y}^\sigma \in [0, 1]$  are both in the interval  $[0, 1]$ , they can be interpreted as probabilities. Define probability distributions  $p^\sigma(x)$  and  $\hat{p}^\sigma(x)$  for  $x \in \{0, 1\}$  by

$$p^\sigma(1) = y^\sigma, \quad p^\sigma(0) = 1 - y^\sigma \quad (47.14)$$

$$\hat{p}^\sigma(1) = \hat{y}^\sigma, \quad \hat{p}^\sigma(0) = 1 - \hat{y}^\sigma \quad (47.15)$$

Then for logistic regression, the following 2 cost functions  $V(b, m)$  can be used as alternatives to the cost function Eq.(47.3) previously given.

$$V(b, m) = \frac{1}{nsam(\vec{x})} \sum_{\sigma} D_{KL}(p^\sigma \| \hat{p}^\sigma) \quad (47.16)$$

and

$$V(b, m) = \frac{1}{nsam(\vec{x})} \sum_{\sigma} CE(p^\sigma \| \hat{p}^\sigma) \quad (47.17)$$

$$= \frac{-1}{nsam(\vec{x})} \sum_{\sigma} \{y^\sigma \ln \hat{y}^\sigma + (1 - y^\sigma) \ln(1 - \hat{y}^\sigma)\} \quad (47.18)$$

$$= \frac{-1}{nsam(\vec{x})} \sum_{\sigma} \ln \{(\hat{y}^\sigma)^{y^\sigma} (1 - \hat{y}^\sigma)^{(1-y^\sigma)}\} \quad (47.19)$$

$$= \frac{-1}{nsam(\vec{x})} \sum_{\sigma} \ln P(\underline{Y} = y^\sigma | \hat{y} = \hat{y}^\sigma) \quad (47.20)$$

$$= - \sum_{x,y} P(x, y) \ln P(\underline{Y} = y | \hat{y} = \hat{y}(x, b, m)) \quad (47.21)$$

Above, we used

$$P(\underline{Y} = Y | \hat{y}) = \hat{y}^Y [1 - \hat{y}]^{1-Y} \quad (47.22)$$

for  $Y \in S_{\underline{Y}} = \{0, 1\}$ . (Bernoulli distribution).

There is no node corresponding to  $\underline{Y}$  in the Bnet of Fig.47.1. Fig.47.2 shows a new Bnet that has a new node called  $\vec{\underline{Y}}$  compared to the Bnet of Fig.47.1. One defines the TPMs for all nodes of Fig.47.2 except  $\vec{\underline{Y}}$  and  $\underline{V}$  the same as for Fig.47.1. For  $\vec{\underline{Y}}$  and  $\underline{V}$ , one defines

$$P(Y^\sigma | \vec{\hat{y}}) = P(\underline{Y} = Y^\sigma | \hat{y}^\sigma) \quad (47.23)$$

$$P(V|\vec{\underline{Y}}, \vec{y}) = \delta(V, \frac{-1}{nsam(\vec{x})} \ln L), \quad (47.24)$$

where  $L = \prod_\sigma P(\underline{Y} = y^\sigma | \hat{y}^\sigma)$ =likelihood.

# Chapter 48

## Linear Deterministic Bnets with External Noise

In this chapter, we will consider bnets which were referred to, prior to the invention of bnets, as: Sewall Wright's **Path Analysis (PA)** and **linear Structural Equations Models (SEM)**. Judea Pearl in his books calls them **linear Structural Causal Models (SCM)**, because they are very convenient for doing causal analysis. We will refer to them as **linear Deterministic with External Noise (LDEN)** diagrams. This chapter is devoted to LDEN diagrams, except that we will say a few words about non-linear DEN diagrams at the end.

A **DEN diagram** is a special kind of bnet. To build a DEN diagram, start with a deterministic bnet  $G$ . The deterministic nodes of  $G$  are called the **endogenous (internal) variables**. Now make a bigger bnet  $\bar{G}$  called a DEN diagram by adding to each node  $a$  of  $G$  a non-deterministic root node  $u_a$  pointing into  $a$  only. The nodes  $u_a$  are called the **exogenous (external) variables**. The exogenous variables make their children noisy. They are assumed to be unobserved and their TPMs are prior probability distributions. Since they are root nodes, they are mutually independent. When we draw a DEN diagram, we will sometimes not draw the exogenous nodes, leaving them implicit.

A **linear DEN diagram (LDEN)** is a DEN diagram whose deterministic nodes have a TPM that is a linear function of the states of the parent nodes.

This chapter uses the notation  $\langle \underline{x}, \underline{y} \rangle$  for the covariance of any two random variables  $\underline{x}, \underline{y}$ . This  $\langle \underline{x}, \underline{y} \rangle$  notation is defined in Chapter C.

### 48.1 Example of LDEN diagram

The TPMs, printed in blue, for the LDEN diagram Fig.48.1, are as follows.

$$P(y|w, z, u_y) = \mathbb{1}(y = \epsilon w + \delta z + u_y) \quad (48.1)$$

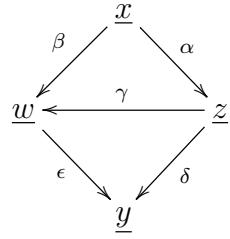


Figure 48.1: Example of a LDEN diagram wherein  $\underline{x}$  splits into two nodes  $\underline{z}$  and  $\underline{w}$ , then merges into node  $\underline{y}$ . There is also an arrow  $\underline{z} \rightarrow \underline{w}$ . Exogenous nodes are not shown. The Greek letters represent real numbers.

$$P(w|x, z, u_{\underline{w}}) = \mathbb{1}(w = \beta x + \gamma z + u_{\underline{w}}) \quad (48.2)$$

$$P(z|x, u_z) = \mathbb{1}(z = \alpha x + u_z) \quad (48.3)$$

$$P(x|u_{\underline{x}}) = \mathbb{1}(x = u_{\underline{x}}) \quad (48.4)$$

Hence,

$$y = \epsilon w + \delta z + u_{\underline{y}} \quad (48.5)$$

$$= \epsilon(\beta x + \gamma z + u_{\underline{w}}) + \delta z + u_{\underline{y}} \quad (48.6)$$

$$= (\epsilon\gamma + \delta)z + \epsilon\beta x + \epsilon u_{\underline{w}} + u_{\underline{y}} \quad (48.7)$$

$$= (\epsilon\gamma + \delta)z + \epsilon\beta u_{\underline{x}} + \epsilon u_{\underline{w}} + u_{\underline{y}} . \quad (48.8)$$

Therefore

$$\left( \frac{\partial y}{\partial z} \right)_{u_{\underline{w}}, u_{\underline{y}}} = \epsilon\gamma + \delta , \quad (48.9)$$

where the partial derivative holds fixed all exogenous variables except  $u_z$ . Note that this partial derivative is a sum of terms, and that each of those terms represents a different directed path from  $\underline{z}$  to  $\underline{y}(\underline{z})$ . This is a general property of LDEN diagrams.

## 48.2 LDEN equations and their 2 solutions

LDEN diagrams are described by a system of linear equations (known as the **structural equations**) of the form

$$\underline{x}_i = \sum_{j=0}^{nx-1} \alpha_{i|j} \underline{x}_j + \underline{u}_i \quad (48.10)$$

for  $i = 0, 1, \dots, nx - 1$ , where the  $\underline{x}_i$  are the internal nodes, the  $\alpha_{i|j}$  are the **path coefficients** (a.k.a. **arrow gains**), and the  $\underline{u}_i$  are the external nodes that inject noise into the system. Some of the  $\alpha_{i|j}$  may be zero, in which case the corresponding arrow  $\underline{x}_j \rightarrow \underline{x}_i$  would not be drawn. The  $\underline{u}_i$  are root nodes with zero covariance with each other.

We can view this as either

1. UNK-CM (unknown covariance matrix) solution  
a linear system of equations with the unknowns  $\underline{x}_i$ . We can solve for these unknowns using basic Linear Algebra. Once we solve for the unknowns, we can calculate the covariances  $\langle \underline{x}_j, \underline{x}_k \rangle$ .
2. UNK-G (unknown gains) solution  
a linear system of equations with the unknowns  $\alpha_{i|j}$ . We can solve for these unknowns using basic Linear Algebra.

Next, we will find the 2 solutions UNK-CM and UNK-G explicitly for arbitrary LDEN diagrams. We will present these solutions gradually, first for fully connected LDEN diagrams, and then for the general case that does not require full connectivity.

## 48.3 Fully connected LDEN diagrams

The bnets that will be considered in this section will all be fully connected. Fully connected bnets are defined in Chapter D.

In this section, we will assume that the nodes  $\underline{x}_j$  are ordered topologically, with the root nodes first. This means that  $\underline{x}_i$  happens after  $\underline{x}_j$  if  $i > j$ . When the nodes are ordered topologically,  $\alpha_{i|j} = 0$  if  $j \geq i$ .

In the fully connected case,  $\alpha_{i|j} \neq 0$  for all  $j < i$ , and for any node  $\underline{x}_i$ , all previous nodes are parents of  $\underline{x}_i$  and we draw arrows  $\underline{x}_j \rightarrow \underline{x}_i$  for  $j = 0, 1, \dots, i - 1$ .

In the not fully connected case, some of the  $\alpha_{i|j}$  with  $j < i$  are zero, in which case the corresponding arrow  $\underline{x}_j \rightarrow \underline{x}_i$  is not drawn.

### 48.3.1 Fully connected LDEN diagram with $nx = 2$

Consider the LDEN diagram of Fig.48.2. This diagram represents the following structural equations:

$$\underline{x}_0 = \underline{u}_0 \quad (48.11a)$$

$$\underline{x}_1 = \alpha_{1|0} \underline{x}_0 + \underline{u}_1 . \quad (48.11b)$$

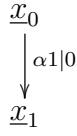


Figure 48.2: Fully connected LDEN diagram with two  $\underline{x}_j$  nodes (exogenous nodes  $\underline{u}_j$  not shown).

### 1. UNK-CM solution

Note that

$$\underline{x}_0 = \underline{u}_0 \quad (48.12a)$$

$$\underline{x}_1 = \alpha_{1|0}\underline{u}_0 + \underline{u}_1 \quad (48.12b)$$

Thus, the  $\underline{x}_i$  can be expressed in terms of the  $\underline{u}_i$ . Using the fact that  $\langle \underline{u}_i, \underline{u}_j \rangle = 0$  for  $i \neq j$ , we get

$$\langle \underline{x}_0, \underline{x}_0 \rangle = \sigma_{\underline{u}_0}^2 \quad (48.13)$$

$$\langle \underline{x}_1, \underline{x}_0 \rangle = \alpha_{1|0}\sigma_{\underline{u}_0}^2 \quad (48.14)$$

$$\langle \underline{x}_1, \underline{x}_1 \rangle = \alpha_{1|0}^2\sigma_{\underline{u}_0}^2 + \sigma_{\underline{u}_1}^2 \quad (48.15)$$

### 2. UNK-G solution

Note that

$$\langle \underline{x}_0, \underline{u}_1 \rangle = 0 \quad (48.16)$$

because the path from  $\underline{x}_0$  to  $\underline{u}_1$  is blocked by a collider. Therefore,

$$\langle \underline{x}_0, \underline{x}_1 \rangle = \alpha_{1|0} \langle \underline{x}_0, \underline{x}_0 \rangle \quad (48.17)$$

so<sup>1</sup>

$$\alpha_{1|0} = \frac{\langle \underline{x}_0, \underline{x}_1 \rangle}{\langle \underline{x}_0, \underline{x}_0 \rangle} = \frac{\partial \underline{x}_1}{\partial \underline{x}_0} \quad (48.18)$$

Thus,  $\alpha_{1|0}$  can be estimated from the covariances  $\langle \underline{x}_i, \underline{x}_j \rangle$ .

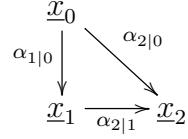


Figure 48.3: Fully connected LDEN diagram with three  $\underline{x}_j$  nodes (exogenous nodes  $\underline{u}_j$  not shown).

### 48.3.2 Fully connected LDEN diagram with $nx = 3$

Consider the LDEN diagram of Fig.48.3. This diagram represents the following structural equations:

$$\underline{x}_0 = \underline{u}_0 \quad (48.19a)$$

$$\underline{x}_1 = \alpha_{1|0}\underline{x}_0 + \underline{u}_1 \quad (48.19b)$$

$$\underline{x}_2 = \alpha_{2|0}\underline{x}_0 + \alpha_{2|1}\underline{x}_1 + \underline{u}_2 . \quad (48.19c)$$

#### 1. UNK-CM solution

Let

$$\underline{x} = \begin{bmatrix} \underline{x}_0 \\ \underline{x}_1 \\ \underline{x}_2 \end{bmatrix}, \quad \underline{u} = \begin{bmatrix} \underline{u}_0 \\ \underline{u}_1 \\ \underline{u}_2 \end{bmatrix} \quad (48.20)$$

and

$$A = \begin{bmatrix} 0 & 0 & 0 \\ \alpha_{1|0} & 0 & 0 \\ \alpha_{2|0} & \alpha_{2|1} & 0 \end{bmatrix} \quad (48.21)$$

Note that

$$\underline{x} = A\underline{x} + \underline{u} \quad (48.22)$$

so

$$\underline{x} = (1 - A)^{-1}\underline{u} \quad (48.23)$$

Thus, the  $\underline{x}_i$  can be expressed in terms of the  $\underline{u}_i$ .

If we define the covariance matrix by

---

<sup>1</sup>We are using the notation  $\frac{\partial b}{\partial a} = \frac{\langle a, b \rangle}{\langle a, a \rangle}$ , for any two random variables  $a, b$

$$C = \langle \underline{x}, \underline{x}^T \rangle , \quad C_{i,j} = \langle \underline{x}_i, \underline{x}_j \rangle \quad (48.24)$$

then<sup>2</sup>

$$C = (1 - A)^{-1} \langle \underline{\epsilon}, \underline{\epsilon}^T \rangle [(1 - A)^{-1}]^T \quad (48.25)$$

$$= (1 - A)^{-1} \text{diag}(\sigma_{\epsilon_i}^2) [(1 - A)^{-1}]^T \quad (48.26)$$

If we define the Jacobian matrix  $J$  by

$$J_{i,j} = \frac{\partial \underline{x}_i}{\partial \underline{x}_j} \quad (48.27)$$

then

$$J = C[\text{diag}(\langle \underline{x}_i, \underline{x}_i \rangle)]^{-1} \quad (48.28)$$

$$= (1 - A)^{-1} \text{diag}(\sigma_{\epsilon_i}^2) [(1 - A)^{-1}]^T [\text{diag}(\langle \underline{x}_i, \underline{x}_i \rangle)]^{-1} \quad (48.29)$$

$C$  has the nice property that it is a symmetric matrix, whereas  $J$  has the nice property that its diagonal elements are all 1.

## 2. UNK-G solution

Note that

$$\langle \underline{x}_0, \underline{x}_1 \rangle = \alpha_{1|0} \langle \underline{x}_0, \underline{x}_0 \rangle \quad (48.30a)$$

$$\langle \underline{x}_0, \underline{x}_2 \rangle = \alpha_{2|0} \langle \underline{x}_0, \underline{x}_0 \rangle + \alpha_{2|1} \langle \underline{x}_0, \underline{x}_1 \rangle \quad (48.30b)$$

$$\langle \underline{x}_1, \underline{x}_2 \rangle = \alpha_{2|0} \langle \underline{x}_1, \underline{x}_0 \rangle + \alpha_{2|1} \langle \underline{x}_1, \underline{x}_1 \rangle \quad (48.30c)$$

Hence

$$\alpha_{1|0} = \frac{\langle \underline{x}_0, \underline{x}_1 \rangle}{\langle \underline{x}_0, \underline{x}_0 \rangle} = \frac{\partial \underline{x}_1}{\partial \underline{x}_0} \quad (48.31)$$

$$\begin{bmatrix} \langle \underline{x}_0, \underline{x}_2 \rangle \\ \langle \underline{x}_1, \underline{x}_2 \rangle \end{bmatrix} = \begin{bmatrix} \langle \underline{x}_0, \underline{x}_0 \rangle & \langle \underline{x}_0, \underline{x}_1 \rangle \\ \langle \underline{x}_1, \underline{x}_0 \rangle & \langle \underline{x}_1, \underline{x}_1 \rangle \end{bmatrix} \begin{bmatrix} \alpha_{2|0} \\ \alpha_{2|1} \end{bmatrix} \quad (48.32)$$

Let

$$\alpha^{(2)} = \begin{bmatrix} \alpha_{2|0} \\ \alpha_{2|1} \end{bmatrix} , \quad \underline{x}^{(2)} = \begin{bmatrix} \underline{x}_0 \\ \underline{x}_1 \end{bmatrix} , \quad \langle \underline{x}^{(2)}, \underline{x}_2 \rangle = \begin{bmatrix} \langle \underline{x}_0, \underline{x}_2 \rangle \\ \langle \underline{x}_1, \underline{x}_2 \rangle \end{bmatrix} \quad (48.33)$$

Define the covariance matrix  $C^{(2)}$  for the third row of  $A$  by

---

<sup>2</sup>We are using the notation  $\text{diag}(a) =$  diagonal matrix with  $a \in \mathbb{R}^n$  along its diagonal.

$$C^{(2)} = \begin{bmatrix} \langle \underline{x}_0, \underline{x}_0 \rangle & \langle \underline{x}_0, \underline{x}_1 \rangle \\ \langle \underline{x}_1, \underline{x}_0 \rangle & \langle \underline{x}_1, \underline{x}_1 \rangle \end{bmatrix} \quad (48.34)$$

Then

$$\langle \underline{x}^{(2)}, \underline{x}_2 \rangle = C^{(2)} \alpha^{(2)} \quad (48.35)$$

so

$$\alpha^{(2)} = [C^{(2)}]^{-1} \langle \underline{x}^{(2)}, \underline{x}_2 \rangle \quad (48.36)$$

Alternatively, let

$$\nabla^{(2)} \underline{x}_2 = \begin{bmatrix} \partial_{\underline{x}_0} \underline{x}_2 \\ \partial_{\underline{x}_1} \underline{x}_2 \end{bmatrix} \quad (48.37)$$

Define the Jacobian matrix for the third row of  $A$  by

$$J_{i,j}^{(2)} = \frac{\partial \underline{x}_i}{\partial \underline{x}_j} \quad (48.38)$$

for  $i, j \in \{0, 1\}$ . Then

$$\nabla^{(2)} \underline{x}_2 = J^{(2)T} \alpha^{(2)} \quad (48.39)$$

so

$$\alpha^{(2)} = [J^{(2)T}]^{-1} \nabla^{(2)} \underline{x}_2 \quad (48.40)$$

From the  $C^{(r)}$  and the  $J^{(r)}$  expressions for  $r = 1, 2$ , we see that the  $\alpha_{i|j}$  can be expressed in terms of the covariances  $\langle \underline{x}_i, \underline{x}_j \rangle$ .

### 48.3.3 Fully connected LDEN diagram with arbitrary $nx$

Let  $\underline{x}_. = (x_i)_{i=0,1,\dots,nx-1}$  and  $\underline{x}_{<i} = (x_k)_{k=0,1,\dots,i-1}$ . Consider a fully connected LDEN diagram with deterministic internal nodes labeled  $\underline{x}_i$ . The  $\underline{x}_i$  labels are assumed to be in topological order (i.e., the parents of node  $\underline{x}_i$  are  $\underline{x}_{<i}$ ). Let the TPMs, printed in blue, for the nodes  $\underline{x}_.$  of the LDEN diagram, be as follows.

$$P(x_i | x_{<i}, u_i) = \mathbb{1}(x_i = \sum_{j < i} \alpha_{i|j} x_j + u_i), \quad (48.41)$$

for some parameters  $\alpha_{i|j} \in \mathbb{R}$ . The external nodes  $\underline{u}_.$  are assumed to be independent so

$$P(u.) = \prod_i P(u_i) \quad (48.42)$$

and

$$\langle \underline{u}_i, \underline{u}_j \rangle = 0 \text{ if } i \neq j . \quad (48.43)$$

Note that

$$P(x.) = \sum_{u.} P(u.) \prod_i P(x_i | x_{<i}, u_i) \quad (48.44)$$

$$= E_{\underline{u}} [\prod_i P(x_i | x_{<i}, u_i)] . \quad (48.45)$$

In terms of random variables, this system is described by the following structural equations:

$$\underline{x}_i = \sum_{j < i} \alpha_{i|j} \underline{x}_j + \underline{u}_i . \quad (48.46)$$

### 1. UNK-CM solution

The structural equations can be written in matrix form as follows. Define a strictly lower triangular matrix  $A$  with the arrow gains  $\alpha_{i|j} \in \mathbb{R}$  as entries. For example, for  $nx = 4$ ,

$$A = \begin{bmatrix} 0 & 0 & 0 & 0 \\ \alpha_{1|0} & 0 & 0 & 0 \\ \alpha_{2|0} & \alpha_{2|1} & 0 & 0 \\ \alpha_{3|0} & \alpha_{3|1} & \alpha_{3|2} & 0 \end{bmatrix} . \quad (48.47)$$

If we now represent the multinodes  $\underline{x}.$  and  $\underline{u}.$  as column vectors  $\underline{x}$  and  $\underline{u}$ , we get

$$\underline{x} = A\underline{x} + \underline{u} . \quad (48.48)$$

Note that

$$\underline{x} = (1 - A)^{-1} \underline{u} \quad (48.49)$$

so the  $\underline{x}_i$  can be expressed in terms of the  $\underline{u}_i$ .

Just like we did for the case  $nx = 3$ , we can now use Eq.(48.49) to express, in terms of  $A$  and the  $\langle \underline{u}_i, \underline{u}_i \rangle = \sigma_{\underline{u}_i}^2$ , the covariance matrix  $C = \langle \underline{x}, \underline{x}^T \rangle$  and the Jacobian matrix  $J$  with  $J_{i,j} = \frac{\partial \underline{x}_i}{\partial \underline{x}_j}$ .

## 2. UNK-G solution

Note that

$$\underline{x}_i = f_i(\underline{u}_{\leq i}) . \quad (48.50)$$

Therefore, if  $i > k$ ,

$$\langle \underline{x}_k, \underline{u}_i \rangle = \langle f_k(\underline{u}_{\leq k}), \underline{u}_i \rangle = 0 . \quad (48.51)$$

Thus, if  $i > k$ ,

$$\langle \underline{x}_k, \underline{x}_i \rangle = \sum_{j < i} \alpha_{i|j} \langle \underline{x}_k, \underline{x}_j \rangle + \langle \underline{x}_k, \underline{u}_i \rangle \quad (48.52)$$

$$= \sum_{j < i} \alpha_{i|j} \langle \underline{x}_k, \underline{x}_j \rangle . \quad (48.53)$$

As shown for the cases  $nx = 2, 3$  above, Eqs.(48.53) can be expressed as a system of equations for each row of the matrix  $A$ , and those systems of equations can be solved to express the  $\alpha_{i|j}$  in terms of the covariances  $\langle \underline{x}_i, \underline{x}_j \rangle$ .

Dividing both sides of Eq.(48.53) by  $\langle \underline{x}_k, \underline{x}_k \rangle$ , we get, for  $i > k$ ,

$$\frac{\partial \underline{x}_i}{\partial \underline{x}_k} = \sum_{j < i} \alpha_{i|j} \frac{\partial \underline{x}_j}{\partial \underline{x}_k} \quad (48.54)$$

## 48.4 Not fully connected LDEN diagrams

When the LDEN diagram is not fully connected, some  $\alpha_{i|j}$  might be zero for  $i > j$ , and the corresponding arrow  $\underline{x}_j \rightarrow \underline{x}_i$  is not drawn. If that is the case, the formulae that we gave above, for the fully connected LDEN diagram, for the UNK-CM solution, still apply, but the formulae that we gave above, for the UNK-G solution, must be modified as follows.

The problem with the previously presented UNK-G solution is that, when we solve for the  $\alpha_{i|j}$  in each row of  $A$ , we are sometimes solving for  $\alpha_{i|j}$  which we know a priori are equal to zero. So basically, we are solving a system of equations with more equations than unknowns, what is called an “overdetermined” system of equations. A simple solution to this quandary is to add to the set of unknown variables  $\alpha_{i|j}$ , a few of the covariances too. That way, we can get a system of equations with the same number of equations as number of unknowns. So which of the covariances should be made into unknowns? A very natural choice is to make the covariance  $\langle \underline{x}_i, \underline{x}_j \rangle$  an unknown if  $\alpha_{i|j} = 0$  for some  $i > j$ . This is what I do in Ref.[77], and it works like a charm. A fully connected LDEN diagram with  $N$  nodes has  $N^2/2 - N/2$  arrows. If  $M$  of those are missing, our final result will be  $M$  constraints among the covariances, and  $N^2/2 - N/2 - M$  equations expressing the non-zero  $\alpha_{i|j}$  in terms of covariances.

## 48.5 LDEN diagram with conditioned nodes

Conditioning on a node  $\underline{x}$  of an LDEN diagram means assuming that  $\underline{x}$  is fixed at a specific value  $x$ . Normally, we assume

$$\langle \underline{\epsilon}_i, \underline{\epsilon}_j \rangle = 0 \quad \text{if } i \neq j \quad (48.55)$$

However, when we condition on some nodes  $\{\underline{x}_i : i \in \mathcal{C}\}$ , the constraint Eq.(48.55) must be modified. Instead, we assume

$$\langle \underline{\epsilon}_i, \underline{\epsilon}_j \rangle = 0 \quad \text{if } i \in \mathcal{C} \text{ or } j \in \mathcal{C}. \quad (48.56)$$

The reason this makes sense is as follows. The  $\underline{\epsilon}_i$  for  $i \in \mathcal{C}$  no longer serve a function because they are futilely pumping noise into a fixed node, so we may set those  $\underline{\epsilon}_i$  to a constant. On the other hand, the  $\underline{\epsilon}_i$  with  $i \notin \mathcal{C}$ , might have become correlated among themselves as a result of the conditioning. For example. we might have conditioned on a collider, and opened an unblocked path between two of those  $\underline{\epsilon}_i$  with  $i \notin \mathcal{C}$ . See Ref.[77] for examples where this occurs.

## 48.6 SCuMpy

Check out my free open source software SCuMpy [77]. SCuMpy ia a Python library for doing both symbolic and numeric calculations for linear Structural Causal Models (SCM) (i.e., LDEN diagrams).

## 48.7 Non-linear DEN diagrams

This chapter is dedicated to linear DEN diagrams. This implicitly assumes that the deterministic nodes  $\underline{x}$ . of the DEN diagram have an interval of real values as their possible states. A trivial but very useful generalization of linear DEN diagrams is to replace Eq.(48.41) for the TPMs of the deterministic nodes of the diagram by

$$P(x_i | x_{<i}, u_i) = \mathbb{1}(x_i = f_i(x_{<i}, u_i)) , \quad (48.57)$$

with structural equations

$$\underline{x}_i = f_i(\underline{x}_{<i}, \underline{u}_i) , \quad (48.58)$$

for  $i = 0, 1, \dots, nx - 1$ . Here the  $f_i$  are possibly non-linear functions that depend on the states  $x_{<i}$  and  $u_i$  of nodes  $\underline{x}_{<i}$  and  $\underline{u}_i$ . If a node  $\underline{x}_i$  has no arrows entering it (i.e., is a root node), then

$$P(x_i | x_{<i}, u_i) = P(x_i) = \delta(x_i, a) \quad (48.59)$$

and

$$\underline{x}_i = a \quad (48.60)$$

for some  $a \in S_{\underline{x}_i}$ .

Besides a linear function, the  $f_i()$  might equal a continuous function such as a polynomial, or a discrete-valued Boolean function such as an OR gate.

# Chapter 49

## Marginalizer Nodes

Suppose we have a bnet node  $\underline{x}$  that has multiple components. For instance, suppose  $\underline{x} = (\underline{x}_1, \underline{x}_2, \underline{x}_3)$ . Then, we can define 3 **marginalizer nodes** with TPMs, shown in blue, as follows

$$P(\underline{\xi}_i = \xi_i | \underline{x} = (x_1, x_2, x_3)) = \delta(\xi_i, x_i) \quad (49.1)$$

for  $\xi_i \in S_{x_i}$  and  $i = 1, 2, 3$ .

Figs.49.1 and 49.2 show 3 different styles for representing marginalizer nodes graphically. In this book, we will use styles (b) or (c). Style (b) is the least ambiguous.

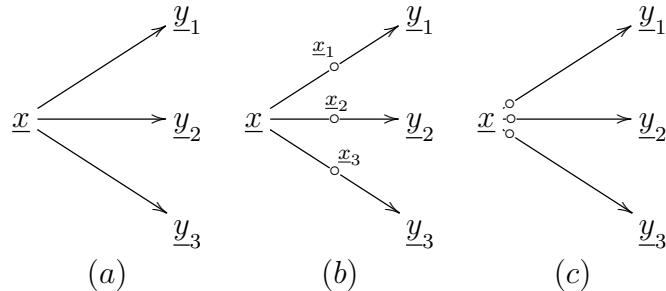


Figure 49.1: 3 styles for representing marginalizer nodes in an arbitrary bnet.

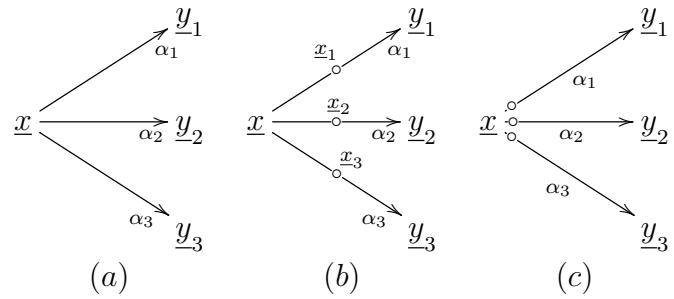


Figure 49.2: 3 styles for representing marginalizer nodes in an LDEN bnet (see Chapter 48).

# Chapter 50

## Markov Blankets

This chapter is based on the Wikipedia article, Ref.[136]. Markov blankets and Markov boundaries of bnets were apparently invented by Judea Pearl. His 1988 book Ref.[50], instead of a research paper, is usually given as the original reference.

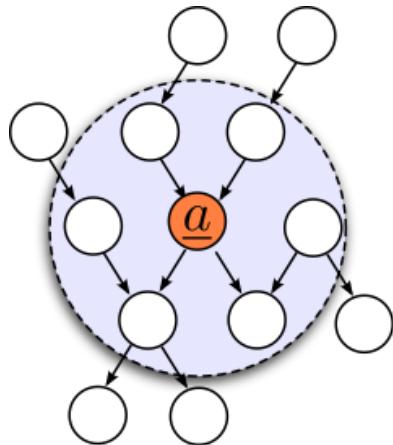


Figure 50.1: In a bnet, the minimal Markov blanket, a.k.a. Markov boundary, of node  $\underline{a}$ .

We will treat vectors of random variables as if they were sets when using the  $\in$ ,  $\subset$  and  $-$  operations. For example, if  $\underline{x} = (\underline{x}_0, \underline{x}_1, \underline{x}_2, \underline{x}_3)$  and  $\underline{b} = (\underline{x}_1, \underline{x}_2)$ , then  $\underline{x}_1 \in \underline{b} \subset \underline{x}$  and  $\underline{x} - \underline{b} = (\underline{x}_0, \underline{x}_3)$ .

Below,  $H(\underline{a} : \underline{b} | \underline{c})$  denotes the conditional mutual information of random variables  $\underline{a}$  and  $\underline{b}$  conditioned on random variable  $\underline{c}$ .  $H(\underline{a} : \underline{b} | \underline{c})$  is used in Shannon Information Theory, where it is defined by

$$H(\underline{a} : \underline{b} | \underline{c}) = \sum_{a,b,c} P(a, b, c) \ln \frac{P(a, b | c)}{P(a | c)P(b | c)}. \quad (50.1)$$

$H(\underline{a} : \underline{b} | \underline{c}) = 0$  iff  $\underline{a}$  and  $\underline{b}$  are independent (uncorrelated) when  $\underline{c}$  is held fixed.

Suppose  $\underline{a} \in \underline{X}$ ,  $\underline{B} \subset \underline{X}$ , but  $\underline{a} \notin \underline{B}$ . Then  $\underline{B}$  is a **Markov blanket** of  $\underline{a}$  if

$$H(\underline{a} : \underline{X} - \underline{a} | \underline{B}) = 0 . \quad (50.2)$$

In other words, one may assume that  $\underline{a}$  depends on  $\underline{B}$  only, and is independent of all random variables in  $\underline{X} - (\underline{a} \cup \underline{B})$ .

The **minimal Markov blanket** is called the **Markov boundary**.

In a bnet, the Markov boundary of a node  $\underline{a}$ , contains:

1. the parents of  $\underline{a}$ ,
2. the children of  $\underline{a}$ ,
3. the parents, other than  $\underline{a}$ , of the children of  $\underline{a}$ .

This is illustrated in Fig.50.1.

From the d-separation theorem (see Chapter 23), we get an intuitive motivation for the definition of Markov boundary. By conditioning on the parents and children of node  $\underline{a}$ , we block almost all, but not all, information from reaching node  $\underline{a}$ . The reason not all info is blocked is that conditioning on a child  $\underline{c}$  of  $\underline{a}$  creates paths from a parent of  $\underline{c}$  to  $\underline{c}$  to  $\underline{a}$ , wherein node  $\underline{c}$  acts as a conditioned collider. To block such paths, we must condition on the parents of  $\underline{c}$  too.

# Chapter 51

## Markov Chain Monte Carlo (MCMC)

Monte Carlo methods are methods for using random number generation to sample probability distributions. The subject of Monte Carlo methods has many branches, as you can see from its Wikipedia category list, Ref.[139]. MCMC (Markov Chain Monte Carlo) is just one of those branches, albeit a major one. Metropolis-Hastings (MH) sampling is a very important MCMC method. Gibbs sampling is a special case of MH sampling. This chapter covers both, MH and Gibbs sampling. It also covers a few other types of sampling.

Throughout this chapter, we use  $P_{\underline{x}} : S_{\underline{x}} \rightarrow [0, 1]$  to denote the target probability distribution that we wish to obtain samples from.

### 51.1 Inverse Cumulative Sampling

For more info about this topic and some original references, see Ref.[123].

This is one of the simplest methods for obtaining samples from a probability distribution  $P_{\underline{x}}$ , but it requires knowledge of the inverse cumulative distribution of  $P_{\underline{x}}$ , which is often not available.

The **cumulative distribution** function is defined by:

$$CUM_{\underline{x}}(x) = P(\underline{x} < x) = \int_{x' < x} dx' P_{\underline{x}}(x') . \quad (51.1)$$

Note that

$$P_{\underline{x}}(x) = \frac{d}{dx} CUM_{\underline{x}}(x) . \quad (51.2)$$

For  $t = 0, 1, \dots, T - 1$ , let

$\underline{u}^{(t)} \in [0, 1]$  = random variable, uniformly distributed over  $[0, 1]$ .

$\vec{\underline{x}}^{(t)} = (\underline{x}^{(t)}[\sigma])_{\sigma=0,1,\dots,nsam(t)-1}$  where  $\underline{x}^{(t)}[\sigma] \in S_{\underline{x}}$  for all  $\sigma$ . Vector of samples collected up to time  $t$ .

The TPMs, printed in blue, for bnet Fig.51.1, are as follows:

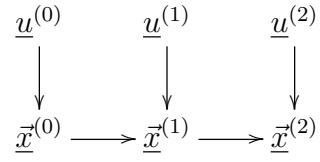


Figure 51.1: bnet for Inverse Cumulative Sampling

$$P(u^{(t)}) = 1 \quad (51.3)$$

$$P(\underline{x}^{(t)} | \underline{x}^{(t-1)}, u^{(t)}) = \delta(\underline{x}^{(t)}, [\underline{x}^{(t-1)}, CUM_{\underline{x}}^{-1}(u^{(t)})]) \quad (51.4)$$

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### Motivation

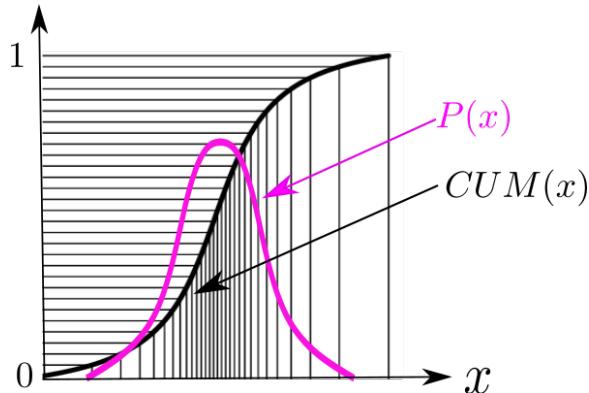


Figure 51.2: Motivation for Inverse Cumulative Sampling.

See Fig.51.2.

Note that if  $\underline{u}$  is uniformly distributed over the interval  $[0, 1]$  and  $a \in [0, 1]$ , then

$$P(\underline{u} < a) = a . \quad (51.5)$$

Thus

$$P(CUM_{\underline{x}}^{-1}(\underline{u}) < x) = P(\underline{u} < CUM_{\underline{x}}(x)) \quad (51.6)$$

$$= CUM_{\underline{x}}(x) . \quad (51.7)$$

Therefore,

$$dP(CUM_{\underline{x}}^{-1}(\underline{u}) < x) = P_{\underline{x}}(x)dx . \quad (51.8)$$

## 51.2 Rejection Sampling

For more info about this topic and some original references, see Ref.[150].

This method samples from a “candidates” probability distribution  $P_c : S_x \rightarrow [0, 1]$ , in cases where sampling directly from the target probability distribution  $P_{\underline{x}} : S_{\underline{x}} \rightarrow [0, 1]$  is not possible.

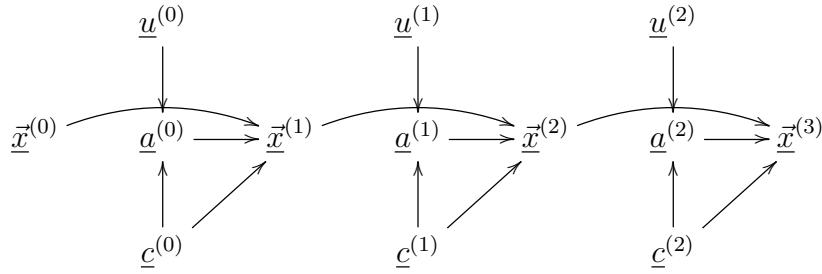


Figure 51.3: bnet for Rejection Sampling

For  $t = 0, 1, \dots, T - 1$ , let

$\underline{u}^{(t)} \in [0, 1] =$  random variable, uniformly distributed over  $[0, 1]$ .

$\underline{a}^{(t)} \in \{0, 1\} =$  accept candidate? (no=0, yes=1)

$\underline{c}^{(t)} \in S_x =$  sample that is a candidate for being accepted

$\bar{\underline{x}}^{(t)} = (\underline{x}^{(t)}[\sigma])_{\sigma=0,1,\dots,nsam(t)-1}$  where  $\underline{x}^{(t)}[\sigma] \in S_x$  for all  $\sigma$ . Vector of samples collected up to time  $t$ .

This algorithm requires a priori definition of a candidate probability distribution  $P_c : S_x \rightarrow \mathbb{R}$  such that

$$P_{\underline{x}}(x) < \beta P_c(x) \quad (51.9)$$

for all  $x \in S_x$ , for some  $\beta \in \mathbb{R}$ .

The TPMs, printed in blue, for bnet Fig.51.3, are as follows:

$$P(\underline{u}^{(t)} = u) = 1 \quad (51.10)$$

$$P(\underline{c}^{(t)} = c) = P_c(c) \quad (51.11)$$

$$P(\underline{a}^{(t)} = a | \underline{c}^{(t)} = c, \underline{u}^{(t)} = u) = \begin{cases} \delta(a, 0) & \text{if } u\beta P_c(c) \geq P_{\underline{x}}(c) \\ \delta(a, 1) & \text{if } u\beta P_c(c) < P_{\underline{x}}(c) \end{cases} \quad (51.12)$$

$$P(\vec{x}^{(t)} | \vec{x}^{(t-1)}, \underline{a}^{(t)} = a, \underline{c}^{(t)} = c) = \begin{cases} \delta(\vec{x}^{(t)}, \vec{x}^{(t-1)}) & \text{if } a = 0 \\ \delta(\vec{x}^{(t)}, [\vec{x}^{(t-1)}, c]) & \text{if } a = 1 \end{cases} \quad (51.13)$$

This last equation is only defined for  $t > 0$ . For  $t = 0$ , the left hand side reduces to  $P(\vec{x}^{(0)})$  which must be specified a priori.

### Motivation

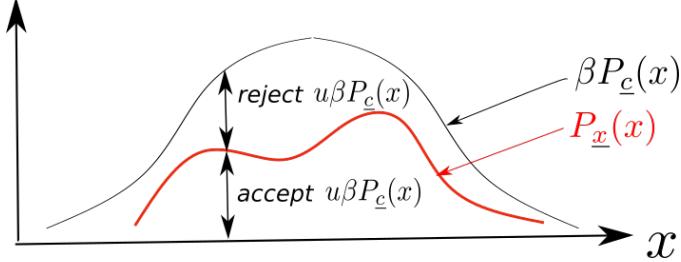


Figure 51.4: Motivation for Rejection Sampling.

See Fig.51.4.

## 51.3 Metropolis-Hastings Sampling

For more info about this topic and some original references, see Refs.[4] and [137].

An advantage of this method is that it can sample unnormalized probability distributions (*constant*) $P_{\underline{x}}$  because it only uses ratios of  $P_{\underline{x}}$  at two different points. Another advantage of this method is that it scales much better than other sampling methods as the number of dimensions of the sampled variable  $\underline{x}$  increases.

This method produces samples that take a finite amount of time to reach steady state. The samples are also theoretically correlated instead of being i.i.d. as one desires. To mitigate for the steady state problem, one discards an initial set of samples (the "burn-in" period). To mitigate for the correlation problem, one calculates the autocorrelation between the samples and keeps only samples separated by a time interval after which the samples cease to be autocorrelated to a good approximation.

For  $t = 0, 1, \dots, T - 1$ , let

$\underline{u}^{(t)} \in [0, 1]$  = random variable, uniformly distributed over  $[0, 1]$ .

$\underline{a}^{(t)} \in \{0, 1\}$  = accept candidate? (no=0, yes=1)

$\underline{c}^{(t)} \in S_{\underline{x}}$  = sample that is a candidate for being accepted

$\underline{m}^{(t)} \in S_{\underline{x}}$  = memory of last accepted sample

$\vec{x}^{(t)} = (\underline{x}^{(t)}[\sigma])_{\sigma=0,1,\dots,n_{sam}(t)-1}$  where  $\underline{x}^{(t)}[\sigma] \in S_{\underline{x}}$  for all  $\sigma$ . Vector of samples collected up to time  $t$ .

A **proposal TPM**  $P_{c|x} : S_{\underline{x}}^2 \rightarrow [0, 1]$  must be specified a priori for this algorithm.

The TPMs, printed in blue, for bnet Fig.51.5, are as follows:

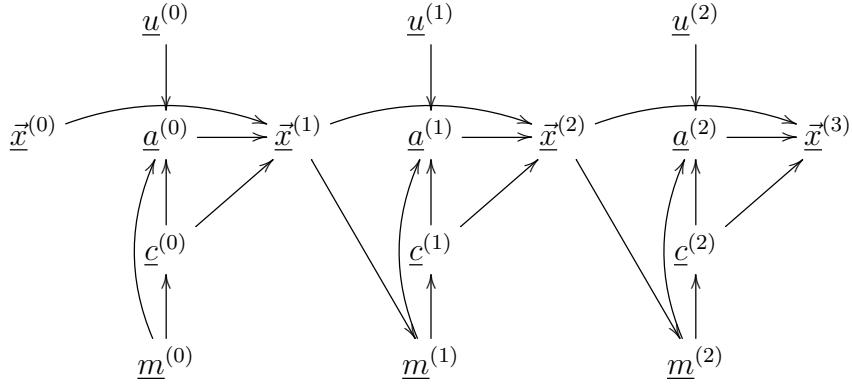


Figure 51.5: bnet for Metropolis-Hastings Sampling

$$P(u^{(t)} = u) = 1 \quad (51.14)$$

$$P(\underline{c}^{(t)} = c | \underline{m}^{(t)} = m) = P_{\underline{c}|\underline{x}}(c|m) \quad (51.15)$$

$$P(\underline{a}^{(t)} = a | \underline{c}^{(t)} = c, \underline{u}^{(t)} = u, \underline{m}^{(t)} = m) = \begin{cases} \delta(a, 0) & \text{if } u \geq \alpha(c|m) \\ \delta(a, 1) & \text{if } u < \alpha(c|m) \end{cases} \quad (51.16)$$

where the **acceptance probability**  $\alpha$  is defined as

$$\alpha(c|m) = \min \left( 1, \frac{P_{\underline{c}|\underline{x}}(m|c) P_{\underline{x}}(c)}{P_{\underline{c}|\underline{x}}(c|m) P_{\underline{x}}(m)} \right) . \quad (51.17)$$

Note that if the proposal distribution is symmetric, then

$$\alpha(c|m) = \min \left( 1, \frac{P_{\underline{x}}(c)}{P_{\underline{x}}(m)} \right) . \quad (51.18)$$

$$P(\vec{x}^{(t)} | \vec{x}^{(t-1)}, \underline{a}^{(t)} = a, \underline{c}^{(t)} = c) = \begin{cases} \delta(\vec{x}^{(t)}, \vec{x}^{(t-1)}) & \text{if } a = 0 \\ \delta(\vec{x}^{(t)}, [\vec{x}^{(t-1)}, c]) & \text{if } a = 1 \end{cases} \quad (51.19)$$

This last equation is only defined for  $t > 0$ . For  $t = 0$ , the left hand side reduces to  $P(\vec{x}^{(0)})$  which must be specified a priori.

$$P(\underline{m}^{(t)} = m | \vec{x}^{(t)}) = \delta(m, \text{last component of } \vec{x}^{(t)}) . \quad (51.20)$$

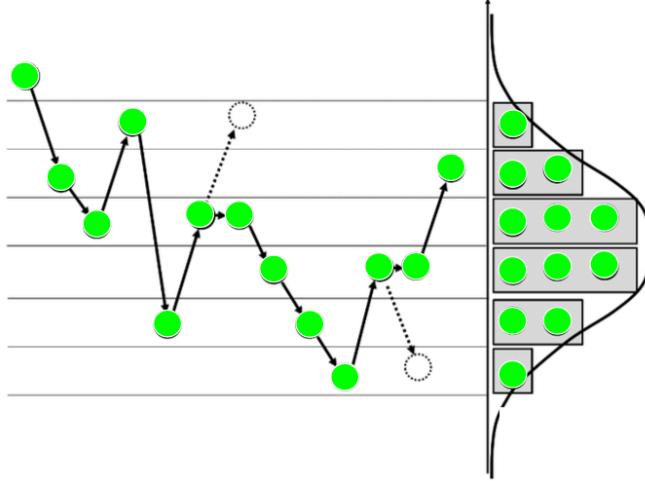


Figure 51.6: Motivation for Metropolis-Hastings Sampling.

This last equation is only defined for  $t > 0$ . For  $t = 0$ , the left hand side reduces to  $P(\underline{m}^{(0)} = m)$  which must be specified a priori.

### Motivation

See Fig.51.6.

Consider a time homogeneous (its TPM is the same for all times) Markov chain with TPM  $P(x'|x) = [T]_{x',x}$ . Its **stationary distribution**, if it exists, is defined as

$$\pi = \lim_{n \rightarrow \infty} T^n \pi_0 . \quad (51.21)$$

Suppose the prob distribution  $P_{\underline{x}}(x)$  that we wish to sample from satisfies

$$P_{\underline{x}}(x) = \pi(x) . \quad (51.22)$$

**Reversibility (detailed balance):** For all  $x, x' \in S_{\underline{x}}$ ,

$$P(x'|x)\pi(x) = P(x|x')\pi(x') . \quad (51.23)$$

Detailed balance is a sufficient (although not necessary) condition for a unique stationary prob distribution  $\pi$  to exist.<sup>1</sup>

Let

$$P(x'|x) = P(\underline{a} = 1|x', x)P_{\underline{c}|x}(x'|x) + \delta(x, x')P(\underline{a} = 0|x) , \quad (51.24)$$

where

$$P(\underline{a} = 0|x) = \sum_{x'} P(\underline{a} = 0|x', x)P_{\underline{c}|x}(x'|x) . \quad (51.25)$$

<sup>1</sup>As explained lucidly in Ref.[4], besides detailed balance, 2 other properties must also be satisfied by the Markov chain, irreducibility and aperiodicity. However, because of how it is constructed, the Metropolis-Hastings algorithm automatically produces a Markov chain that has those 2 properties.

**Claim 81** If

$$P(a = 1|x', x) = \alpha(x'|x) , \quad (51.26)$$

then detailed balance is satisfied.

**proof:** Assume  $x \neq x'$ .

$$P(x'|x)P(x) = P(\underline{a} = 1|x', x)P_{\underline{c}|\underline{x}}(x'|x)P_{\underline{x}}(x) \quad (51.27)$$

$$= \min \left( 1, \frac{P_{\underline{c}|\underline{x}}(x|x')P_{\underline{x}}(x')}{P_{\underline{c}|\underline{x}}(x'|x)P_{\underline{x}}(x)} \right) P_{\underline{c}|\underline{x}}(x'|x)P_{\underline{x}}(x) \quad (51.28)$$

$$= \min (P_{\underline{c}|\underline{x}}(x'|x)P_{\underline{x}}(x), P_{\underline{c}|\underline{x}}(x|x')P_{\underline{x}}(x')) \quad (51.29)$$

$$= P(x|x')P(x') \quad (51.30)$$

QED

## 51.4 Gibbs Sampling

For more info about this topic and some original references, see Ref.[117].

Gibbs sampling is a special case of Metropolis-Hastings sampling. Gibbs sampling is ideally suited for application to a bnet, because it is stated in terms of the conditional prob distributions of  $N$  random variables, and conditional prob distributions are part of the definition of a bnet.

Consider a bnet with nodes  $\underline{x}_0, \underline{x}_1, \dots, \underline{x}_{N-1}$

Identify the random variable  $\underline{x} = (\underline{x}_0, \underline{x}_1, \dots, \underline{x}_{N-1})$  with the random variable  $\underline{x}$  used in Metropolis-Hastings sampling. For Gibbs sampling, we use the following proposal distribution:

$$P_{\underline{c}|\underline{x}}(c|m) = \prod_{j=0}^{N-1} P(c_j | [m_i]_{i \neq j}) . \quad (51.31)$$

Eq.(51.31) can be simplified using Markov Blankets (see Chapter 50) to the following:

$$P_{\underline{c}|\underline{x}}(c|m) = \prod_{j=0}^{N-1} P(c_j | [m_i : \forall i \ni \underline{x}_i \in MB(\underline{x}_j)]) , \quad (51.32)$$

where, for any node  $\underline{a}$ , we denote its Markov blanket by  $MB(\underline{a})$ .

An alternative proposal distribution that leads to much faster convergence is as follows. The idea is to make the components  $c_j^{(t)}$  of candidate sample  $c^{(t)}$  depend on the previous components  $(c_i^{(t)})_{i < j}$ . See the bnet Fig.51.7. The TPM for the nodes of that bnet are

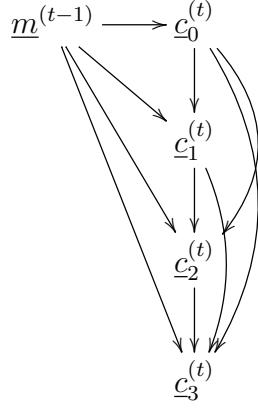


Figure 51.7: In Gibbs sampling, the proposal distribution  $P_{\underline{c}|\underline{x}}$  can be defined by making the components  $c_j^{(t)}$  of candidate sample  $c^{(t)}$  depend on the previous components  $(c_i^{(t)})_{i < j}$ .

$$P(\underline{c}_j^{(t)} = c_j | (\underline{c}_i^{(t)})_{i < j} = (c_i)_{i < j}, \underline{m}^{(t-1)} = m) = P(c_j | (c_i)_{i < j}, (m_i)_{i > j}) \quad (51.33)$$

for  $j = 0, 1, \dots, N - 1$ . This implies

$$P_{\underline{c}|\underline{x}}(\underline{c}^{(t)} = c | \underline{m}^{(t-1)} = m) = \prod_{j=0}^{N-1} P(c_j | (c_i)_{i < j}, (m_i)_{i > j}). \quad (51.34)$$

As before, we can condition only on the Markov blanket of each node  $\underline{x}_j$ .

$$P_{\underline{c}|\underline{x}}(\underline{c}^{(t)} = c | \underline{m}^{(t-1)} = m) = \prod_{j=0}^{N-1} P(c_j | (c_i)_{i < j}, (m_i)_{i > j}, \text{ use only } c_i \text{ and } m_i \ni \underline{x}_i \in MB(\underline{x}_j)). \quad (51.35)$$

## 51.5 Importance Sampling

For more info about this topic and some original references, see Ref.[121].

Suppose random variables  $\underline{x}[\sigma] \in S_{\underline{x}}$  for  $\sigma = 0, 1, \dots, nsam - 1$  are i.i.d. with probability distribution  $P_{\underline{x}}$ . Then

$$E_{\underline{x}}[f(x)] \approx \frac{1}{nsam} \sum_{\sigma=0}^{nsam-1} f(x[\sigma]) \quad (51.36)$$

for any  $f : S_{\underline{x}} \rightarrow \mathbb{R}$ . Sometimes, instead of using i.i.d. samples  $\underline{x}[\sigma] \in S_{\underline{x}}$  where  $\underline{x}[\sigma] \sim P_{\underline{x}}$ , we wish to use i.i.d. samples  $\underline{y}[\sigma] \in S_{\underline{x}}$  where  $\underline{y}[\sigma] \sim P_{\underline{y}}$ .

$$E_{\underline{x}}[f(\underline{x})] = \sum_x P_{\underline{x}}(x) f(x) \quad (51.37)$$

$$= \sum_x P_{\underline{y}}(x) \frac{P_{\underline{x}}(x)}{P_{\underline{y}}(x)} f(x) \quad (51.38)$$

$$= E_{\underline{y}}\left[\frac{P_{\underline{x}}(y)}{P_{\underline{y}}(y)} f(y)\right] \quad (51.39)$$

Sampling from  $P_{\underline{y}}(y)$  instead of  $P_{\underline{x}}(x)$  might reduce (or increase) variance for a particular  $f : S_{\underline{x}} \rightarrow \mathbb{R}$ .

$$Var_{\underline{x}}[f(x)] = E_{\underline{x}}[(f(x))^2] - (E_{\underline{x}}[f(x)])^2 \quad (51.40)$$

$$Var_{\underline{y}}\left[\frac{P_{\underline{x}}(y)}{P_{\underline{y}}(y)} f(y)\right] = E_{\underline{y}}\left[\left(\frac{P_{\underline{x}}(y)}{P_{\underline{y}}(y)} f(y)\right)^2\right] - (E_{\underline{y}}\left[\frac{P_{\underline{x}}(y)}{P_{\underline{y}}(y)} f(y)\right])^2 \quad (51.41)$$

$$= E_{\underline{x}}\left[\frac{P_{\underline{x}}(x)}{P_{\underline{y}}(x)} (f(x))^2\right] - (E_{\underline{x}}[f(x)])^2 \quad (51.42)$$

# Chapter 52

## Markov Chains

A Markov Chain is simply a bnet with the graph structure of a chain. For example, Fig.52.1 shows a chain with  $n = 4$  nodes.

$$\underline{x}_0 \longrightarrow \underline{x}_1 \longrightarrow \underline{x}_2 \longrightarrow \underline{x}_3$$

Figure 52.1: Markov chain with  $n = 4$  nodes.

Because of its graph structure, the TPM of each node only depends on the state of the previous node:

$$P(x_t | (x_a)_{a \neq t}) = P(x_t | x_{t-1}), \quad (52.1)$$

where  $(x_a)_{a \neq t}$  are all the nodes except  $x_t$  itself and  $t = 1, 2, \dots, n - 1$ .

If there exists a single TPM  $P_{\underline{x}_1 | \underline{x}_0}$  such that

$$P(x_t | x_{t-1}) = P_{\underline{x}_1 | \underline{x}_0}(x_t | x_{t-1}) \quad (52.2)$$

for  $t = 1, 2, \dots, n - 1$ , then we say that the Markov chain is **time homogeneous**.

**Claim 82** (*Data Processing Inequality (DPI)*)

Consider a Markov chain  $\underline{x}_0 \rightarrow \underline{x}_1 \cdots \rightarrow \underline{x}_{n-1}$ . Suppose  $0 \leq a < m < b \leq n - 1$ . Then

$$H(\underline{x}_a : \underline{x}_b) \leq \min[H(\underline{x}_a : \underline{x}_m), H(\underline{x}_m : \underline{x}_b)] \quad (52.3)$$

See Ref.[107] for references where the DPI is proven. This inequality confirms our intuitive expectations that the information transmitted (i.e., the mutual information(MI)) from  $\underline{a}$  to  $\underline{b}$  (or vice versa since MI is symmetric) is smaller or equal to the one transmitted from  $\underline{a}$  to  $\underline{m}$  or from  $\underline{m}$  to  $\underline{b}$  because  $\underline{a}$  and  $\underline{b}$  are “farther apart” and “some info can get lost during transmission through the mediator node  $\underline{m}$ ”.

# Chapter 53

## Mediation Analysis

This chapter is mostly based on Refs.[53, 51] by Pearl.

To fully understand this chapter, the reader should first read Chapter 12 where do and imagine operators are defined.

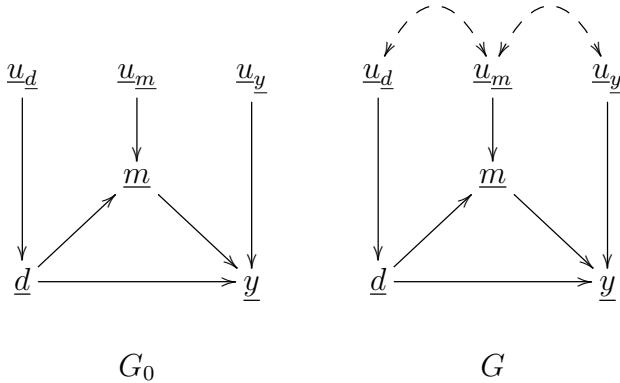


Figure 53.1: DEN bnets  $G_0$  and  $G$  are used to discuss mediation analysis. In graph  $G_0$ , the external variables are independent, whereas in graph  $G$  they are not.

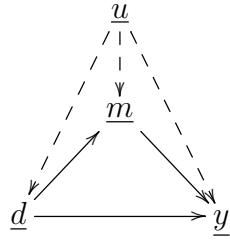
The term “mediation analysis” (MA) refers to the analysis by Pearl of the DEN bnet  $G$  in Fig.53.1. We will discuss MA in terms of DEN bnets, just as Pearl does. However, note that much of what we will say applies also to the general (i.e., not necessarily a DEN) bnet  $G_{gen}$  show in Fig. 53.2.

In the DEN bnet  $G$ , node  $\underline{d}$  influences node  $\underline{y}$  both directly and via the mediator node  $\underline{m}$ . The structural equations for  $G$  are of the form:

$$\underline{d} = \underline{u}_d \quad (53.1a)$$

$$\underline{m} = f_m(\underline{d}, \underline{u}_m) \quad (53.1b)$$

$$\underline{y} = f_y(\underline{d}, \underline{m}, \underline{u}_y). \quad (53.1c)$$



$$G_{gen}$$

Figure 53.2: General bnet used to discuss mediation analysis. Node  $\underline{u}$  is a hidden confounder.

Thus,

$$\underline{y} = f_{\underline{y}}(\underline{u}_d, f_m(\underline{u}_d, \underline{u}_m), \underline{u}_y) . \quad (53.2)$$

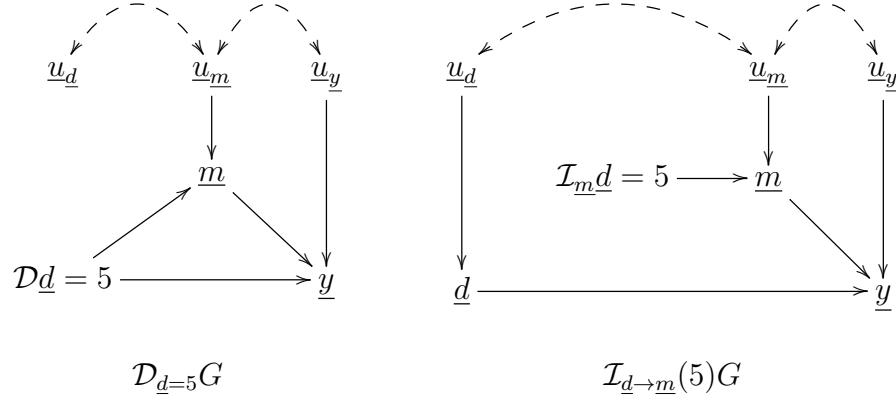


Figure 53.3: Graph  $G$  of Fig.53.1 after applying do operator  $\mathcal{D}_{\underline{d}=5}$  and imagine operator  $\mathcal{I}_{\underline{d} \rightarrow \underline{m}}(5)$ .

If we apply  $\mathcal{D}_{\underline{d}=5}G$  to Eqs.(53.1), we get

$$\underline{d} = 5 \quad (53.3a)$$

$$\underline{m} = f_m(\underline{d}, \underline{u}_m) \quad (53.3b)$$

$$\underline{y} = f_{\underline{y}}(\underline{d}, \underline{m}, \underline{u}_y) . \quad (53.3c)$$

Eqs.53.3 are represented graphically in Fig.53.3. We will often denote the random

variable  $\underline{y}$  in Eqs.(53.3) by the more explicit symbol  $y_{\mathcal{D}_{d=5}G}$ . Pearl often refers to this  $\underline{y}$  by the less explicit symbol  $Y_5$  or  $Y_5(u)$  where  $u = (u_{\underline{m}}, u_{\underline{y}}) = u_{!d}$ .

If we apply  $\mathcal{I}_{d \rightarrow \underline{m}}(5)G$  to Eqs.(53.1), we get

$$\underline{d} = \underline{u}_d \quad (53.4a)$$

$$\underline{m} = f_{\underline{m}}(5, \underline{u}_m) \quad (53.4b)$$

$$\underline{y} = f_{\underline{y}}(\underline{d}, \underline{m}, \underline{u}_y). \quad (53.4c)$$

Eqs.53.4 are represented graphically in Fig.53.3. We will often denote the random variable  $\underline{y}$  in Eqs.(53.4) by the more explicit symbol  $y_{\mathcal{I}_{d \rightarrow \underline{m}}(5)G}$ . Pearl often refers to this  $\underline{y}$  by the less explicit symbol  $Y_5$  or  $Y_5(u)$  where  $u = (u_{\underline{d}}, u_{\underline{m}}, u_{\underline{y}})$ .

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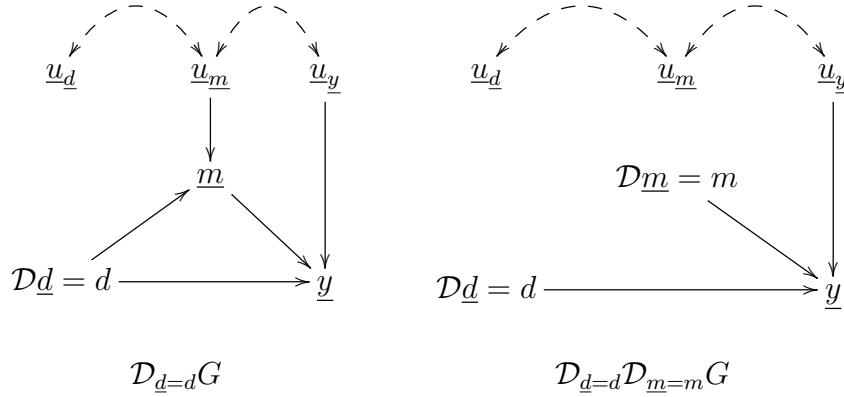


Figure 53.4: Graph  $G$  of Fig.53.1 after applying the do operators  $\mathcal{D}_{\underline{d}=d}$  and  $\mathcal{D}_{\underline{d}=d}\mathcal{D}_{\underline{m}=m}$ .

Define

$$\mathcal{Y}_d = E[y_{\mathcal{D}_{\underline{d}=d}G}] = \sum_y y P(y | \mathcal{D}\underline{d} = d) \quad (53.5)$$

and

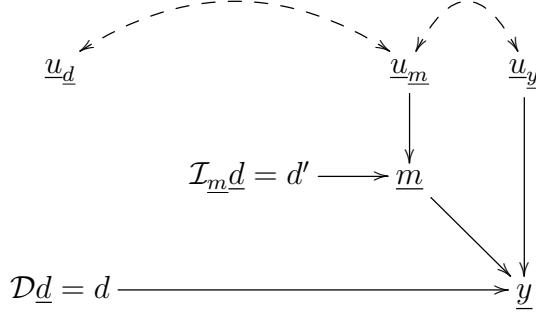
$$\mathcal{Y}_d^m = E[y_{\mathcal{D}_{\underline{d}=d}\mathcal{D}_{\underline{m}=m}G}] = \sum_y y P(y | \mathcal{D}\underline{d} = d, \mathcal{D}\underline{m} = m) \quad (53.6)$$

The two DEN diagrams  $\mathcal{D}_{\underline{d}=d}G$  and  $\mathcal{D}_{\underline{d}=d}\mathcal{D}_{\underline{m}=m}G$  used in the definitions of  $\mathcal{Y}_d$  and  $\mathcal{Y}_d^m$  are given in Fig.53.4.

Now define the Total Effect (TE), and the Controlled Direct Effect (CDE) by

$$TE = \mathcal{Y}_1 - \mathcal{Y}_0 \quad (53.7)$$

$$CDE(m) = \mathcal{Y}_1^m - \mathcal{Y}_0^m \quad (53.8)$$



$$D_{d=d} I_{d \rightarrow y}(d') G$$

Figure 53.5: Graph  $G$  of Fig.53.1 after applying the imagine operator  $\mathcal{I}$  to arrow  $\underline{d} \rightarrow \underline{m}$  and the do operator to node  $\underline{d}$ .

Define

$$\bar{\mathcal{Y}}_d^{d'} = E[y_{D_{d=d} I_{d \rightarrow y}(d') G}] = \sum_y y P(y | D_d = d, I_{\underline{m}} \underline{d} = d') \quad (53.9)$$

Fig.53.5 shows the diagram  $D_{d=d} I_{d \rightarrow y}(d') G$  used in the definition of  $\bar{\mathcal{Y}}_d^{d'}$ .

Note that

$$\bar{\mathcal{Y}}_d^{d'} = \sum_m \mathcal{Y}_d^m P(\underline{m} = m | d') \quad (53.10)$$

if there is no arrow  $\underline{u}_m \rightarrow \underline{m}$ . This expresses  $P(y | D_d = d, I_d = d')$  in terms of  $P(y | D_d = d, D_m = m)$ .

Define

$$\bar{\mathcal{Y}}_d^{d'-} = \bar{\mathcal{Y}}_d^{d'} - \bar{\mathcal{Y}}_d^d \quad (53.11)$$

and

$$\bar{\mathcal{Y}}_{d-}^{d'} = \bar{\mathcal{Y}}_d^{d'} - \bar{\mathcal{Y}}_d^d \quad (53.12)$$

Now define the Natural Direct Effect (NDE), and the Natural Indirect Effect (NIE) by

$$NDE_d^{d'} = \bar{\mathcal{Y}}_d^{d'-} \quad (53.13)$$

$$NIE_d^{d'} = \bar{\mathcal{Y}}_{d-}^{d'} . \quad (53.14)$$

Note that

$$NDE_1^0 - NIE_1^0 = -\bar{\mathcal{Y}}_0^0 + \bar{\mathcal{Y}}_1^1 \quad (53.15)$$

$$= TE . \quad (53.16)$$

### Linear Case

Consider the LDEN of Fig.53.6. One has

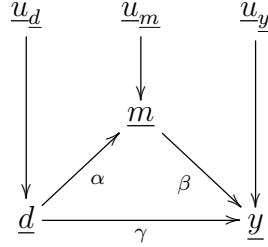


Figure 53.6: LDEN that is used to discuss mediation analysis.

$$\underline{d} = \underline{u}_d \quad (53.17a)$$

$$\underline{m} = \alpha \underline{d} + \underline{u}_m \quad (53.17b)$$

$$\underline{y} = \gamma \underline{d} + \beta \underline{m} + \underline{u}_y . \quad (53.17c)$$

$$\mathcal{Y}_d = (\gamma + \alpha\beta)d \quad (53.18)$$

$$\mathcal{Y}_d^m = \gamma d + \beta m \quad (53.19)$$

$$\bar{\mathcal{Y}}_d^{d'} = \gamma d + \alpha\beta d' \quad (53.20)$$

$$TE = \mathcal{Y}_1 - \mathcal{Y}_0 = \gamma + \alpha\beta \quad (53.21)$$

$$CDE(m) = \mathcal{Y}_1^m - \mathcal{Y}_0^m = \gamma \quad (53.22)$$

$$NDE_1^0 = \bar{\mathcal{Y}}_1^{0-} = \gamma \quad (53.23)$$

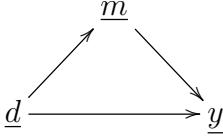
$$NIE_1^0 = \bar{\mathcal{Y}}_{1-}^0 = -\alpha\beta \quad (53.24)$$

As expected,  $NDE_1^0 - NIE_1^0 = TE$ .

$TE$  and the “controlled effect”  $CDE(m)$  contain do operators but no imagine operators so one can do do-intervention experiments to calculate them. On the other hand, the “natural effects”  $NDE_1^0$  and  $NIE_1^0$  contain imagine operators (and therefore counterfactual distributions) so it’s not obvious how to calculate them, or even

whether it is possible to do so. The next claim shows how to calculate  $\bar{\mathcal{Y}}_d^{d'}$  in certain cases. In technical jargon, the claim gives sufficient conditions for  $\mathcal{DI}$ -identifiability of  $\bar{\mathcal{Y}}_d^{d'}$ .  $NDE_1^0$  and  $NIE_1^0$  can be calculated once  $\bar{\mathcal{Y}}_d^{d'}$  is known.

**Claim 83** (*Unconfounded Mediation, from Ref.[53]*)

If  then

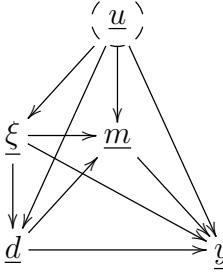
$$P(y|\mathcal{D}\underline{d} = d, \mathcal{I}\underline{m}d = d') = \sum_m P(y|d, m)P(m|d') \quad (53.25)$$

$$\begin{array}{ccc} \mathcal{I}\underline{d} = d' & & \mathcal{I}\underline{d} = d' \longrightarrow \sum m \\ \searrow & & \swarrow \\ \mathcal{D}\underline{d} = d \longrightarrow y & = & \mathcal{D}\underline{d} = d \longrightarrow y \end{array} \quad (53.26)$$

**proof:** See Claim 55.

**QED**

**Claim 84** (*Mediation with universal prior  $\xi$  and universal confounder  $\underline{u}$ , from Ref.[53]*)

If  then

$$P(y|\mathcal{D}\underline{d} = d, \mathcal{I}\underline{m}d = d') = \sum_{\xi} \sum_m P(y|d, m, \xi)P(m|d', \xi)P(\xi) \quad (53.27)$$

$$\begin{array}{ccc} \mathcal{I}\underline{d} = d' & & \mathcal{I}\underline{d} = d' \xrightarrow{\sum \xi} \sum m \\ \searrow & & \swarrow \\ \mathcal{D}\underline{d} = d \longrightarrow y & = & \mathcal{D}\underline{d} = d \longrightarrow y \end{array} \quad (53.28)$$

**proof:** See Claim 56.

**QED**

Actually,

$$\sum_m P(y|d, m)P(m|d') = \sum_{\xi} \sum_m P(y|d, m, \xi)P(m|d', \xi)P(\xi) \quad (53.29)$$

so the adjustment formulae in Claims 83 and 84 are equivalent, but if the available dataset contains info about  $\xi$ , then the adjustment formula that uses that  $\xi$  info should be used, as it will be more sensitive to deviations from the DAG model being hypothesized.

# Chapter 54

## Mendelian Randomization

Mendelian Randomization (MR) is an application of the method of Instrumental Variables (IVs) to genetics. It's considered an "observational study". It's used as a substitute to an RCT (i.e., experimental study), when an RCT can't be done.

IVs are discussed in Chapter 41. Here is a quick review of the essential points of that chapter.

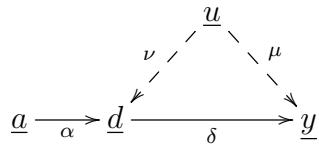


Figure 54.1: MR assumes this bnet

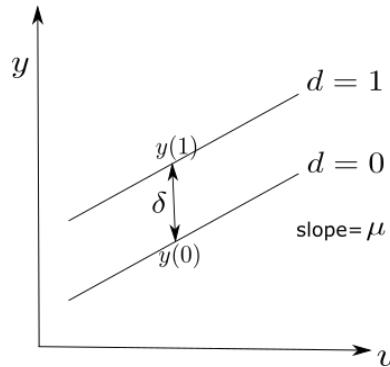


Figure 54.2: Pictorial representation of  $ATE = y(1) - y(0) = \delta$ .

The bnet of Fig.54.1 obeys the following equations:

$$\begin{cases} \underline{y} = \delta \underline{d} + \mu \underline{u} + \underline{u}_y \\ \underline{d} = \alpha \underline{a} + \nu \underline{u} + \underline{u}_d \end{cases} \quad (54.1)$$

where  $\underline{u}_y$  and  $\underline{u}_d$  are external, uncorrelated noises.

If one solves for  $\delta$ , one gets<sup>1</sup>

$$ATE = \delta = \frac{\frac{\partial y}{\partial \underline{a}}}{\frac{\partial \underline{d}}{\partial \underline{a}}} \quad (54.2)$$

This formula for  $\delta$  can be estimated using Linear Regression. See Fig.54.2 for a pictorial representation of  $\delta$ .

---

What these random variables stand for in MR:

$\underline{a}$  : genotype (inherited genetic variant trait). This is the IV.

$\underline{u}$  : hidden variable, "confounders" (good controls)

$\underline{d} \in \{0, 1\}$ : exposure

$\underline{y} \in \{0, 1\}$ : outcome

---

Example

$\underline{a}$  : has genotype that is strongly associated with heavy smokers?

$\underline{u}$  : city dweller?

$\underline{d}$ : smoker?

$\underline{y}$ : died of lung cancer?

---

### Assumptions of MR (should be tested)

- $\underline{a} \rightarrow \underline{d}$ , but no  $\underline{a} \rightarrow \underline{y}$
- no confounder  $\underline{c}$  such that  $\underline{c} \rightarrow \underline{a}, \underline{y}$
- no feedback (a.k.a. reverse causation) arrows  $\underline{y} \rightarrow \underline{a}$ .

Using genotype for  $\underline{a}$  makes these assumptions more likely.

---

<sup>1</sup>As usual in this book, we define  $\frac{\partial \underline{y}}{\partial \underline{x}} = \frac{\langle \underline{x}, \underline{y} \rangle}{\langle \underline{x}, \underline{x} \rangle}$  for any random variables  $\underline{x}, \underline{y}$ .

# Chapter 55

## Message Passing and Bethe Free Energy

This chapter is based on Refs. [83] and [170].

### 55.1 2MRFs

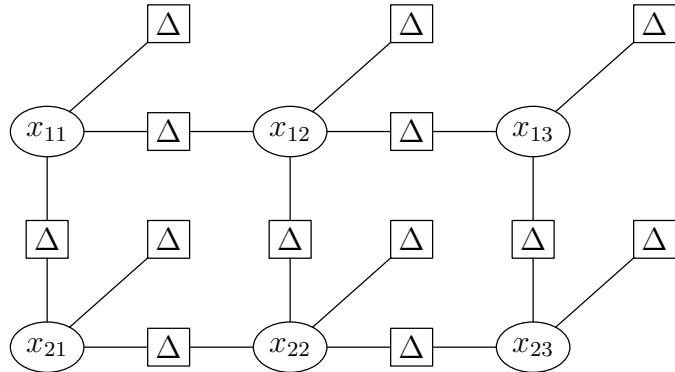


Figure 55.1: Example of factor graph for a 2MRF. In this figure, a boxed  $\Delta$  between variables  $x_i$  and  $x_j$ , denotes the propagator function  $\Delta(x_i, x_j)$ . Also, a boxed  $\Delta$  connected to a single variable  $x_i$ , denotes the function  $\Delta(x_i, k)$ , where  $k$  is a fixed number. If we view this factor graph as a representation of a 3 dimensional device with the leaf nodes  $\Delta$  in the back part and everything else in the front part, then the back part can represent the light inputs from a scene, and the front part can represent the analysis being done with the light inputs.

Factor graphs are discussed in Chapter 27.

A pairwise Markov Random Field (2MRF) is a statistical model whose probability distribution is of the form

$$p(x) = \mathcal{N}(!x) \prod_{i-j} \Delta(x_i, x_j) \quad (55.1)$$

where  $x = (x_1, x_2, \dots, x_n)$ , where  $i - j$  represents the edge that connects nodes  $i$  and  $j$  in an undirected graph  $G$ , and where the product is over all edges of  $G$ .  $p(x)$  can be represented graphically by a factor graph.

Fig.55.1 shows an example of a 2MRF represented as a factor graph.

The **Ising model** is another prototypical example of a 2MRF. Let  $T$  be the temperature of a system,

$$\theta = \frac{1}{T}, \quad (55.2)$$

and  $x = (x_1, x_2, \dots, x_n) \in \{-1, 1\}^{nx}$ . The Ising model is defined for  $J, h(x_i) \in \mathbb{R}$  by

$$\epsilon(x) = -J \sum_{i-j} x_i x_j - \sum_i h(x_i) \quad (55.3)$$

$$P(x) = \frac{e^{\frac{-\epsilon(x)}{T}}}{Z_\theta} \quad (55.4)$$

Note that a bnet can be easily converted to an equivalent 2MRF. You just set  $\Delta(x_i, k) = p(x_i)$  if  $x_i$  is a root node of the bnet, and  $\Delta(x_i, x_j) = p(x_i|x_j)$  if  $x_i$  isn't a root node. One must then choose the arrow directions of the bnet. A natural choice is to choose the bnet arrows so that they all point from an  $x_i$  to a  $\Delta$ .

In what follows, we shall use **messages (a.k.a. cavity fields)**  $m_{a \Rightarrow i}(x_i)$ , Note that in our notation for messages, the letter  $i$  appears twice, and both occurrences are next to each other. This is always the case in our notation for messages.

Henceforth, we will refer to the functions  $\Delta(x_i, x_j)$  as **propagators**, to make contact with Physics.

Henceforth, we shall use the notation  $\partial i$  to denote all nodes  $j$  that are neighbors of node  $i$ .  $\partial i$  is called the **neighborhood or boundary** of  $i$ .

## 55.2 Message Passing Intuition

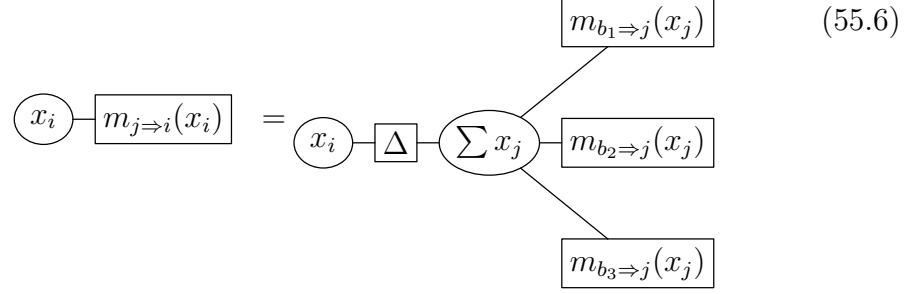
Next we present some results that will be derived later in the chapter, but which we will first present now without proof, and explain how they make sense intuitively. Assume that the functions  $\Delta(x_i, x_j)$  are known for all edges  $i - j$ , and that the full probability distribution  $p(x)$  of the model is given by Eq.(55.1).

1. Calculate message  $m_{j \Rightarrow i}(x_i)$  in terms of messages leaving  $x_j$ . This is called the **message updating rule**.

One has that

$$m_{j \Rightarrow i}(x_i) = \sum_{x_j} \Delta(x_i, x_j) \prod_{b \in \partial j \setminus i} m_{b \Rightarrow j}(x_j) \quad (55.5)$$

This can be represented graphically by

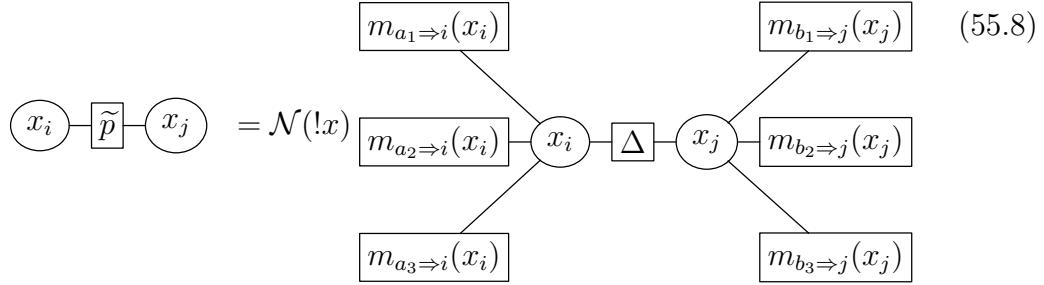


2. Calculate  $\tilde{p}(x_i, x_j)$  for any edge  $i - j$  in terms of messages entering  $x_i$  and leaving  $x_j$

One has that

$$\tilde{p}(x_i, x_j) = \mathcal{N}(!x) \Delta(x_i, x_j) \prod_{a \in \partial i \setminus j} m_{a \Rightarrow i}(x_i) \prod_{b \in \partial j \setminus i} m_{b \Rightarrow j}(x_j) \tag{55.7}$$

This can be represented graphically by

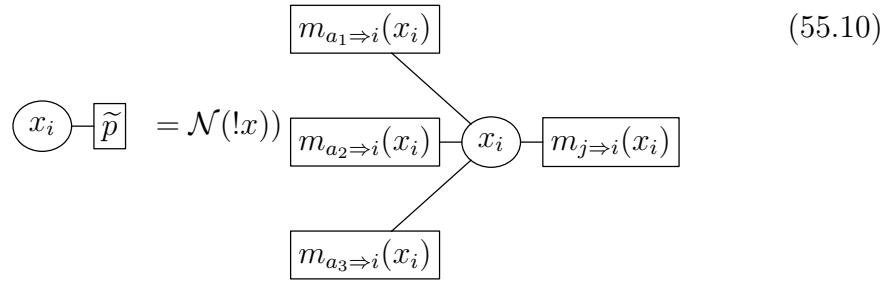


3. Calculate  $\tilde{p}(x_i)$  in terms of messages entering  $x_i$

One has that

$$\tilde{p}(x_i) = \sum_{x_j} \tilde{p}(x_i, x_j) \tag{55.9}$$

This can be represented graphically by

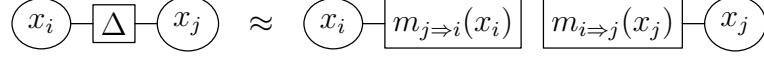


Why it works?

Suppose we approximate the propagator  $\Delta(x_i, x_j)$  by

$$\Delta(x_i, x_j) \approx m_{j \Rightarrow i}(x_i)m_{i \Rightarrow j}(x_j) \quad (55.11)$$

This can be represented graphically by



$$(x_i) \rightarrow \Delta \rightarrow (x_j) \approx (x_i) \rightarrow [m_{j \Rightarrow i}(x_i)] \quad [m_{i \Rightarrow j}(x_j)] \rightarrow (x_j) \quad (55.12)$$

Then the results 1,2,3 above can be justified as follows.

1.

$$m_{j \Rightarrow i}(x_i) \approx \sum_{x_j} \underbrace{m_{j \Rightarrow i}(x_i)m_{i \Rightarrow j}(x_j)}_{\Delta(x_i, x_j)} \prod_{b \in \partial j \setminus i} m_{b \Rightarrow j}(x_j) \quad (55.13)$$

$$= m_{j \Rightarrow i}(x_i) \sum_{x_j} \prod_{b \in \partial j} m_{b \Rightarrow j}(x_j) \quad (55.14)$$

$$= \mathcal{N}(!x)m_{j \Rightarrow i}(x_i) \quad (55.15)$$

2.

$$\tilde{p}(x_i, x_j) = \sum_{x \setminus x_i, x_j} \tilde{p}(x) \quad (55.16)$$

$$\approx \mathcal{N}(!x) \sum_{x \setminus x_i, x_j} \prod_{i=j} \underbrace{m_{j \Rightarrow i}(x_i)m_{i \Rightarrow j}(x_j)}_{\Delta(x_i, x_j)} \quad (55.17)$$

$$\approx \mathcal{N}(!x)\Delta(x_i, x_j) \prod_{a \in \partial i \setminus j} m_{a \Rightarrow i}(x_i) \prod_{b \in \partial j \setminus i} m_{b \Rightarrow j}(x_j) \quad (55.18)$$

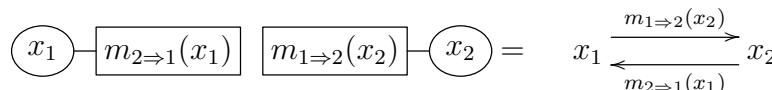
3.

$$\tilde{p}(x_i) = \sum_{x_j} \tilde{p}(x_i, x_j) \quad (55.19)$$

$$\approx \mathcal{N}(!x) \sum_{x_j} \underbrace{m_{j \Rightarrow i}(x_i)m_{i \Rightarrow j}(x_j)}_{\Delta(x_i, x_j)} \prod_{a \in \partial i \setminus j} m_{a \Rightarrow i}(x_i) \prod_{b \in \partial j \setminus i} m_{b \Rightarrow j}(x_j) \quad (55.20)$$

$$\approx \mathcal{N}(!x) \prod_{a \in \partial i} m_{a \Rightarrow i}(x_i) \quad (55.21)$$

Henceforth, we will occasionally use the following more compressed notation for the factor graph of a 2MRF. Instead of using circles for variables and squares for functions, we will use arrows pointing from  $x_1$  to  $x_2$  and vice versa.



$$(x_1) \rightarrow [m_{2 \Rightarrow 1}(x_1)] \rightarrow (x_2) = x_1 \xrightarrow[m_{2 \Rightarrow 1}(x_1)]{m_{1 \Rightarrow 2}(x_2)} x_2 \quad (55.22)$$

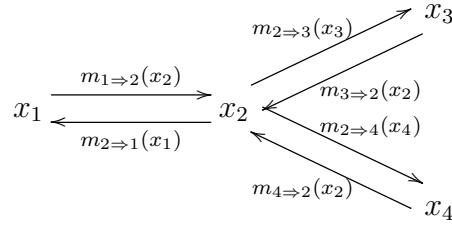


Figure 55.2: Example of compressed factor graph for a 2MRF.

Next, we give an example of how to use message passing to find the marginal  $\tilde{p}(x_i)$  for any node  $x_i$ . Refer to Fig55.2 for this example.

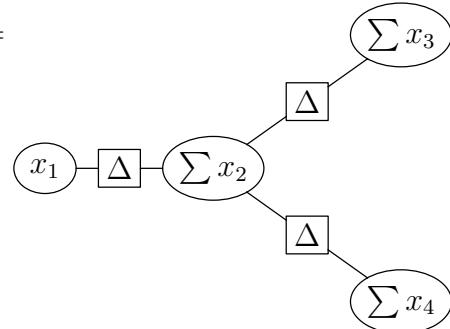
Using the message updating rule successively, we get

$$\tilde{p}(x_1) = \mathcal{N}(!x)m_{2\Rightarrow 1}(x_1) \quad (55.23)$$

$$= \mathcal{N}(!x) \sum_{x_2} \Delta(x_1, x_2) m_{3\Rightarrow 2}(x_2) m_{4\Rightarrow 2}(x_2) \quad (55.24)$$

$$= \mathcal{N}(!x) \sum_{x_2} \Delta(x_1, x_2) \sum_{x_3} \Delta(x_2, x_3) \sum_{x_4} \Delta(x_2, x_4) \quad (55.25)$$

$$= \quad \sum_{x_3} \quad (55.26)$$



This algorithm is guaranteed to work only for trees. In practice, one starts by calculating the messages pointing up from the leaf nodes of the tree. Then one calculates the messages pointing up from the parents of the leaf nodes of the tree. And so forth until one calculates all the messages pointing up from the leaf nodes to the root node of the tree. Then one goes in the opposite direction, first calculating messages pointing down from the root node to its children, from the children of the root node to their children. And so forth. By the end, all upward and downward pointing messages have been calculated. From this,  $\tilde{p}(x_i)$  for all  $i$  can be calculated.  $\tilde{p}(x_i)$  is the product of all messages pointing into  $x_i$ .

### 55.3 $-\ln Z_\theta$ = Free Energy (FE)

Suppose  $\theta, \epsilon(x) \in \mathbb{R}^{ni}$  and  $x = (x_1, x_2, \dots, x_{nx}) \in \mathbb{R}^{nx}$ . Define the **partition function**  $Z_\theta$  by

$$Z_\theta = \sum_x e^{-\theta^T \epsilon(x)} \quad (55.27)$$

and the probability distribution  $P(x|h)$  by

$$\underbrace{P(x|\theta)}_{e^{LL_\theta(x)}} = \exp(-\theta^T \epsilon(x) - \ln Z_\theta) \quad (55.28)$$

$$= \frac{e^{-\theta^T \epsilon(x)}}{Z} \quad (55.29)$$

$\epsilon(x)$  is called a **sufficient statistic** for  $\underline{x}$  because  $P(x|\theta)$  is a functional (i.e., a function of a function) of  $\epsilon(x)$ . Note that by taking first and higher order derivatives of  $\ln Z_\theta$  with respect to  $\theta_i$ , we can calculate the statistics of  $\epsilon_i(x)$ .

$$-\partial_{\theta_i} \ln Z_\theta = \frac{1}{Z_\theta} \sum_x \epsilon_i(x) e^{-\theta^T \epsilon(x)} \quad (55.30)$$

$$= E_{\underline{x}|\theta}[\epsilon_i(\underline{x})] = \langle \epsilon_i \rangle \quad (55.31)$$

$$\partial_{\theta_j} \partial_{\theta_i} \ln Z_\theta = \partial_{\theta_j} \frac{1}{Z_\theta} \sum_x -\epsilon_i(x) e^{-\theta^T \epsilon(x)} \quad (55.32)$$

$$= \left\{ \begin{array}{l} \frac{1}{Z_\theta} \sum_x \epsilon_j(x) \epsilon_i(x) e^{-\theta^T \epsilon(x)} \\ + \frac{-1}{Z_\theta^2} \left[ \sum_x -\epsilon_j(x) e^{-\theta^T \epsilon(x)} \right] \left[ \sum_x -\epsilon_i(x) e^{-\theta^T \epsilon(x)} \right] \end{array} \right\} \quad (55.33)$$

$$= \langle \epsilon_j \epsilon_i \rangle - \langle \epsilon_j \rangle \langle \epsilon_i \rangle \quad (55.34)$$

$$= \langle \epsilon_j, \epsilon_i \rangle \quad (55.35)$$

Define the log likelihood  $LL_\theta(x)$  by

$$LL_\theta(x) = -\theta^T \epsilon(x) - \ln Z_\theta \quad (55.36)$$

and the **entropy**  $S$  by <sup>1</sup>

$$S = - \sum_x P(x|\theta) LL_\theta(x) \quad (55.37)$$

$$= - \sum_x P(x|\theta) \ln P(x|\theta) \quad (55.38)$$

---

<sup>1</sup>In Thermodynamics, the entropy is denoted by the letter  $S$ . In Shannon Information Theory, and elsewhere in this book, it is denoted by the letter  $H$ .

Define the **internal energy**  $U$  by

$$U = \sum_x P(x|\theta) \epsilon_\theta(x) \quad (55.39)$$

$$-S = -\theta^T U - \ln Z_\theta \quad (55.40)$$

$$\partial_{U_i} S = \theta_i \quad (55.41)$$

$S$  is concave.  $S$  and  $-\ln Z_\theta = F/T$  are concave dual functions.<sup>2</sup>

### Relationship to Thermodynamics

In Thermodynamics,  $U$  is the internal energy and  $S$  is the entropy of a system at **temperature**  $T$ . Define  $\theta \in \mathbb{R}$  to be the inverse temperature

$$\theta = \frac{1}{T} \quad (55.42)$$

Define the **free energy**  $F$  by<sup>a</sup>

$$F = -T \ln Z_\theta \quad (55.43)$$

$$= -T \ln \sum_x e^{-\frac{\epsilon(x)}{T}} \quad (55.44)$$

Then

$$U - TS = F \quad (55.45)$$

So the free energy equals the internal energy minus the energy held in disordered form.

---

<sup>a</sup>In this chapter, we call  $-\ln Z$  the free energy too.

## 55.4 $-\ln Z_{\theta^*} = \text{Minimum FE}$

Suppose we consider  $P(x|\theta)$  for two different parameter  $\theta$  and  $\tilde{\theta}$ . Define

$$p(x) = P(x|\theta), \quad \tilde{p}(x) = P(x|\tilde{\theta}) \quad (55.46)$$

The Kullback-Leibler divergence is always non-negative so:

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<sup>2</sup>Concave dual functions are discussed in Chapter 99

$$0 \leq D_{KL}(\tilde{p}(x) \| p(x)) \quad (55.47)$$

$$= \sum_x \tilde{p}(x) \ln \frac{\tilde{p}(x)}{p(x)} \quad (55.48)$$

$$= -\tilde{S} - \sum_x \tilde{p}(x) [-(\theta)^T \epsilon(x) - \ln Z_\theta] \quad (55.49)$$

$$= -\tilde{S} + (\theta)^T \tilde{U} + \ln Z_\theta \quad (\tilde{S}, \tilde{U} \text{ correspond to parameter } \tilde{\theta}) \quad (55.50)$$

$$-\ln Z_\theta \leq -\tilde{S} + (\theta)^T \tilde{U} \quad (55.51)$$

Let

$$\theta^* = \operatorname{argmin}_\theta \left[ -\tilde{S} + (\theta)^T \tilde{U} \right] \quad (55.52)$$

Henceforth, we will refer to  $-\ln Z_\theta$  as the **FE (Free Energy)** and to  $-\ln Z_{\theta^*}$  as the **minimum FE**.

Relationship to convex/concave dual functions<sup>3</sup>

$$\tilde{S} = \min_\theta \left[ (\theta)^T \tilde{U} + \ln Z_\theta \right] \quad (55.53)$$

$$-\ln Z_\theta = \min_{\tilde{U}} \left[ (\theta)^T \tilde{U} - \tilde{S} \right] \quad (55.54)$$

$\tilde{S}$  and  $-\ln Z_\theta$  are concave dual functions.

$$-\ln Z_{\theta^*} = (\theta^*)^T \tilde{U} - \tilde{S} \quad (55.55)$$

## 55.5 $-\ln Z_\theta^{tree} = \text{Tree FE (a.k.a. Bethe FE)}$

$\tilde{p}(x)$  is said to satisfy **Mean Field Approximation (MFA)** or **independent variables approximation (IVA)** if its variables  $x_i$  are independently distributed:

$$\tilde{p}^{ind}(x) = \prod_k \tilde{p}(x_k) \quad (55.56)$$

In the MFA, the entropy is

---

<sup>3</sup>Convex/concave dual functions are discussed in Chapter 99

$$\tilde{S}^{ind} = - \sum_x \tilde{p}(x) \ln \prod_i \tilde{p}(x_i) \quad (55.57)$$

$$= - \sum_{x_i} \tilde{p}(x_i) \ln \tilde{p}(x_i) \quad (55.58)$$

$$= \sum_i \tilde{H}(\underline{x}_i) \quad (55.59)$$

A slightly more complicated case than the MFA is when  $\tilde{p}(x)$  is defined on a tree graph  $G^{tree}$  with edges  $i - j$ . In such a case, it will take just a few examples of trees  $G^{tree}$  to convince the reader that in general, for any tree  $G^{tree}$ ,  $\tilde{p}(x)$  must have the following form:

$$\tilde{p}^{tree}(x) = \tilde{p}^{ind}(x) \prod_{i-j} \frac{\tilde{p}(x_i, x_j)}{\tilde{p}(x_i)\tilde{p}(x_j)} \quad (55.60)$$

Hence,

$$\tilde{S}^{tree} = - \sum_i \sum_{x_i} \tilde{p}^{tree}(x_i) \ln \tilde{p}^{tree}(x_i) \quad (55.61)$$

$$= \sum_i \tilde{H}(\underline{x}_i) - \sum_{i-j} \sum_{x_i, x_j} \tilde{p}(x_i, x_j) \ln \frac{\tilde{p}(x_i, x_j)}{\tilde{p}(x_i)\tilde{p}(x_j)} \quad (55.62)$$

$$= \sum_i \tilde{H}(\underline{x}_i) - \sum_{i-j} \tilde{H}(\underline{x}_i : \underline{x}_j) \quad (55.63)$$

Note that  $\tilde{S}^{tree}$  can be written in terms of the joint entropy  $\tilde{H}(\underline{x}_i, \underline{x}_j)$  instead of the mutual entropy  $\tilde{H}(\underline{x}_i : \underline{x}_j)$ .

$$\tilde{S}^{tree} = - \sum_i (d_i - 1) \tilde{H}(\underline{x}_i) + \sum_{i-j} \tilde{H}(\underline{x}_i, \underline{x}_j) \quad (55.64)$$

where  $d_i$  is the number of neighbors of node  $i$ .

The following approximation is often called the **Bethe approximation**

$$-\ln Z_{\theta^*} \approx -\ln Z_{\theta^*}^{tree} \quad (55.65)$$

## 55.6 $-\ln Z_{\theta^*}^{tree}$ = Tree Minimum FE, and message passing

In this section, we will evaluate  $-\ln Z_{\theta^*}^{tree}$  exactly using a message passing ansatz (an ansatz is an initial guess).

If we replace  $\tilde{S}$  by  $\tilde{S}^{tree}$  in Eq.(55.55), we get

$$-\ln Z_{\theta^*}^{tree} = \min_{\tilde{U}} \left[ (\theta)^T \tilde{U} - \tilde{S}^{tree} \right] \quad (55.66)$$

But note that

$$(\theta)^T \tilde{U} = \sum_i \theta_i \sum_x \tilde{p}(x) \epsilon_i(x) \quad (55.67)$$

$$= \sum_x \tilde{p}(x) \underbrace{\sum_i \theta_i \epsilon_i(x)}_{\text{call } \Theta(x)} \quad (55.68)$$

so Eq.(55.66) becomes

$$-\ln Z_{\theta^*}^{tree} = \min_{\tilde{p}} \left[ \sum_x \tilde{p}(x) \Theta(x) - \sum_i \tilde{H}(\underline{x}_i) + \sum_{i-j} \tilde{H}(\underline{x}_i : \underline{x}_j) \right] \quad (55.69)$$

subject to  $\sum_x \tilde{p}(x) = 1$  and  $\tilde{p}(x) \geq 0$  for all  $x$ .

**Claim 85**  $-\ln Z_{\theta^*}^{tree}$  is achieved if

$$\tilde{p}(x) = \mathcal{N}(!x) e^{-\Theta(x)} \quad (55.70)$$

$$\Theta(x) = \sum_i \Theta(x_i) + \sum_{i-j} \Theta(x_i, x_j) \quad (55.71)$$

(This form for  $\tilde{p}(x)$  and  $\Theta(x)$  agrees with Eq.(55.60))

$$m_{t \Rightarrow s}(x_s) = e^{\lambda_{t \Rightarrow s}(x_s)} \quad (55.72)$$

$$\tilde{p}(x_i) = \mathcal{N}(!x) e^{-\Theta(x_i)} \prod_{a \in \partial i} m_{a \Rightarrow i}(x_i) \quad (55.73)$$

$$\tilde{p}(x_i, x_j) = \mathcal{N}(!x) e^{-\Theta(x_i, x_j) - \Theta(x_i) - \Theta(x_j)} \left[ \prod_{a \in \partial i \setminus j} m_{a \Rightarrow i}(x_i) \right] \left[ \prod_{b \in \partial j \setminus i} m_{b \Rightarrow j}(x_j) \right] \quad (55.74)$$

**proof:**

We want to minimize the following Lagrangian with respect to variations  $\delta \tilde{p}(x_i)$  of  $\tilde{p}(x)$ , for each  $i$ .

$$\mathcal{L} = \left\{ \begin{array}{l} \sum_x \tilde{p}(x) \Theta(x) \\ + \sum_i (1 - d_i) \sum_{x_i} \tilde{p}(x_i) \ln \tilde{p}(x_i) \\ + \sum_{i-j} \sum_{x_i, x_j} \tilde{p}(x_i, x_j) \ln \tilde{p}(x_i, x_j) \\ + \lambda [\sum_x \tilde{p}(x) - 1] \end{array} \right\} \quad (55.75)$$

The term proportional to the Lagrange multiplier  $\lambda$  enforces the constraint  $\sum_x \tilde{p}(x) = 1$ . Note that in general,

$$\delta \tilde{p}(x) = \sum_i \delta \tilde{p}(x_i) \quad (55.76)$$

so if we only vary  $\tilde{p}(x_i)$ ,

$$\delta F(\tilde{p}(x)) = \frac{\partial F(\tilde{p}(x))}{\partial \tilde{p}(x)} \delta \tilde{p}(x) \quad (55.77)$$

$$= \frac{\partial F(\tilde{p}(x))}{\partial \tilde{p}(x)} \delta \tilde{p}(x_i) \quad (55.78)$$

for any well behaved function  $F : \mathbb{R} \rightarrow \mathbb{R}$ . Hence

$$\delta \mathcal{L} = \sum_x \delta \tilde{p}(x_i) \left\{ \begin{array}{l} \Theta(x) \\ + \sum_i (1 - d_i) [1 + \ln \tilde{p}(x_i)] \\ + \sum_{i-j} [1 + \ln \tilde{p}(x_i, x_j)] \\ + \lambda \end{array} \right\} \quad (55.79)$$

for any variation  $\delta \tilde{p}(x_i)$ . Setting the coefficient of  $\delta \tilde{p}(x_i)$  to zero now yields

$$0 = \left\{ \begin{array}{l} \Theta(x) \\ + \sum_i [1 + \ln \tilde{p}(x_i)] \\ + \sum_{i-j} \left[ 1 + \ln \frac{\tilde{p}(x_i, x_j)}{\tilde{p}(x_i) \tilde{p}(x_j)} \right] \\ + \lambda \end{array} \right\} \quad (55.80)$$

for each  $i$ . If we now substitute the equations that are hypotheses to this claim, we get

$$0 = \left\{ \begin{array}{l} \Theta(x) \\ - \sum_i \Theta(x_i) \\ - \sum_{i-j} \Theta(x_i, x_j) \end{array} \right\} \quad (55.81)$$

$$0 = \left\{ \begin{array}{l} + \sum_i \ln \prod_{a \in \partial i} m_{a \Rightarrow i}(x_i) \\ + \sum_{i-j} \ln \frac{[\prod_{a \in \partial i \setminus j} m_{a \Rightarrow i}(x_i)] [\prod_{b \in \partial j \setminus i} m_{b \Rightarrow j}(x_j)]}{\prod_{a \in \partial i} m_{a \Rightarrow i}(x_i) \prod_{b \in \partial j} m_{b \Rightarrow j}(x_j)} \\ + \lambda \end{array} \right\} \quad (55.82)$$

$$= \left\{ \begin{array}{l} \sum_i \sum_{a \in \partial i} \lambda_{a \Rightarrow i}(x_i) \\ - \sum_{i-j} [\lambda_{j \Rightarrow i}(x_i) + \lambda_{i \Rightarrow j}(x_j)] \\ + \lambda \end{array} \right\} \quad (55.83)$$

$$= \lambda \quad (55.84)$$

So the hypotheses to this claim indeed do satisfy  $\delta \mathcal{L} = 0$  for all variations  $\delta \tilde{p}(x_i)$ , for each  $i$ , with Lagrange multiplier  $\lambda = 0$ .

**QED**

# Chapter 56

## Message Passing, Pearl's theory

This chapter is mostly based on chapter 4 of Ref.[50] by Pearl. Refs.[91], and [42] were also helpful in writing this chapter.

In his book Ref.[50], Pearl explains two types of Message Passing (i.e., distributed computing in a bnet). In Chapter 4, he discusses one type of MP which he calls Belief Propagation (BP) or Belief Updating. In Chapter 5, he introduces a second type of MP which he calls Belief Revision, but which I prefer to call Explanation Optimization (EO). This chapter will be devoted to BP only.

BP was first proposed for bnets in 1982 Ref.[49] by Judea Pearl to simplify the exact evaluation of the probability of one node conditioned on other nodes of a bnet (exact inference). It gives exact results for trees and polytrees (i.e., bnets with a single connected component and no loops). For bnets with loops, it gives approximate results (loopy belief propagation), and it has been generalized to the junction tree algorithm (see Chapter 43) which can do exact inference for general bnets with loops. The basic idea behind the junction tree algorithm is to eliminate loops by clustering them into single nodes.

### 56.1 Distributed Soldier Counting

Consider a group of soldiers marching single file. Fig.56.1 shows several methods by which a member of the group can obtain a count of the soldiers without breaking the line to do global operations. This can be done in a distributed fashion, with every soldier doing only local operations (i.e., each soldier can only send messages to either the soldier in front or the one in back). Such distributed soldier counting is a rudimentary type of BP. In the next section, we will generalize this BP for soldiers to BP for a Markov chain.

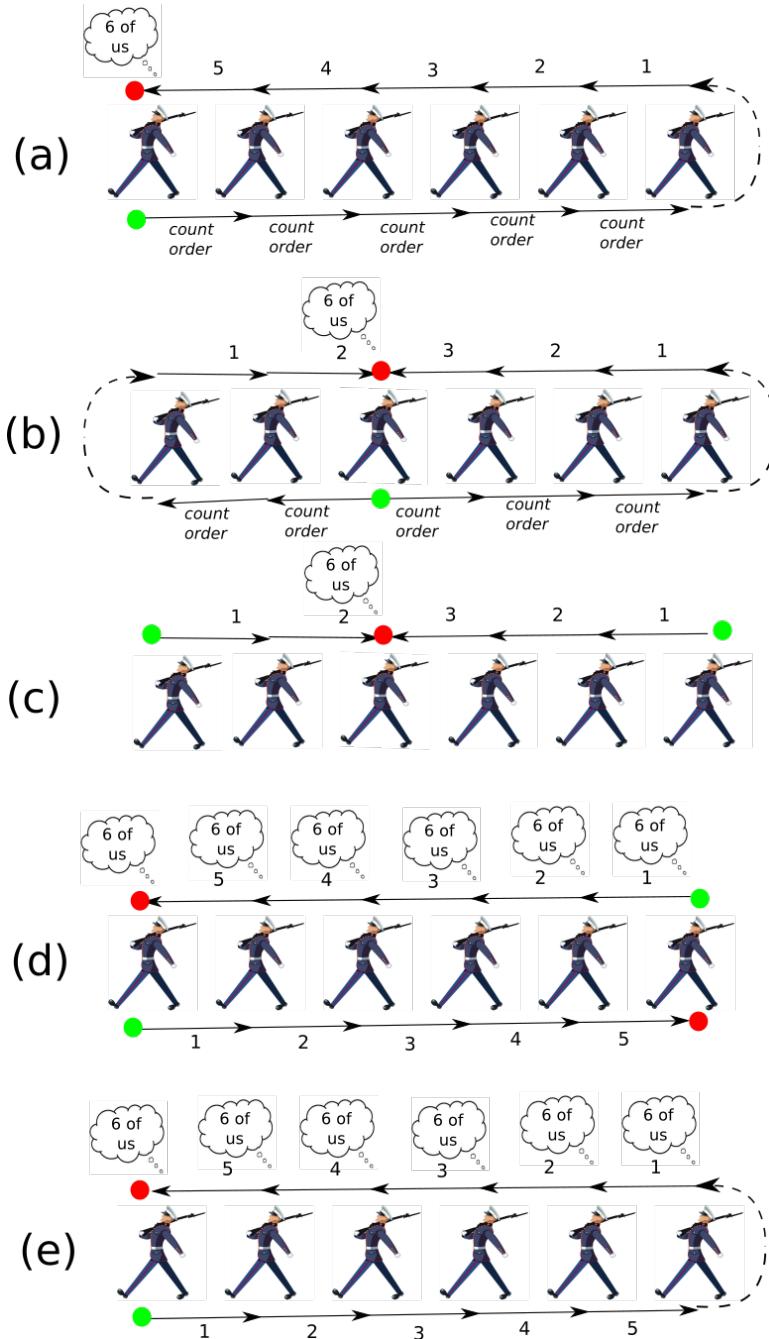


Figure 56.1: Distributed soldier counting (This example comes from Chapter 4 of Ref.[50]). Green dots indicate the beginning and red dots the end of a count. Only first soldier can calculate total count in (a). Only third soldier can calculate total count in (b,c). All soldiers can calculate the total count in (d,e). One starting point in (a,b,e). Two ends as starting points in (c,d).

## 56.2 Spring Systems

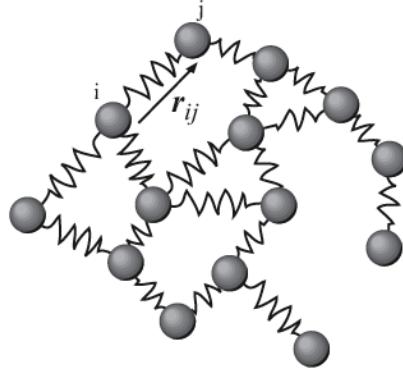


Figure 56.2: Spring system. Point masses connected by springs.

See Ref.[155] for an introduction to spring systems. Ideal springs between the point mass nodes would not be sufficient. One would have to add damping to the springs so as to reach an equilibrium. Time dependent forces (loads) pointing into or out of the page, applied to the point masses, would generate signals that would propagate like BP messages.

## 56.3 BP for Markov Chains

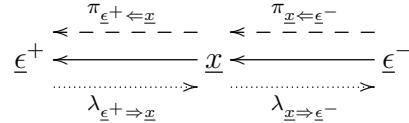


Figure 56.3: 3 node Markov chain  $\underline{\epsilon}^+ \leftarrow \underline{x} \leftarrow \underline{\epsilon}^-$ . The  $\pi$  messages (probability functions) travel downstream (i.e., they carry info in the direction of the graph arrows, towards the future) and are indicated by a dashed arrow or by a left double arrow  $\Leftarrow$ . The  $\lambda$  messages (likelihood functions) travel upstream (i.e., they carry info opposite to direction of the graph arrows, towards the past) and are indicated by a dotted arrow or by a right double arrow  $\Rightarrow$ .  $\underline{\epsilon}^+$  stands for future evidence and  $\underline{\epsilon}^-$  for past evidence.

Consider the 3 node Markov chain  $\underline{\epsilon}^+ \leftarrow \underline{x} \leftarrow \underline{\epsilon}^-$  shown in Fig.56.3. Define<sup>1</sup>

---

<sup>1</sup>The pattern behind these definitions, in case it eludes you, is as follows: the  $\pi$ 's always carry

$$\pi_{\underline{\epsilon}^+ \leftarrow \underline{x}}(x) = P(x|\epsilon^-) \text{ (past of } \underline{x}) \quad (56.1)$$

$$\lambda_{\underline{\epsilon}^+ \Rightarrow \underline{x}}(x) = P(\epsilon^+|x) \text{ (future of } \underline{x}) \quad (56.2)$$

$$\pi_{\underline{x} \leftarrow \underline{\epsilon}^-}(\epsilon^-) = P(\epsilon^-) = \delta(\epsilon^-, \epsilon_0^-) \text{ (past of } \underline{\epsilon}^-) \quad (56.3)$$

$$\lambda_{\underline{x} \Rightarrow \underline{\epsilon}^-}(\epsilon^-) = P(\epsilon^+|\epsilon^-) \text{ (future of } \underline{\epsilon}^-) . \quad (56.4)$$

Furthermore, define the Belief BEL in  $x$  to be

$$BEL_{\underline{x}}(x) = P(x|\epsilon) , \quad (56.5)$$

where

$$\underline{\epsilon} = \underline{\epsilon}^+ \cup \underline{\epsilon}^- . \quad (56.6)$$

It follows that

$$BEL_{\underline{x}}(x) = P(x|\epsilon^+, \epsilon^-) = \quad (56.7)$$

$$= \mathcal{N}(!x)P(\epsilon^+, x, \epsilon^-) \quad (56.8)$$

$$= \mathcal{N}(!x)P(\epsilon^+|x)P(x|\epsilon^-) \quad (56.9)$$

$$= \mathcal{N}(!x)\lambda_{\underline{\epsilon}^+ \Rightarrow \underline{x}}(x)\pi_{\underline{\epsilon}^+ \leftarrow \underline{x}}(x) . \quad (56.10)$$

Note that Bayes rule would affirm that<sup>2</sup>

$$P(x|\epsilon^+) = \mathcal{N}(!x) \underbrace{P(\epsilon^+|x)}_{\lambda_{\underline{\epsilon}^+ \Rightarrow \underline{x}}(x)} P(x) . \quad (56.11)$$

Thus, Eq.(56.10) is like a 2-sided Janus Bayes rule.

Note that the  $\pi$  messages and  $\lambda$  messages propagate independently of each other, via the TPM  $P(x|\epsilon^-)$ :

$$\underbrace{\pi_{\underline{\epsilon}^+ \leftarrow \underline{x}}(x)}_{P(x|\epsilon_0^-)} = \sum_{\epsilon^-} P(x|\epsilon^-) \underbrace{\pi_{\underline{x} \leftarrow \underline{\epsilon}^-}(\epsilon^-)}_{\delta(\epsilon^-, \epsilon_0^-)} \quad (56.12a)$$

$$\underbrace{\lambda_{\underline{x} \Rightarrow \underline{\epsilon}^-}(\epsilon^-)}_{P(\epsilon^+|\epsilon^-)} = \sum_x P(x|\epsilon^-) \underbrace{\lambda_{\underline{\epsilon}^+ \Rightarrow \underline{x}}(x)}_{P(\epsilon^+|x)} \quad (56.12b)$$

---

information about the past and the  $\lambda$ 's about the future. But the past or future of what? Of the argument of the function. Out of the two random variables in the subscript of the function, the one on the right hand side of the subscript, the one which is adjacent but beneath the argument, is always the argument.

<sup>2</sup>As usual in this book,  $\mathcal{N}(!x)$  means a constant that is independent of  $x$ .

Eqs.(56.12) suggest that we define an edge bnet for the  $\pi$  and  $\lambda$  messages (these messages live in the edges between the nodes  $\underline{\epsilon}^+, \underline{x}, \underline{\epsilon}^-$ ). Such an edge bnet, shown in Fig.56.4, is complementary to bnet for the nodes themselves. We will call it the **BP 2-track bnet** for the bnet Fig.56.3, because it has two “tracks”, one for  $\pi$  messages and another for  $\lambda$  ones. The TPMs, printed in blue, for bnet Fig.56.4, are as follows:

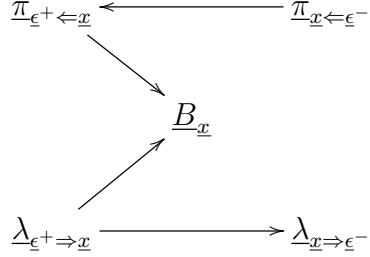


Figure 56.4: BP 2-track bnet for the bnet Fig.56.3.

$$P(\pi_{\underline{x} \leftarrow \underline{\epsilon}^-}) = \prod_{\epsilon^-} \mathbb{1}(\pi_{\underline{x} \leftarrow \underline{\epsilon}^-}(\epsilon^-) = P(\epsilon^-)) \quad (56.13)$$

$$P(\pi_{\underline{\epsilon}^+ \leftarrow \underline{x}} | \pi_{\underline{x} \leftarrow \underline{\epsilon}^-}) = \prod_x \mathbb{1} \left( \pi_{\underline{\epsilon}^+ \leftarrow \underline{x}}(x) = \sum_{\epsilon^-} P(x|\epsilon^-) \pi_{\underline{x} \leftarrow \underline{\epsilon}^-}(\epsilon^-) \right) \quad (56.14)$$

$$P(B_{\underline{x}} | \pi_{\underline{\epsilon}^+ \leftarrow \underline{x}}, \lambda_{\underline{\epsilon}^+ \Rightarrow \underline{x}}) = \prod_x \mathbb{1}(B_{\underline{x}}(x) = BEL_{\underline{x}}(x)) \quad (56.15)$$

$$P(\lambda_{\underline{\epsilon}^+ \Rightarrow \underline{x}}) = \prod_x \mathbb{1}(\lambda_{\underline{\epsilon}^+ \Rightarrow \underline{x}}(x) = P(\epsilon^+|x)) \quad (56.16)$$

$$P(\lambda_{\underline{x} \Rightarrow \underline{\epsilon}^-} | \lambda_{\underline{\epsilon}^+ \Rightarrow \underline{x}}) = \prod_{\epsilon^-} \mathbb{1} \left( \lambda_{\underline{x} \Rightarrow \underline{\epsilon}^-}(\epsilon^-) = \sum_x P(x|\epsilon^-) \lambda_{\underline{\epsilon}^+ \Rightarrow \underline{x}}(x) \right) \quad (56.17)$$

---

So far in this section, we have considered Markov chains with 3 nodes. Before concluding our discussion of BP for Markov chains, let us consider BP for a slightly longer chain. Let us consider the 5 node Markov chain  $\underline{\epsilon}^+ \leftarrow \underline{b} \leftarrow \underline{x} \leftarrow \underline{a} \leftarrow \underline{\epsilon}^-$  shown

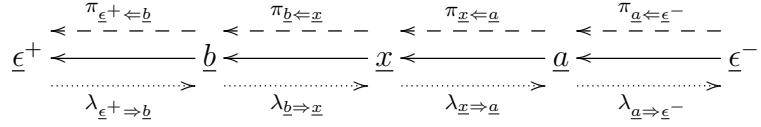


Figure 56.5: 5 node Markov chain

in Fig.56.5. We have already dealt with the end nodes of a Markov chain in the 3 node Markov chain example above, so in the 5 node case, let us focus on the internal (i.e., not at an end) node  $\underline{x}$  and its neighbors  $\underline{a}$  and  $\underline{b}$ . Define

$$\pi_{\underline{b} \leftarrow \underline{x}}(x) = P(x|\epsilon^-) \text{ (past of } \underline{x}) , \quad (56.18)$$

$$\lambda_{\underline{b} \Rightarrow \underline{x}}(x) = P(\epsilon^+|x) \text{ (future of } \underline{x}) , \quad (56.19)$$

$$\pi_{\underline{x} \leftarrow \underline{a}}(a) = P(a|\epsilon^-) \text{ (past of } \underline{a}) \quad (56.20)$$

and

$$\lambda_{\underline{x} \Rightarrow \underline{a}}(a) = P(\epsilon^+|a) \text{ (future of } \underline{a}) . \quad (56.21)$$

Define the Belief BEL in  $x$  to be

$$BEL_{\underline{x}}(x) = P(x|\epsilon) , \quad (56.22)$$

where

$$\epsilon = \underline{\epsilon}^+ \cup \underline{\epsilon}^- . \quad (56.23)$$

Then

$$BEL_{\underline{x}}(x) = \mathcal{N}(!x)P(\epsilon^+|x)P(x|\epsilon^-) \quad (56.24)$$

$$= \mathcal{N}(!x)\lambda_{\underline{b} \Rightarrow \underline{x}}(x)\pi_{\underline{b} \leftarrow \underline{x}}(x) . \quad (56.25)$$

In analogy with the case of BP for a 3 node Markov chain, we can define the bnet Fig.56.6, which we refer to as the **BP 2-track bnet** for Fig.56.5. The TPMs, printed in blue, for bnet Fig.56.6, are as follows:

$$P(\pi_{\underline{b} \leftarrow \underline{x}} | \pi_{\underline{x} \leftarrow \underline{a}}) = \prod_x \mathbb{1} \left( \pi_{\underline{b} \leftarrow \underline{x}}(x) = \sum_a P(x|a)\pi_{\underline{x} \leftarrow \underline{a}}(a) \right) \quad (56.26)$$

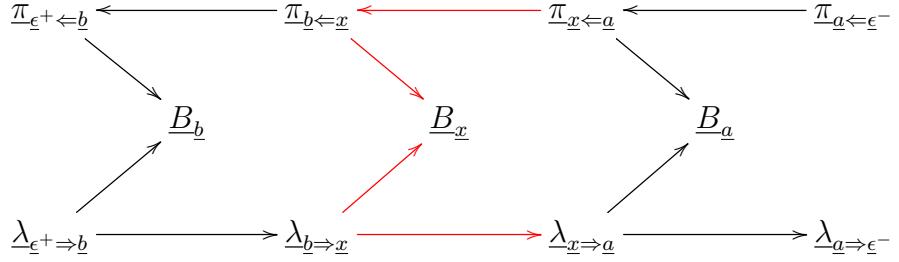


Figure 56.6: BP 2-track bnet for the bnet Fig.56.5.

$$P(B_{\underline{x}} | \pi_{\underline{b} \leftarrow \underline{x}}, \lambda_{\underline{b} \Rightarrow \underline{x}}) = \prod_x \mathbb{1}(B_{\underline{x}}(x) = BEL_{\underline{x}}(x)) \quad (56.27)$$

$$P(\lambda_{\underline{x} \Rightarrow \underline{a}} | \lambda_{\underline{b} \Rightarrow \underline{x}}) = \prod_a \mathbb{1}\left(\lambda_{\underline{x} \Rightarrow \underline{a}}(a) = \sum_x P(x|a) \lambda_{\underline{b} \Rightarrow \underline{x}}(x)\right) \quad (56.28)$$

Let us represent the Markov chain of Fig.56.5 by  $\underline{x}_{nx-1} \leftarrow \dots \leftarrow \underline{x}_2 \leftarrow \underline{x}_1 \leftarrow \underline{x}_0$  where  $nx = 5$ . For any node  $\underline{x}_i$  with parent  $\underline{p}_{\underline{x}_i} = \underline{x}_{i-1}$  and child  $\underline{c}_{\underline{x}_i} = \underline{x}_{i+1}$ , define the **memory matrix**  $\mathcal{M}_{\underline{x}_i}$  for node  $\underline{x}_i$  as

$$\mathcal{M}_{\underline{x}_i} = [\mathcal{M}_{\underline{x}_i}^+, \mathcal{M}_{\underline{x}_i}^-], \quad (56.29)$$

where  $+$  =future,  $-$  =past, and

$$\mathcal{M}_{\underline{x}_i}^+ = \begin{bmatrix} \pi_{\underline{c}_{\underline{x}_i} \leftarrow \underline{x}_i}(\cdot) \\ \lambda_{\underline{c}_{\underline{x}_i} \Rightarrow \underline{x}_i}(\cdot) \end{bmatrix}, \quad \mathcal{M}_{\underline{x}_i}^- = \begin{bmatrix} \pi_{\underline{x}_i \leftarrow \underline{p}_{\underline{x}_i}}(\cdot) \\ \lambda_{\underline{x}_i \Rightarrow \underline{p}_{\underline{x}_i}}(\cdot) \end{bmatrix}. \quad (56.30)$$

Note that

$$\mathcal{M}_{\underline{x}_i}^- = \mathcal{M}_{\underline{p}_{\underline{x}_i}}^+ \quad (56.31)$$

for all nodes  $\underline{x}_i$ . We will refer to Eqs.(56.31) as the **memory overlap conditions**.

We will also use a permuted version of the memory matrix

$$\mathcal{M}'_{\underline{x}_i} = [\mathcal{M}_{\underline{x}_i}^{OUT}, \mathcal{M}_{\underline{x}_i}^{IN}], \quad (56.32)$$

where

$$\mathcal{M}_{\underline{x}_i}^{OUT} = \begin{bmatrix} \pi_{\underline{c}_{\underline{x}_i} \leftarrow \underline{x}_i}(\cdot) \\ \lambda_{\underline{x}_i \Rightarrow \underline{p}_{\underline{x}_i}}(\cdot) \end{bmatrix}, \quad \mathcal{M}_{\underline{x}_i}^{IN} = \begin{bmatrix} \pi_{\underline{x}_i \leftarrow \underline{p}_{\underline{x}_i}}(\cdot) \\ \lambda_{\underline{c}_{\underline{x}_i} \Rightarrow \underline{x}_i}(\cdot) \end{bmatrix}. \quad (56.33)$$

Unfortunately, 2-track bnets cannot be generalized in any obvious way from Markov chains to more complicated DAGs. An alternative to 2-track bnets that still

$$\underline{\mathcal{M}}_{\epsilon^+} \longleftarrow \underline{\mathcal{M}}_b \longleftarrow \underline{\mathcal{M}}_x \longleftarrow \underline{\mathcal{M}}_a \longleftarrow \underline{\mathcal{M}}_{\epsilon^-}$$

Figure 56.7: BP Memory Bnet for the bnet Fig.56.5.

carries message info in its nodes, are memory bnets. An **BP memory bnet** is a bnet which takes each node of an original bnet and adds a local memory to it. More specifically, it keeps that DAG but replaces each node  $\underline{x}_i$  by a memory  $\underline{\mathcal{M}}_{\underline{x}_i}$ . Fig.56.7 shows the memory bnet for the bnet Fig.56.5. The TPM, printed in blue, for the node  $\underline{\mathcal{M}}_x$  of the memory bnet Fig.56.7, is as follows

$$P(\underline{\mathcal{M}}_{\underline{x}_i} | \underline{\mathcal{M}}_{n \in nb(\underline{x}_i)}) = AB , \quad (56.34)$$

where

$$A = \mathbb{1}(\underline{\mathcal{M}}_{\underline{x}_i}^- = \underline{\mathcal{M}}_{\underline{px}_i}^+) , \quad (56.35)$$

and

$$B = \mathbb{1}(\underline{\mathcal{M}}_{\underline{x}_i}^{OUT} = \mathcal{C}(\underline{\mathcal{M}}_{\underline{x}_i}^{IN})) . \quad (56.36)$$

The function  $\mathcal{C}$ , which we will call the **BP local computation**, maps  $\underline{\mathcal{M}}_{\underline{x}_i}^{IN}$  into  $\underline{\mathcal{M}}_{\underline{x}_i}^{OUT}$ . More explicitly,  $\mathcal{C}$  is defined so that

$$B = \underbrace{P(\pi_{\underline{b} \leftarrow \underline{x}} | \pi_{\underline{x} \leftarrow \underline{a}})}_{B_\pi} \underbrace{P(\lambda_{\underline{x} \Rightarrow \underline{a}} | \lambda_{\underline{b} \Rightarrow \underline{x}})}_{B_\lambda} , \quad (56.37)$$

where  $B_\pi$  and  $B_\lambda$  are given by Eqs.(56.26) and (56.28), respectively.

The BP memory bnet Fig. 56.7 is a deterministic bnet. A deterministic bnet is basically just a coupled system of equations (CSE) for some unknowns  $x_i$ . A CSE per se does not include with it a method for solving for the  $x_i$ . Such methods are not unique. For example, for the distributed soldier counting problem, the various methods that we described for counting soldiers are just different methods for solving the same CSE. One can describe a method for solving a CSE using a dynamical bnet.<sup>3</sup> To solve the CSE represented by the memory bnet Fig.56.7, we will use the dynamical bnet Fig.56.8. Henceforth, we will refer to Fig.56.8 as an **BP dynamical bnet** for Fig.56.7.

Next, we will explain the meaning of Fig.56.8. Fig.56.8 is a step by step recipe (i.e., algorithm) for solving a CSE, where the unknowns are memory matrices. Each step encoded in Fig.56.8 corresponds to a specific message sending event, where the messages are sent along the edges of the Markov chain Fig.56.5. These message

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<sup>3</sup>The term dynamical bnet was used in Chapter 25 to mean a time inhomogeneous Markov chain, but here we are stretching its meaning to include Markov chains that aren't time inhomogeneous.

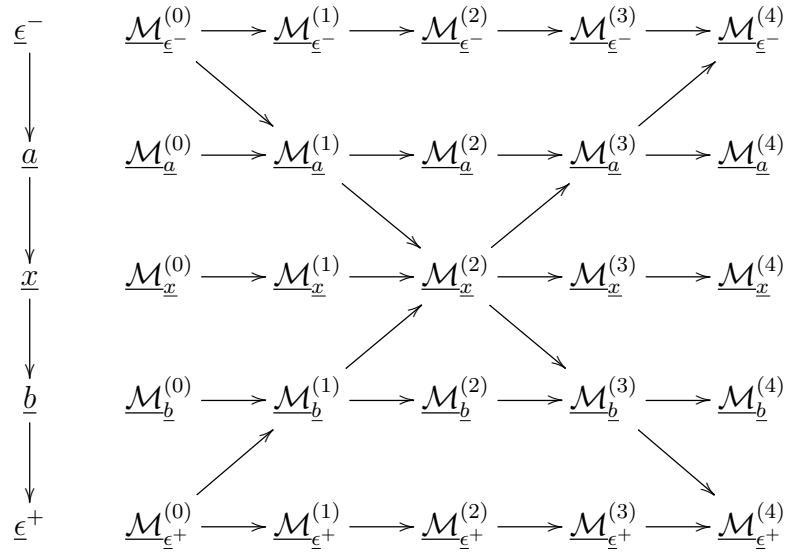


Figure 56.8: BP dynamical bnet for the bnet Fig.56.7.

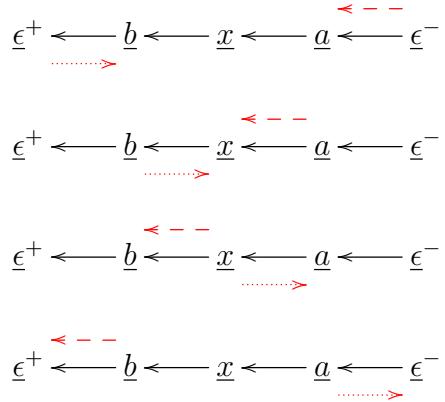


Figure 56.9: Steps encoded in the bnet Fig.56.8. Note the similarity of this figure to Fig.56.1 (d) for soldier counting.

sending events are portrayed in chronological order in Fig.56.9. In that figure,  $\pi$  messages are indicated by dashed red arrows, and  $\lambda$  messages by dotted red arrows. These steps, or message sending events, lead to an updating of the memory matrices that we are solving for. Each step propagates information between the memory nodes. In the usual Pearl BP algo, the evidence nodes initiate the BP chain of message passing events. These events continue until the memory matrices reach an equilibrium and the CSE is solved.

To use bnet Fig.56.8, we need to specify the **initial conditions** (i.e., the value

of  $\mathcal{M}_{\underline{x}_i}^{(0)}$  for all  $i$ ). For that, one can use

$$\pi_{\underline{px}_0 \leftarrow x_0}^{(0)} = P(x_0) , \quad (56.38)$$

$$\lambda_{\underline{cx}_i \Rightarrow \underline{x}_{nx-1}}^{(0)}(x_{nx-1}) = \delta(x_{nx-1}, x'_{nx-1}) . \quad (56.39)$$

All other  $\mathcal{M}_{\underline{x}_i}^{(0)}$  entries for all  $i$  can be set to 1.

The TPMs, printed in blue, for bnet Fig.56.8, are as follows.

$$P(\mathcal{M}_{\underline{x}_i}^{(t)} | \mathcal{M}_{\underline{n} \in nb(\underline{x}_i)}^{(t-1)}, \mathcal{M}_{\underline{x}_i}^{(t-1)}) = AB , \quad (56.40)$$

where

$$A = \begin{cases} \mathbb{1}(\mathcal{M}_{\underline{x}_i}^{(t)-} = \mathcal{M}_{\underline{px}_i}^{(t-1)+}) & \text{if input from } \underline{px}_i \\ \mathbb{1}(\mathcal{M}_{\underline{x}_i}^{(t)+} = \mathcal{M}_{\underline{cx}_i}^{(t-1)-}) & \text{if input from } \underline{cx}_i \end{cases} , \quad (56.41)$$

and

$$B = \mathbb{1}(\mathcal{M}_{\underline{x}_i}^{(t)OUT} = \mathcal{C}(\mathcal{M}_{\underline{x}_i}^{(t)IN})) . \quad (56.42)$$

The function  $\mathcal{C}$ , which we will call the **BP local computation**, maps  $\mathcal{M}_{\underline{x}_i}^{(t)IN}$  into  $\mathcal{M}_{\underline{x}_i}^{(t)OUT}$ . More explicitly,  $\mathcal{C}$  is defined so that

$$B = B_\pi B_\lambda \quad (56.43)$$

where

$$B_\pi = \prod_x \mathbb{1} \left( \underbrace{\pi_{\underline{b} \leftarrow \underline{x}}^{(t)}(x)}_{OUT} = \sum_a P(x|a) \underbrace{\pi_{\underline{x} \leftarrow \underline{a}}^{(t)}(a)}_{IN} \right) \quad (56.44)$$

and

$$B_\lambda = \prod_a \mathbb{1} \left( \underbrace{\lambda_{\underline{x} \Rightarrow \underline{a}}^{(t)}(a)}_{OUT} = \sum_x P(x|a) \underbrace{\lambda_{\underline{b} \Rightarrow \underline{x}}^{(t)}(x)}_{IN} \right) . \quad (56.45)$$

The basic idea behind Eq.(56.42), which we will call the **memory updating equation**, is simple: the memory overlap conditions translate the information from time  $t - 1$  to  $t$ , and then the local computation translates  $IN$  to  $OUT$  at fixed time  $t$ .

## 56.4 BP Algorithm for Polytrees

Consider Fig.56.10, which illustrates a bnet node  $\underline{x}$  receiving and sending messages to its neighbors. The  $\pi$  messages (probability functions) travel downstream (i.e., they carry info in the direction of the graph arrows, towards the future) and are indicated by a dashed arrow or by a left double arrow  $\Leftarrow$ . The  $\lambda$  messages (likelihood functions) travel upstream (i.e., they carry info opposite to direction of the graph arrows, towards the past) and are indicated by a dotted arrow or by a right double arrow  $\Rightarrow$ .

Note that argument  $arg$  of the  $\pi(arg)$  and  $\lambda(arg)$  functions is always the same as the letter in the subscript that is closest to the argument.

Note that in Fig.56.10, we indicate messages that travel "downstream" (resp., "upstream"), by arrows with dashed (resp., dotted) lines as shafts. Mnemonic: think of the shaft as a velocity vector field for the message. You travel faster when you swim downstream as opposed to upstream.

$pa(\underline{x})$  = parents of node  $\underline{x}$

$ch(\underline{x})$  = children of node  $\underline{x}$

$nb(\underline{x}) = pa(\underline{x}) \cup ch(\underline{x})$  = neighbors of node  $\underline{x}$

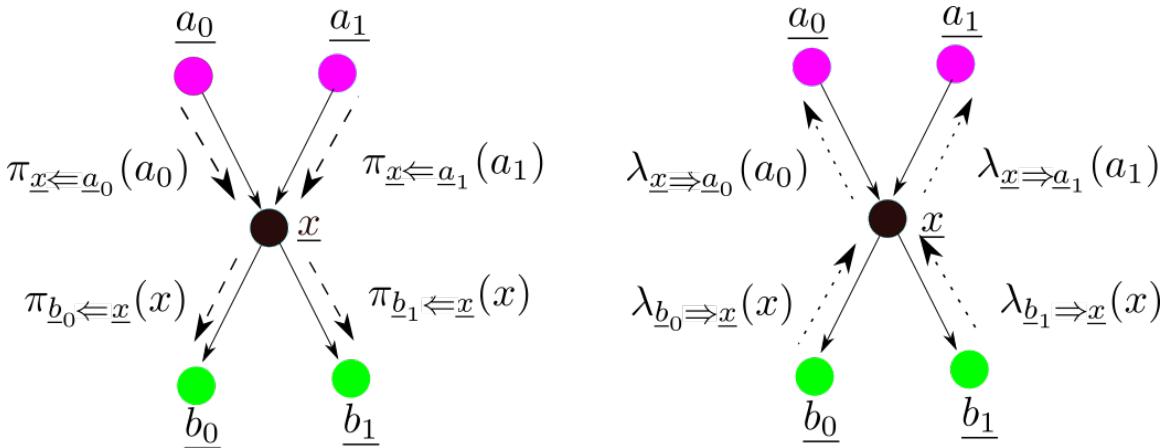


Figure 56.10: Node  $\underline{x}$  receiving and sending messages to its neighbors. (neighbors=parents and children).

We define a **memory matrix**  $\mathcal{M}_{\underline{x}}$  for node  $\underline{x}$  as

$$\mathcal{M}_{\underline{x}} = [\mathcal{M}_{\underline{x}}^+, \mathcal{M}_{\underline{x}}^-] , \quad (56.46)$$

where  $+$  =future,  $-$  =past, and

$$\mathcal{M}_{\underline{x}}^+ = [ \pi_{b \Leftarrow \underline{x}}(\cdot) \quad \lambda_{b \Rightarrow \underline{x}}(\cdot) ]_{b \in ch(\underline{x})} = [\mathcal{M}_{b,\underline{x}}^+]_{b \in ch(\underline{x})} , \quad (56.47)$$

$$\mathcal{M}_{\underline{x}}^- = \left[ \begin{array}{c} \pi_{\underline{x} \leftarrow \underline{a}}(\cdot) \\ \lambda_{\underline{x} \Rightarrow \underline{a}}(\cdot) \end{array} \right]_{\underline{a} \in pa(\underline{x})} = [\mathcal{M}_{\underline{x}, \underline{a}}^-]_{\underline{a} \in pa(\underline{x})}. \quad (56.48)$$

Note that

$$\mathcal{M}_{\underline{x}, \underline{a}}^- = \mathcal{M}_{\underline{a}, \underline{x}}^+ \quad (56.49)$$

for every arrow  $\underline{x} \leftarrow \underline{a}$ . We will refer to Eqs.(56.49) as the **memory overlap conditions**.

We will also use a permuted version of the memory matrix

$$\mathcal{M}'_{\underline{x}} = [\mathcal{M}_{\underline{x}}^{OUT}, \mathcal{M}_{\underline{x}}^{IN}], \quad (56.50)$$

where

$$\mathcal{M}_{\underline{x}}^{OUT} = \left( \begin{array}{c} [\pi_{\underline{b} \leftarrow \underline{x}}(\cdot)]_{\underline{b} \in ch(\underline{x})} \\ [\lambda_{\underline{x} \Rightarrow \underline{b}}(\cdot)]_{\underline{b} \in pa(\underline{x})} \end{array} \right) = [\mathcal{M}_{\underline{x}, \underline{n}}^{OUT}]_{\underline{n} \in nb(\underline{x})}, \quad (56.51)$$

$$\mathcal{M}_{\underline{x}}^{IN} = \left( \begin{array}{c} [\pi_{\underline{x} \leftarrow \underline{a}}(\cdot)]_{\underline{a} \in pa(\underline{x})} \\ [\lambda_{\underline{b} \Rightarrow \underline{x}}(\cdot)]_{\underline{b} \in ch(\underline{x})} \end{array} \right) = [\mathcal{M}_{\underline{x}, \underline{n}}^{IN}]_{\underline{n} \in nb(\underline{x})}. \quad (56.52)$$

For times  $t = 0, 1, \dots, T - 1$ , we calculate  $\mathcal{M}_{\underline{x}}^{(t)}$  in two steps: first we calculate  $\mathcal{M}_{\underline{x}}^{(t)IN}$  from earlier memories at time  $t - 1$ , then we calculate  $\mathcal{M}_{\underline{x}}^{(t)OUT}$ :

An **evidence node** is a node whose TPM is a delta function set to a particular state of the node. We will assume, without loss of generality, that all evidence nodes are leaf nodes. If that is not the case, any evidence node  $\underline{e}$  that is not a leaf node, can be given a new companion leaf node  $\underline{l}$  connected to  $\underline{e}$  by an arrow  $\underline{l} \leftarrow \underline{e}$ , and such that  $\underline{l}$  has a delta function TPM.

1. Calculating  $\mathcal{M}_{\underline{x}}^{(t)IN}$  from signals received from  $\underline{n} \in nb(\underline{x})$ , sent at earlier time  $t - 1$ :

Set

$$\mathcal{M}_{\underline{x}, \underline{a}}^{(t)-} |_{\pi} = \mathcal{M}_{\underline{a}, \underline{x}}^{(t-1)+} |_{\pi}, \quad (56.53)$$

for all  $\underline{a} \in pa(\underline{x})$ , and

$$\mathcal{M}_{\underline{b}, \underline{x}}^{(t)+} |_{\lambda} = \mathcal{M}_{\underline{x}, \underline{b}}^{(t-1)-} |_{\lambda}, \quad (56.54)$$

for all  $\underline{b} \in ch(\underline{x})$ . By  $X|_{\lambda}$  (resp.,  $X|_{\pi}$ ) we mean the  $\lambda$  (resp.,  $\pi$ ) component of  $X$ .

2. Calculating  $\mathcal{M}_{\underline{x}}^{(t)OUT}$  from already calculated  $\mathcal{M}_{\underline{x}}^{(t)IN}$ :

Let  $\underline{a}^{na} = (\underline{a}_i)_{i=0,1,\dots,na-1}$  denote the parents of  $\underline{x}$  and  $\underline{b}^{nb} = (\underline{b}_i)_{i=0,1,\dots,nb-1}$  its children.

Define

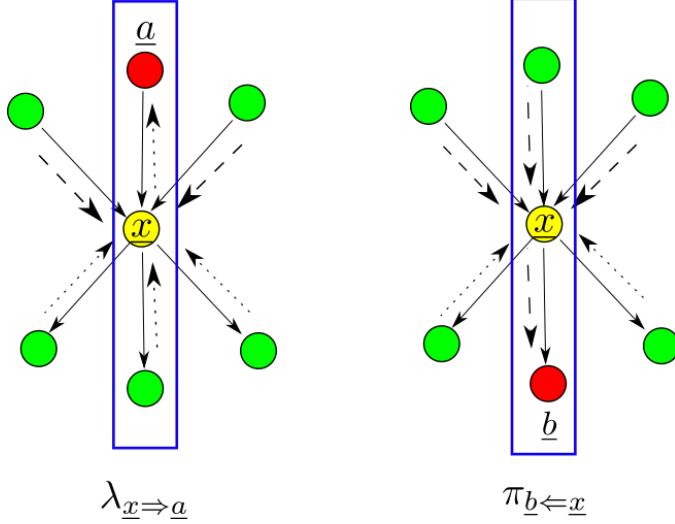


Figure 56.11: Subgraph of a bnet showing two cases (RULE 1 and RULE 2) of message info flow. The yellow node is a gossip monger. It receives messages from all the green nodes, and then it relays a joint message to the red node. Union of green nodes and the red node = full neighborhood of yellow node. There are two possible cases: the red node is either a parent or a child of the yellow one. As usual, we use arrows with dashed (resp., dotted) shafts for downstream (resp., upstream) messages. Blue boxes indicate Markov chain case.

$$\pi_{\underline{x}}(x) = \sum_{a^{na}} P(x|a^{na}) \prod_i \pi_{\underline{x} \Leftarrow \underline{a}_i}(a_i) \quad (56.55)$$

$$= E_{\underline{a}^{na}}[P(x|a^{na})] \quad (56.56)$$

(boundary case: if  $\underline{x}$  is a root node, use  $\pi_{\underline{x}}(x) = P(x)$ .) and

$$\lambda_{\underline{x}}(x) = \prod_i \lambda_{\underline{b}_i \Rightarrow \underline{x}}(x) . \quad (56.57)$$

(boundary case: if  $\underline{x}$  is a leaf node, use  $\lambda_{\underline{x}}(x) = 1$ .)

- **RULE 1: (red parent)**

From the  $\lambda_{\underline{x} \Rightarrow \underline{a}}$  panel of Fig.56.11, we get

$$\underbrace{\lambda_{\underline{x} \Rightarrow \underline{a}_i}(a_i)}_{OUT} = \mathcal{N}(!a_i) \sum_x \left[ \underbrace{\lambda_{\underline{x}}(x)}_{IN} \sum_{(a_k)_{k \neq i}} \left( P(x|a^{na}) \prod_{k \neq i} \underbrace{\pi_{\underline{x} \Leftarrow \underline{a}_k}(a_k)}_{IN} \right) \right] \quad (56.58)$$

$$= \mathcal{N}(!a_i) \sum_x [\lambda_{\underline{x}}(x) E_{(\underline{a}_k)_{k \neq i}}[P(x|a^{na})]] \quad (56.59)$$

$$= \mathcal{N}(!a_i) E_{(\underline{a}_k)_{k \neq i}} E_{\underline{x}|a^{na}} \lambda_{\underline{x}}(x) \quad (56.60)$$

(boundary case: if  $\underline{x}$  is a root node, use  $\lambda_{\underline{x} \Rightarrow a_i}(a_i) = \mathcal{N}(!a_i)$ .)

- **RULE 2: (red child)**

From the  $\pi_{b \leftarrow \underline{x}}$  panel of Fig.56.11, we get

$$\underbrace{\pi_{b_i \leftarrow \underline{x}}(x)}_{OUT} = \mathcal{N}(!x) \underbrace{\pi_{\underline{x}}(x)}_{IN} \prod_{k \neq i} \underbrace{\lambda_{b_k \Rightarrow \underline{x}}(x)}_{IN} \quad (56.61)$$

(boundary case: if  $\underline{x}$  is a leaf node, use  $\pi_{b_i \leftarrow \underline{x}}(x) = \mathcal{N}(!x)\pi_{\underline{x}}(x)$ .)

In the above equations, if the range set of a product is empty, then define the product as 1; i.e.,  $\prod_{k \in \emptyset} F(k) = 1$ .

---

**Claim:** Define

$$BEL^{(t)}(x) = \mathcal{N}(!x)\lambda_{\underline{x}}^{(t)}(x)\pi_{\underline{x}}^{(t)}(x) . \quad (56.62)$$

Then

$$\lim_{t \rightarrow \infty} BEL^{(t)}(x) = P(x|\epsilon) . \quad (56.63)$$

This says that the belief in  $\underline{x} = x$  converges to  $P(x|\epsilon)$  and it equals the product of messages received from all parents and children of  $\underline{x} = x$ .

#### 56.4.1 How BP algo for polytrees reduces to the BP algo for Markov chains

It is instructive to see how the BP algo for polytrees reduces to BP algo for Markov chains.

For a Markov chain, node  $\underline{x}$  has a single parent (i.e., ancestor)  $\underline{a}$  and a single child  $\underline{b}$ .

Therefore, Eqs.(56.55) and (56.57) reduce to

$$\pi_{\underline{x}}(x) = \sum_a P(x|a)\pi_{\underline{x} \leftarrow \underline{a}}(a) \quad (56.64)$$

and

$$\lambda_{\underline{x}}(x) = \lambda_{\underline{b} \Rightarrow \underline{x}}(x) . \quad (56.65)$$

RULE 1 given by Eq.(56.58) reduces to

$$\lambda_{\underline{x} \Rightarrow \underline{a}}(a) = \mathcal{N}(!a) \sum_x \lambda_{\underline{x}}(x)P(x|a) \quad (56.66)$$

$$= \mathcal{N}(!a) \sum_x \lambda_{\underline{b} \Rightarrow \underline{x}}(x)P(x|a) \quad (56.67)$$

RULE 2 given by Eq.(56.61) reduces to

$$\pi_{b \leftarrow \underline{x}}(x) = \mathcal{N}(!x)\pi_{\underline{x}}(x) \quad (56.68)$$

$$= \sum_a P(x|a)\pi_{\underline{x} \leftarrow \underline{a}}(a). \quad (56.69)$$

## 56.5 Derivation of BP Algorithm for Polytrees

This derivation is taken from the 1988 book Ref.[50] by Judea Pearl, where it is presented very lucidly. We only made some minor changes in notation.

### Notation

The BP algorithm yields an expansion for  $P(x|\epsilon)$ .

$x$ = the focus node, arbitrary node of bnet that we are focusing on to calculate its  $P(x|\epsilon)$ .

$(a_i)_{i=0,1,\dots,na-1}$ . = parent nodes (mnemonic: a=ancestor) of  $\underline{x}$

$(b_i)_{i=0,1,\dots,nb-1}$ . = children nodes of  $\underline{x}$ .

$\underline{\epsilon}$ = set of nodes for which there is evidence; that is,  $\underline{\epsilon} = \epsilon$ , so the state of these nodes is fixed.

$\epsilon_{\underline{x}}^- = \underline{\epsilon} \cap an(\underline{x})$  (evidence in past of  $\underline{x}$ )<sup>4</sup>

$\epsilon_{\underline{x}a_i}^- = \epsilon_{\underline{x}}^- \cap an(a_i)$ .

Note that  $\epsilon_{\underline{x}}^- = \bigcup_i \epsilon_{\underline{x}a_i}^-$

$\epsilon_{\underline{x}}^+ = \underline{\epsilon} \cap [de(\underline{x}) \cup \underline{x}]$  (evidence in future of  $\underline{x}$ )

$\epsilon_{\underline{x}b_i}^+ = \epsilon_{\underline{x}}^+ \cap [de(b_i) \cup b_i]$ .

Note that  $\epsilon_{\underline{x}}^+ = \bigcup_i \epsilon_{\underline{x}b_i}^+$

Note that  $\underline{\epsilon} = \epsilon_{\underline{x}}^+ \cup \epsilon_{\underline{x}}^-$

$$\pi_{\underline{x}}(x) = P(x|\epsilon_{\underline{x}}^-) \quad (56.70)$$

$$\pi_{\underline{x} \leftarrow \underline{a}_i}(a_i) = P(a_i|\epsilon_{\underline{x}a_i}^-) \quad (56.71)$$

$$\pi_{b_i \leftarrow \underline{x}}(x) = P(x|\epsilon_{\underline{x}b_i}^-) \quad (56.72)$$

$$\lambda_{\underline{x}}(x) = P(\epsilon_{\underline{x}}^+|x) \quad (56.73)$$

$$\lambda_{b_i \Rightarrow \underline{x}}(x) = P(\epsilon_{\underline{x}b_i}^+|x) \quad (56.74)$$

$$\lambda_{\underline{x} \Rightarrow \underline{a}_i}(a_i) = P(\epsilon_{\underline{x}a_i}^+|a_i) \quad (56.75)$$

---

<sup>4</sup>Careful: Chapter 4 of Ref.[50] uses – indicate the future and + to indicate the past. This is the opposite of our notation.

---

**Expansions of  $\lambda_{\underline{x}}(x)$  and  $\pi_{\underline{x}}(x)$  into products of single node messages.**

$$\underbrace{P(x|\epsilon_{\underline{x}}^-)}_{\pi_{\underline{x}}(x)} = P(x| \cup_i \epsilon_{\underline{x}a_i}^-) \quad (56.76)$$

$$= \sum_{a^{na}} P(x|a^{na}) P(a^{na}| \cup_i \epsilon_{\underline{x}a_i}^-) \quad (56.77)$$

$$= \sum_{a^{na}} P(x|a^{na}) \prod_i \underbrace{P(a_i|\epsilon_{\underline{x}a_i}^-)}_{\pi_{\underline{x} \leftarrow a_i}(a_i)} \quad (56.78)$$

$$\underbrace{P(\epsilon_{\underline{x}}^+|x)}_{\lambda_{\underline{x}}(x)} = \prod_i \underbrace{P(\epsilon_{\underline{x}b_i}^+|x)}_{\lambda_{\underline{b}_i \Rightarrow \underline{x}}(x)} \quad (56.79)$$

---

Note that past and future evidences  $\epsilon_{\underline{x}}^-$  and  $\epsilon_{\underline{x}}^+$  that are causally connected to  $\underline{x}$  are conditionally independent at fixed  $\underline{x}$ :

$$P(\epsilon_{\underline{x}}^+, \epsilon_{\underline{x}}^-|x) = P(\epsilon_{\underline{x}}^+|x)P(\epsilon_{\underline{x}}^-|x). \quad (56.80)$$

This observation is key to the proof of the following claim:

**Claim 86**

$$P(x|\epsilon_{\underline{x}}^+, \epsilon_{\underline{x}}^-) = P(\epsilon_{\underline{x}}^+|x)P(x|\epsilon_{\underline{x}}^-) \frac{1}{P(\epsilon_{\underline{x}}^+|\epsilon_{\underline{x}}^-)} \quad (56.81)$$

$$= \mathcal{N}(!x)P(\epsilon_{\underline{x}}^+|x)P(x|\epsilon_{\underline{x}}^-) \quad (56.82)$$

$$= \mathcal{N}(!x) (\epsilon_{\underline{x}}^+ \leftarrow x \leftarrow \epsilon_{\underline{x}}^-) \quad (56.83)$$

$$= \mathcal{N}(!x)\lambda_{\underline{x}}(x)\pi_{\underline{x}}(x) \quad (56.84)$$

**proof:**

$$P(x|\epsilon_{\underline{x}}^+, \epsilon_{\underline{x}}^-) = P(\epsilon_{\underline{x}}^+, \epsilon_{\underline{x}}^-|x) \frac{P(x)}{P(\epsilon_{\underline{x}}^+, \epsilon_{\underline{x}}^-)} \quad (56.85)$$

$$= P(\epsilon_{\underline{x}}^+|x)P(\epsilon_{\underline{x}}^-|x) \frac{P(x)}{P(\epsilon_{\underline{x}}^+, \epsilon_{\underline{x}}^-)} \quad (56.86)$$

$$= P(\epsilon_{\underline{x}}^+|x)P(x|\epsilon_{\underline{x}}^-) \frac{P(\epsilon_{\underline{x}}^-)}{P(\epsilon_{\underline{x}}^+, \epsilon_{\underline{x}}^-)} \quad (56.87)$$

$$= P(\epsilon_{\underline{x}}^+|x)P(x|\epsilon_{\underline{x}}^-) \frac{1}{P(\epsilon_{\underline{x}}^+|\epsilon_{\underline{x}}^-)} \quad (56.88)$$

**QED**

Next we prove BP rules 1 and 2.

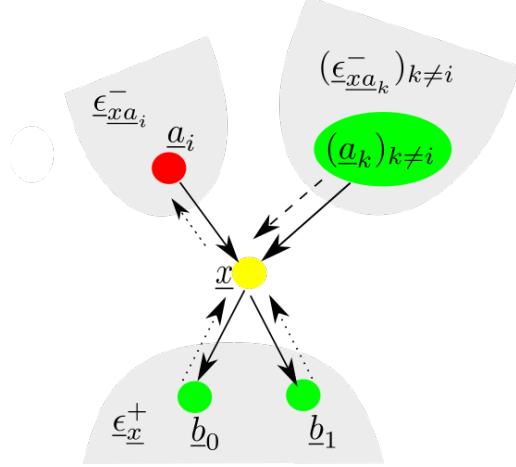


Figure 56.12: This figure is used in the derivation of the BP RULE 1.

- **RULE 1 (red parent)**

Note that

$$\epsilon_x^+ \cup \cup_{k \neq i} \epsilon_{xa_k}^- = (\epsilon_x^+ \cup \epsilon_x^-) - \epsilon_{xa_i}^- \quad (56.89)$$

$$= \epsilon_{xa_i}^+ \quad (56.90)$$

Let  $y = (a_k)_{k \neq i}$  and  $\epsilon_y^- = (\epsilon_{xa_k}^-)_{k \neq i}$ .

$$\underbrace{P(\epsilon_{xa_i}^+ | a_i)}_{\lambda_{\underline{x} \Rightarrow \underline{a}_i}(a_i)} = P(\epsilon_x^+, \epsilon_y^- | a_i) \quad (56.91)$$

$$= \sum_x \sum_y P(\epsilon_x^+, \epsilon_y^- | x, y) P(x, y | a_i) \quad (56.92)$$

$$= \sum_x \sum_y P(\epsilon_x^+ | x) P(\epsilon_y^- | y) P(x | y, a_i) P(y | a_i) \quad (56.93)$$

$$= P(\epsilon_y^-) \sum_x \sum_y P(\epsilon_x^+ | x) \frac{P(y | \epsilon_y^-)}{P(y)} P(x | y, a_i) \underbrace{P(y | a_i)}_{= P(y)} \quad (56.94)$$

$$= \mathcal{N}(!a_i) \sum_x \sum_y P(\epsilon_x^+ | x) P(x | \underbrace{y, a_i}_{a^{na}}) P(y | \epsilon_y^-) \quad (56.95)$$

$$= \mathcal{N}(!a_i) \sum_x \underbrace{P(\epsilon_x^+ | x)}_{\lambda_{\underline{x}}(x)} \sum_{(a_k)_{k \neq i}} P(x | a^{na}) \prod_{k \neq i} \underbrace{P(a_k | \epsilon_{xa_k}^-)}_{\pi_{\underline{x} \leftarrow \underline{a}_k}(a_k)} \quad (56.96)$$

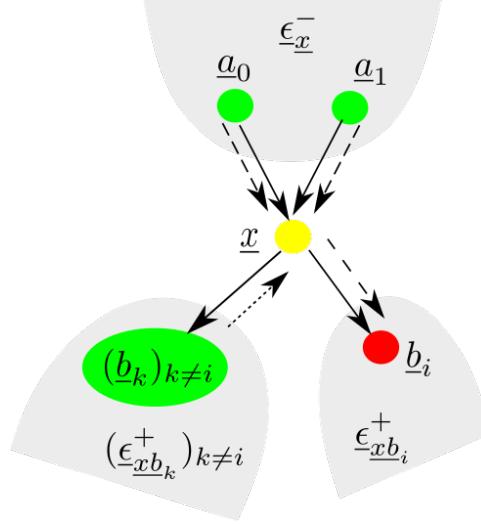


Figure 56.13: This figure is used in the derivation of the BP RULE 2.

- **RULE 2 (red child)**

Note that

$$(\cup_{k \neq i} \epsilon_{\underline{x}b_k}^+) \cup \epsilon_{\underline{x}}^- = (\epsilon_{\underline{x}}^+ \cup \epsilon_{\underline{x}}^-) - \epsilon_{\underline{x}b_i}^+ \quad (56.97)$$

$$= \epsilon_{\underline{x}b_i}^- \quad (56.98)$$

$$\underbrace{P(x|\epsilon_{\underline{x}b_i}^-)}_{\pi_{\underline{b}_i \Leftarrow \underline{x}}(x)} = P(x|(\epsilon_{\underline{x}b_k}^+}_{k \neq i})_{k \neq i}, \epsilon_{\underline{x}}^-) \quad (56.99)$$

$$= \mathcal{N}(!x) P((\epsilon_{\underline{x}b_k}^+}_{k \neq i}|x) P(x|\epsilon_{\underline{x}}^-) \quad (56.100)$$

$$= \mathcal{N}(!x) \left( \prod_{k \neq i} \underbrace{P(\epsilon_{\underline{x}b_k}^+|x)}_{\lambda_{\underline{b}_k \Rightarrow \underline{x}}(x)} \right) \underbrace{P(x|\epsilon_{\underline{x}}^-)}_{\pi_{\underline{x}}(x)} \quad (56.101)$$

## 56.6 Example of BP algo for a Tree

In this section, we describe how to apply the BP algo to the tree bnet Fig.56.14. In Fig.56.14, if we replace each integer  $i$  by the random variable  $\underline{A}_i$ , we get an **original bnet**, and if we replace each  $i$  by  $\underline{\mathcal{M}}_{\underline{A}_i}$ , we get the **BP memory bnet** of the original bnet. In Fig.56.14, the magenta nodes are evidence nodes and the green ones aren't.

We want to solve for the memory matrices of the memory bnet. To do so, we use the **BP dynamical bnet** Fig.56.15. The steps encoded in the dynamical bnet are shown in Fig.56.16. Fig.56.16 has frames in chronological order, showing the direction of travel of the  $\pi\&\lambda$  information. This sequence of frames also indicates the order in which we solve for the entries of the memory matrices. The information first emanates from the evidence nodes. It propagates generally upstream, although some nodes can generate downstream flow. Some of the info reaches the root node and is reflected there. The root node is the only one that is capable of reflection (i.e., instant output along an arrow, in response to input along that arrow). Eventually, all info reaches the leaf nodes via downstream propagation and is absorbed there.

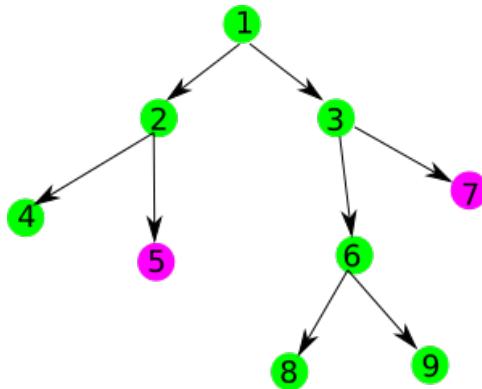


Figure 56.14: Example tree bnet used to illustrate BP.

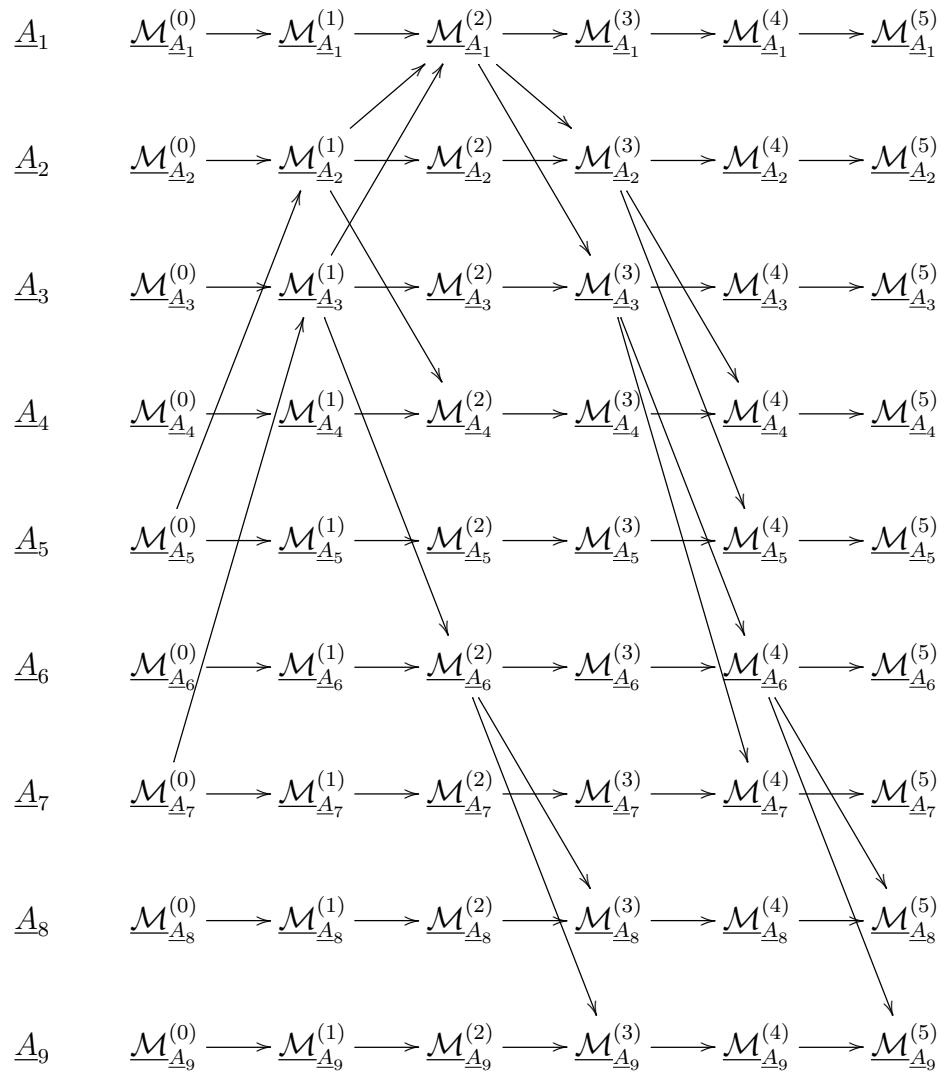


Figure 56.15: BP dynamical bnet for the bnet Fig.56.14.

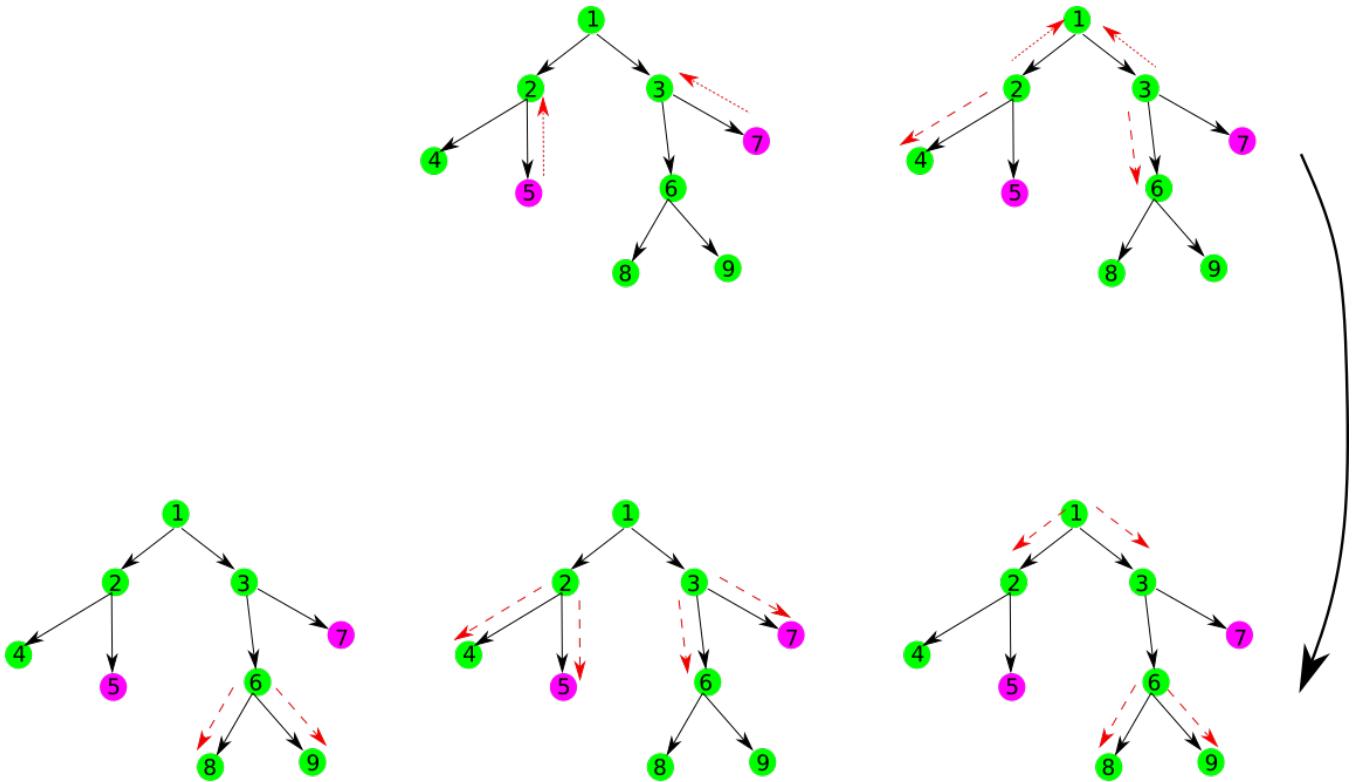


Figure 56.16: Steps encoded in the bnet Fig.56.15.

## 56.7 Bipartite bnets

By a **bipartite bnet** we will mean a bnet in which all nodes are either root nodes (parentless) or leaf nodes (childless). BP simplifies when dealing with bipartite bnets. Next, we will explain how it simplifies. But before doing so, let us define tree bnets and show how these can be replaced by equivalent bipartite bnets.

A **tree bnet** is a bnet for which all nodes have exactly one parent except for the apex root node which has none. A tree bnet is very much like the filing system in a computer.

One can map a tree bnet (the “source”) into an equivalent bipartite bnet (the “image”) as follows. Replace each arrow

$$\underline{x} \longrightarrow \underline{y} \quad (56.102)$$

of the tree bnet by

$$\underline{x} \longrightarrow P_{\underline{y}|\underline{x}} \longleftarrow \underline{y} . \quad (56.103)$$

For example, the tree bnet Fig.56.17 has the image bipartite bnet given by Fig.56.18. The bnet Fig.56.19 is just a different way of drawing the bnet Fig.56.18.

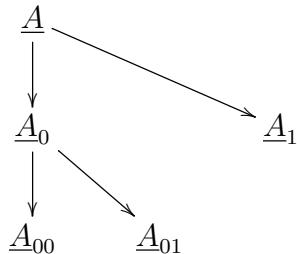


Figure 56.17: Example of a tree bnet.

The TPMs, printed in blue, for the image bipartite bnet Fig.56.18, are as follows. We express the TPMs of the image bnet in terms of the TPMs of the source bnet Fig.56.17. Let

$$P(P_{\underline{y}|\underline{x}}|x, y) = P_{\underline{y}|\underline{x}}(y|x)\delta(P_{\underline{y}|\underline{x}}, 1) + (1 - P_{\underline{y}|\underline{x}}(y|x))\delta(P_{\underline{y}|\underline{x}}, 0) \quad (56.104)$$

for all the leaf nodes  $\underline{P}_{\underline{y}|\underline{x}} \in \{0, 1\}$  of the image bipartite bnet. Also, let

$$P_{\underline{y}}(y) = \text{arbitrary prior} \quad (56.105)$$

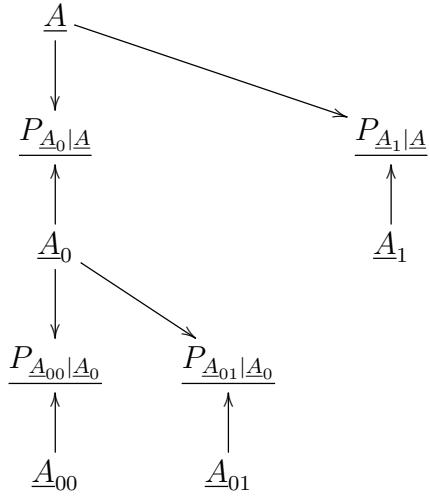


Figure 56.18: Bipartite bnet corresponding to tree bnet Fig.56.17.

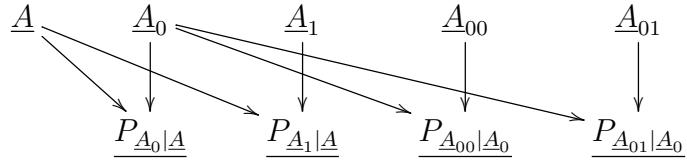


Figure 56.19: Different way of drawing the bnet Fig.56.18.

for all the root nodes  $\underline{y}$  of the image bipartite bnet except when  $\underline{y}$  corresponds to the root node  $\underline{A}$  of the source tree bnet. In that exceptional case,

$$P_{\underline{y}}(\underline{y}) = P_{\underline{A}}(\underline{y}) . \quad (56.106)$$

## 56.8 BP for bipartite bnets (BP-BB)

For a bipartite bnet as defined above, with root nodes  $\underline{x}_i$  and leaf nodes  $\underline{f}_\alpha$ , let

$$nb(i) = \{\alpha : \underline{f}_\alpha \in nb(\underline{x}_i)\} , \quad (56.107)$$

$$nb(\alpha) = \{i : \underline{x}_i \in nb(\underline{f}_\alpha)\} , \quad (56.108)$$

$$m_{\alpha \Leftarrow i}(x_i) = \pi_{\underline{f}_\alpha \Leftarrow \underline{x}_i}(x_i) , \quad (56.109)$$

$$m_{\alpha \Rightarrow i}(x_i) = \lambda_{\underline{f}_\alpha \Rightarrow \underline{x}_i}(x_i) , \quad (56.110)$$

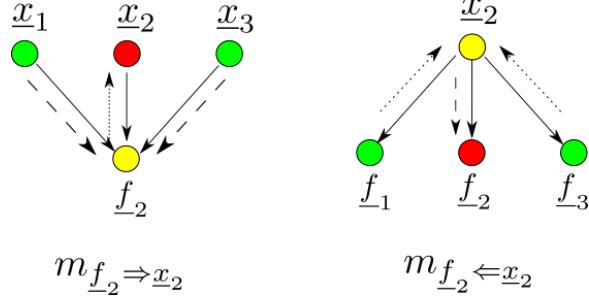


Figure 56.20: Fig.56.11 becomes this figure for the special case of a bipartite bnet. Union of green nodes and the red node = full neighborhood of yellow node. There are two possible cases: the red node is either a parent or a child of the yellow node.

Next we will show how to find  $m_{\alpha \Leftarrow i}^{(t)}$  and  $m_{\alpha \Rightarrow i}^{(t)}$  from  $m_{\alpha \Leftarrow i}^{(t-1)}$  and  $m_{\alpha \Rightarrow i}^{(t-1)}$ .

### 1. Traversing an $x$ (i.e., root) node.

See the  $m_{\underline{f}_2 \Leftarrow \underline{x}_2}$  panel of Fig.56.20.

For  $i = 0, 1, \dots, nx - 1$ , if  $\alpha \in nb(i)$ , then,

$$m_{\alpha \Leftarrow i}^{(t)}(x_i) = \prod_{\beta \in nb(i) - \alpha} m_{\beta \Rightarrow i}^{(t-1)}(x_i) , \quad (56.111)$$

whereas if  $\alpha \notin nb(i)$

$$m_{\alpha \Leftarrow i}^{(t)}(x_i) = m_{\alpha \Leftarrow i}^{(t-1)}(x_i) . \quad (56.112)$$

### 2. Traversing an $f$ (i.e., leaf) node.

See the  $m_{\underline{f}_2 \Rightarrow \underline{x}_2}$  panel of Fig.56.20.

For  $\alpha = 0, 1, \dots, nf - 1$ , if  $i \in nb(\alpha)$ , then

$$m_{\alpha \Rightarrow i}^{(t)}(x_i) = \sum_{(x_k)_{k \in nb(\alpha) - i}} f_\alpha(x_{nb(\alpha)}) \prod_{k \in nb(\alpha) - i} m_{\alpha \Leftarrow k}^{(t-1)}(x_k) \quad (56.113)$$

$$= E_{(x_k)_{k \in nb(\alpha) - i}}^{(t-1)} [f_\alpha(x_{nb(\alpha)})] , \quad (56.114)$$

whereas if  $i \notin nb(\alpha)$

$$m_{\alpha \Rightarrow i}^{(t)}(x_i) = m_{\alpha \Rightarrow i}^{(t-1)}(x_i) . \quad (56.115)$$

In the above equations, if the range set of a product is empty, then define the product as 1; i.e.,  $\prod_{k \in \emptyset} F(k) = 1$ .

---

**Claim:**

$$P(x_i|\epsilon) = \lim_{t \rightarrow \infty} \mathcal{N}(!x_i) \prod_{\alpha \in nb(i)} m_{\alpha \Rightarrow i}^{(t)}(x_i) \quad (56.116)$$

and

$$P(x_{nb(\alpha)}|\epsilon) = \lim_{t \rightarrow \infty} \mathcal{N}(!x_{nb(\alpha)}) f_\alpha(x_{nb(\alpha)}) \prod_{k \in nb(\alpha)} m_{\alpha \Leftarrow k}^{(t)}(x_k) . \quad (56.117)$$

### 56.8.1 BP-BB and general BP agree on Markov chains

It is instructive to compare the belief values (i.e.,  $P(x_i|\epsilon)$ ) obtained by applying the general (i.e., polytree) BP and BP-BB algorithms to a Markov chain. Next we show that both algorithms yield the same belief values.

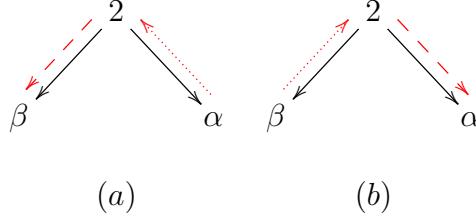


Figure 56.21: Traversing a root node of a Markov chain (a) Propagation towards left (i.e., towards future). (b) Propagation towards right (i.e., towards past).

Consider the BP-BB rule for traversing a root node. When traveling towards the left as in Fig.56.21 (a), it implies that

$$m_{\alpha \Rightarrow 2}(x_2) = m_{\beta \Leftarrow 2}(x_2) , \quad (56.118)$$

and when traveling towards the right as in Fig.56.21 (b), it implies that

$$m_{\beta \Rightarrow 2}(x_2) = m_{\alpha \Leftarrow 2}(x_2) . \quad (56.119)$$

Now consider the BP-BB rule for traversing a leaf node. When traveling to the left as in Fig.56.22 (a), it implies that

$$\underbrace{m_{\alpha \Rightarrow 2}(x_2)}_{\lambda} = \sum_{x_1} P(x_2|x_1) \underbrace{m_{\alpha \Leftarrow 1}(x_1)}_{\pi} . \quad (56.120)$$

One can rewrite the left and right hand sides (LHS, RHS) of Eq.(56.120) as follows

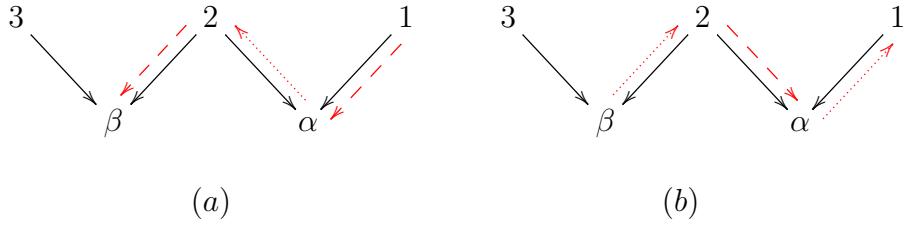


Figure 56.22: Traversing a leaf node of a Markov chain (a)Propagation towards left (i.e., towards future). (b)Propagation towards right (i.e., towards past).

$$RHS = \sum_{x_1} P(x_2|x_1) \pi_{\alpha \Leftarrow 1}(x_1) , \quad (56.121)$$

and

$$LHS = m_{\alpha \Rightarrow 2}(x_2) = m_{\beta \Leftarrow 2}(x_2) = \pi_{\beta \Leftarrow 2}(x_2) , \quad (56.122)$$

Therefore

$$\pi_{\beta \Leftarrow 2}(x_2) \sum_{x_1} P(x_2|x_1) \pi_{\alpha \Leftarrow 1}(x_1) . \quad (56.123)$$

Once again, consider the BP-BB rule for traversing a leaf node. When traveling to the right as in Fig.56.22 (b), it implies that

$$\underbrace{m_{\alpha \Rightarrow 1}(x_1)}_{\lambda} = \sum_{x_2} P(x_2|x_1) \underbrace{m_{\alpha \Leftarrow 2}(x_2)}_{\pi} . \quad (56.124)$$

One can rewrite the left and right hand sides (LHS, RHS) of Eq.(56.124) as follows

$$RHS = \sum_{x_2} P(x_2|x_1) \pi_{\alpha \Leftarrow 2}(x_2) \quad (56.125)$$

$$= \sum_{x_2} P(x_2|x_1) \lambda_{\alpha \Rightarrow 1}(x_1) , \quad (56.126)$$

and

$$LHS = \lambda_{\alpha \Rightarrow 1}(x_1) . \quad (56.127)$$

Therefore,

$$\lambda_{\alpha \Rightarrow 1}(x_1) = \sum_{x_2} P(x_2|x_1) \lambda_{\beta \Rightarrow 2}(x_2) . \quad (56.128)$$

Finally, note that Eq.(56.116) becomes

$$P(x_2|\epsilon) = \mathcal{N}(!x_2)m_{\beta \Rightarrow 2}(x_2)m_{\alpha \Rightarrow 2}(x_2) \quad (56.129)$$

$$= \mathcal{N}(!x_2)m_{\alpha \Leftarrow 2}(x_2)m_{\alpha \Rightarrow 2}(x_2) \quad (56.130)$$

$$= \mathcal{N}(!x_2)\pi_{\alpha \Leftarrow 2}(x_2)\lambda_{\alpha \Rightarrow 2}(x_2) \quad (56.131)$$

$$= \mathcal{N}(!x_2)P(x_2|\epsilon^-)P(x_2|\epsilon^+) \quad (56.132)$$

and Eq.(56.117) becomes

$$P(x_2, x_1) = \mathcal{N}(!x_2, !x_1)P(x_2|x_1)m_{\alpha \Leftarrow 1}(x_1)m_{\alpha \Leftarrow 2}(x_2) \quad (56.133)$$

$$= \mathcal{N}(!x_2, !x_1)P(x_2|x_1)\pi_{\alpha \Leftarrow 1}(x_1)\pi_{\alpha \Leftarrow 2}(x_2). \quad (56.134)$$

### 56.8.2 BP-BB and general BP agree on tree bnets.

It is instructive to compare the belief values (i.e.,  $P(x_i|\epsilon)$ ) obtained by applying the general (i.e., polytree) BP and BP-BB algorithms to a tree bnet. Next we show that both algorithms yield the same belief values.

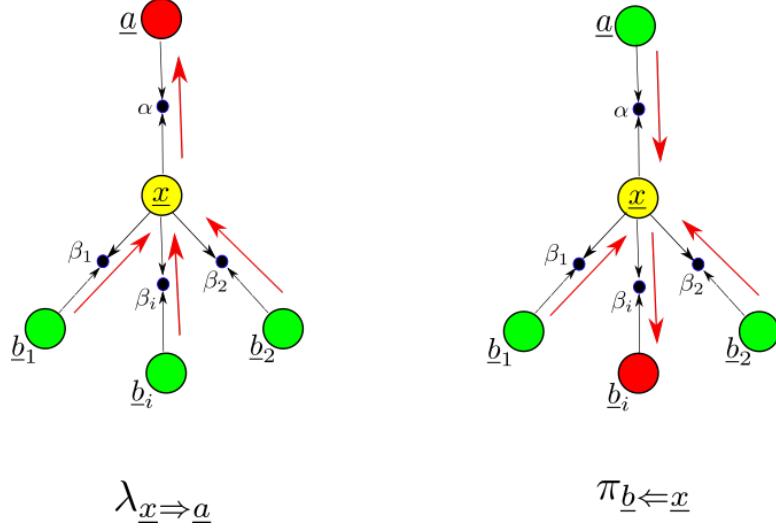


Figure 56.23: Subgraph of a tree bnet. This is the same as Fig.56.11, except that here the yellow node has a single parent because this is a subgraph of a tree bnet, not of an arbitrary bnet like Fig.56.11. The subgraph has been converted to a subgraph of a bipartite bnet by inserting a collider leaf node, labeled by a Greek letter, at the center of each edge of the tree bnet. Red arrows indicate the direction of message info flow.

Applying to the left panel of Fig.56.23 the BP-BB rule for traversing a root node, we get

$$m_{\alpha \Leftarrow \underline{x}}(x) = \prod_i m_{\beta_i \Rightarrow \underline{x}}(x) . \quad (56.135)$$

Applying to the left panel of Fig.56.23 the BP-BB rule for traversing a leaf node, we get

$$m_{\alpha \Rightarrow \underline{a}}(a) = \mathcal{N}(!a) \sum_x m_{\alpha \Leftarrow \underline{x}}(x) P(x|a) . \quad (56.136)$$

Combining Eqs.(56.135) and (56.136), we get

$$m_{\alpha \Rightarrow \underline{a}}(a) = \mathcal{N}(!a) \sum_x P(x|a) \prod_i m_{\beta_i \Rightarrow \underline{x}}(x) , \quad (56.137)$$

which can be rewritten as

$$\lambda_{\underline{x} \Rightarrow \underline{a}}(a) = \mathcal{N}(!a) \sum_x P(x|a) \underbrace{\prod_i \lambda_{b_i \Rightarrow \underline{x}}(x)}_{\lambda_{\underline{x}}(x)} . \quad (56.138)$$

Eq.(56.138) is just RULE 1 for general BP.

Applying to the right panel of Fig.56.23 the BP-BB rule for traversing a root node, we get

$$m_{\beta_i \Leftarrow \underline{x}}(x) = \mathcal{N}(!x) m_{\alpha \Rightarrow \underline{x}}(x) \prod_{k \neq i} m_{\beta_k \Rightarrow \underline{x}}(x) \quad (56.139)$$

Applying to the right panel of Fig.56.23 the BP-BB rule for traversing a leaf node, we get

$$m_{\alpha \Rightarrow \underline{x}}(x) = \sum_a P(x|a) m_{\alpha \Leftarrow \underline{a}}(a) \quad (56.140)$$

$$= \sum_a P(x|a) \pi_{\underline{x} \Leftarrow \underline{a}}(a) \quad (56.141)$$

$$= \pi_{\underline{x}}(x) . \quad (56.142)$$

Combining Eqs.(56.139) and (56.142), we get

$$\pi_{\underline{b}_i \Leftarrow \underline{x}}(x) = \mathcal{N}(!x) \pi_{\underline{x}}(x) \prod_{k \neq i} \lambda_{b_k \Rightarrow \underline{x}}(x) . \quad (56.143)$$

Eq.(56.143) is just RULE 2 of general BP.

## 56.9 BP-BB and sum-product decomposition

BP-BB yields what is often referred to as a **sum-product decomposition**. I don't like that name because it is unnecessarily confusing, and it fails to convey the recursive nature<sup>5</sup> of the decomposition. I prefer to call it a **recursive sum of products (RSOP) decomposition**, and will call it so henceforth in this chapter.

Expressing the marginals of a bnet as RSOPs, which is what BP does, reduces the complexity of the calculation. (i.e., the total number of additions and multiplications that need to be performed) That makes using the BP algo very advantageous. For instance, consider a Markov chain  $\underline{x}_{n-1} \leftarrow \dots \leftarrow \underline{x}_1 \leftarrow \underline{x}_0$ , where  $x_i \in \{0, 1, 2\}$  for all  $i$ . Note that if we calculate  $P(x_{n-1})$  as follows

$$P(x_{n-1}) = \left[ \sum_{x_{n-2}} P(x_{n-1}|x_{n-2}) \dots \left[ \sum_{x_1} P(x_2|x_1) \left[ \sum_{x_0} P(x_1|x_0)P(x_0) \right] \dots \right] \right], \quad (56.144)$$

we need to perform  $2(n - 1)$  additions and  $3(n - 1)$  multiplications. On the other hand, if we calculate  $P(x_{n-1})$  as follows

$$P(x_{n-1}) = \sum_{x_{n-2}} \dots \sum_{x_1} \sum_{x_0} P(x_{n-1}|x_{n-2}) \dots P(x_2|x_1)P(x_1|x_0)P(x_0), \quad (56.145)$$

we need to perform  $3^n - 1$  additions and  $3^n(n - 1)$  multiplications.

---

<sup>5</sup>By "recursive nature", we mean bootstrapped definitions that lead to nested sums. The recursive nature of BP is evident from RULES 1 and 2 that define  $\lambda$ 's and  $\pi$ 's in terms of other  $\lambda$ 's and  $\pi$ 's.

## Chapter 57

# Message Passing in Quantum Mechanics

See Ref.[75].

# Chapter 58

## Meta-learners for estimating ATE

This section is based on the final 2 chapters of Ref.[14].

The Average Treatment Effect (ATE) is defined in Chapter 72.

Economists are huge fans of Linear Regression (LR), and traditionally calculate ATE using LR. But in recent times, they have begun to calculate ATE using Machine Learning (ML) instead. This chapter describes various methods that economists and others have devised for calculating ATE with ML. These methods are called **meta-learners** because they involve multiple ML or LR steps.

Using ML to calculate ATE captures non-linear trends whose exclusion might sometimes lead to a poor result. On the other hand, ML is more expensive computationally than LR, and it introduces the danger of overfitting, a danger which is nonexistent with LR.

Below, we represent each Linear Regression (LR) step as follows. We list a dataset; i.e., a set of tuples indexed by the individuals  $\sigma$  of a population  $\Sigma$  such that  $|\Sigma| = nsam$ . The independent variables of the LR (i.e.,  $x^\sigma$ ) are unboxed and the dependent variable (a.k.a. target feature) (i.e.,  $y^\sigma$ ) is shown inside a box. Then we show an arrow with the superscript “LR-fit”, followed by the fit function obtained by performing the LR.<sup>1</sup>

$$\{(\sigma, x^\sigma = [x_i^\sigma], \boxed{y^\sigma}) : \sigma \in \Sigma\} \xrightarrow{\text{LR-fit}} \hat{y}(x) = \alpha + x_i \beta_i \quad (58.1)$$

Analogously, below, we represent each Supervised Machine Learning (ML) step as follows.

$$\{(\sigma, x^\sigma, \boxed{y^\sigma}) : \sigma \in \Sigma\} \xrightarrow{\text{ML-fit}} \hat{y}(x) \quad (58.2)$$

Henceforth, we will use  $\delta(x) (\approx \text{ATE})$  to denote the treatment effect.

- **S (Single)-learner**

---

<sup>1</sup>In this chapter, we will occasionally use the Einstein summation convention; i.e., implicit sum over repeated indices.

$$\{(\sigma, x^\sigma, d^\sigma, \boxed{y^\sigma}) : \sigma \in \Sigma\} \xrightarrow{\text{ML-fit}} \hat{y}(d, x) \quad (58.3)$$

$$\delta(x) = \hat{y}(1, x) - \hat{y}(0, x) \quad (58.4)$$

- **T (Twin)-learner**

$$\{(\sigma, x^\sigma, d^\sigma = 0, \boxed{y^\sigma}) : \sigma \in \Sigma\} \xrightarrow{\text{ML-fit}} \hat{y}_0(x) \quad (58.5)$$

$$\{(\sigma, x^\sigma, d^\sigma = 1, \boxed{y^\sigma}) : \sigma \in \Sigma\} \xrightarrow{\text{ML-fit}} \hat{y}_1(x) \quad (58.6)$$

$$\delta(x) = \hat{y}_1(x) - \hat{y}_0(x) \quad (58.7)$$

- **X (Cross)-learner**

do T-learner, get  $\hat{y}_0(x), \hat{y}_1(x)$

$$\{(\sigma, x^\sigma, d^\sigma = 0, \boxed{y^\sigma - \hat{y}_1(x^\sigma)}) : \sigma \in \Sigma\} \xrightarrow{\text{ML-fit}} \mathcal{Y}_0(x) \quad (58.8)$$

$$\{(\sigma, x^\sigma, d^\sigma = 1, \boxed{y^\sigma - \hat{y}_0(x^\sigma)}) : \sigma \in \Sigma\} \xrightarrow{\text{ML-fit}} \mathcal{Y}_1(x) \quad (58.9)$$

$$\delta(x) = \frac{1}{2}[\mathcal{Y}_1(x) - \mathcal{Y}_0(x)] \quad (58.10)$$

- **De-biased (a.k.a. Orthogonal) ML**

Standard supervised ML is performed with two features, the independent feature and the dependent or target feature. Supervised ML has a target feature. Unsupervised ML doesn't.

In **De-biased LR**, we do LR with two residuals. Let's call them the **independent residual** and the **dependent or target residual**. These two residuals are calculated with the help of two previously performed LR steps.

In **De-biased ML**, we do ML or LR (either one) with two residuals. These two residuals are calculated with the help of two previously performed ML steps (instead of two LR steps).

The FWL theorem discussed in Chapter 28 shows how to do De-biased LR. Next, we will describe how to do De-biased ML.

We start by doing two ML steps:

$$\{(\sigma, x^\sigma, \boxed{d^\sigma}) : \sigma \in \Sigma\} \xrightarrow{\text{ML-fit}} \hat{d}(x) \quad (58.11)$$

$$\{(\sigma, x^\sigma, \boxed{y^\sigma}) : \sigma \in \Sigma\} \xrightarrow{\text{ML-fit}} \hat{y}(x) \quad (58.12)$$

After these two ML steps, we do either LR or ML to get  $\delta(x)$ .

Let

$$\Delta d^\sigma = d^\sigma - \hat{d}(x^\sigma) \quad (58.13)$$

$$\Delta y^\sigma = y^\sigma - \hat{y}(x^\sigma) \quad (58.14)$$

Options for the final learning step that calculates  $\delta(x)$ :

1. Do a standard LR to get a  $\delta(x)$  that is a constant (i.e.,  $x$  independent):

$$\{(\sigma, \Delta d^\sigma, \boxed{\Delta y^\sigma}) : \sigma \in \Sigma\} \xrightarrow{\text{LR-fit}} \mathcal{Y}(\Delta d) = \alpha + \Delta d \delta \quad (58.15)$$

$$\delta = \text{coefficient of } \Delta d \text{ in } \mathcal{Y}(\Delta d). \quad (58.16)$$

2. Do a LR with a  $x * d$  cross term to get a  $\delta(x)$  that is linear in  $x$ :

$$\{(\sigma, x^\sigma, \Delta d^\sigma, \boxed{\Delta y^\sigma}) : \sigma \in \Sigma\} \xrightarrow{\text{LR-fit}} \mathcal{Y}(\Delta d, x) = \alpha_0 + x\beta_0 + \Delta d(\alpha_1 + x\beta_1) \quad (58.17)$$

$$\delta(x) = \mathcal{Y}(\Delta d|_{d=1}, x) - \mathcal{Y}(\Delta d|_{d=0}, x) = \alpha_1 + x\beta_1 \quad (58.18)$$

3. Do ML with a weighted cost function to get a general fit  $\hat{\delta}(x)$ .

The cost function used in standard ML (see Eq.(58.2)) is:

$$\mathcal{C} = \frac{1}{nsam} \sum_{\sigma} [y^\sigma - \hat{y}(x^\sigma)]^2 \quad (58.19)$$

Define the cost function in this case as

$$\mathcal{C} = \frac{1}{nsam} \sum_{\sigma} \left[ \Delta y^\sigma - \hat{\delta}(x^\sigma) \Delta d^\sigma \right]^2 \quad (58.20)$$

$$= \frac{1}{nsam} \sum_{\sigma} [\Delta d^\sigma]^2 \left[ \frac{\Delta y^\sigma}{\Delta d^\sigma} - \hat{\delta}(x^\sigma) \right]^2 \quad (58.21)$$

This is a weighted cost function with weights  $[\Delta d^\sigma]^2$ .

$$\{(\sigma, x^\sigma, \boxed{\frac{\Delta y^\sigma}{\Delta d^\sigma}}) : \sigma \in \Sigma\} \xrightarrow{\text{ML-fit}} \hat{\delta}(x) \quad (58.22)$$

4. Do ML with  $\Delta d^\sigma$  as an independent feature to get a general fit  $\hat{\delta}(\Delta d, x)$ :

$$\{(\sigma, x^\sigma, \Delta d^\sigma, \boxed{\frac{\Delta y^\sigma}{\Delta d^\sigma}}) : \sigma \in \Sigma\} \xrightarrow{\text{ML-fit}} \hat{\delta}(\Delta d, x) \quad (58.23)$$

$$\delta(x) = \hat{\delta}(\Delta d|_{d=1}, x) \quad (58.24)$$

# Chapter 59

## Missing Data, Imputation

This chapter assumes that the reader has read some parts of Chapter 26 on the Expectation Maximization (EM) algo and Chapter 51 on Markov Chain Monte Carlo (MCMC).

	$h_0$	$x_0$	$x_1$	$x_2$	
1	NA	0	1	1	
2	NA	0	0	0	
3	NA	1	1	0	
4	NA	NA	1	NA	
5	NA	0	NA	1	
6	NA	0	0	1	

	$h_0$	$x_0$	$x_1$	$x_2$	$m$
1	NA	0	1	1	(0,0,0)
2	NA	0	0	0	(0,0,0)
3	NA	1	1	0	(0,0,0)
4	NA	0		0	
		0		1	
		1		0	(1,0,1)
		1		1	
5	NA	0	0	1	(0,1,0)
6	NA	0	0	1	(0,0,0)

Table 59.1: **Left Table:** Dataset with  $nsam = 6$  and some missing entries, for 4 binary variables  $h_0, x_0, x_1, x_2$ . NA=not available. The  $h_0$  column is completely missing because  $h_0$  is an unobserved variable. **Right Table:** All possibilities for  $x_i = NA$  cells of left table have been enumerated. A new column labeled  $m$  has been added.  $m_i = \mathbb{1}(x_i \text{ is missing})$  for  $i = 0, 1, 2$ .

Suppose that you have compiled a **dataset**  $\vec{x} = (x[\sigma])_{\sigma=0,1,\dots,nsam-1}$  where  $x = (x_0, x_1, \dots, x_{nx-1})$  from a study or survey. It consists of  $nsam$  number of samples (sample= row), and  $nx$  columns (each column is a different feature, or observation). Suppose that some of the cells in this matrix are empty. Throwing away all the incomplete rows is okay if the number of incomplete rows is much smaller than  $nsam$ . If not, throwing them away would throw away a substantial amount of information contained in all the filled cells in those incomplete rows, plus it might bias your dataset. This chapter deals with how to fill those empty cells with plausible fake data. A fancy name for this process is **imputation**. There is no unique way of

fabricating fake data, but some fakes are better than others by some metrics. This chapter will consider two popular ways (EM and MCMC) of filling those empty cells with their “most likely” values based on the cells of the dataset that aren’t missing, and also based on some bnet model that is expected to describe well the dataset.

Notation:  $\vec{a} = (\underline{a}[\sigma])_{\sigma=0,1,\dots,nsam-1}$ , where  $nsam$  is the number of samples. Will sometimes denote  $a[\sigma]$  by  $a^\sigma$ .

For concreteness, we will apply the concepts of this chapter to the dataset with missing data given by Table 59.1.

## 59.1 Imputation via EM

We begin by augmenting Fig.26.1 (the first figure in Chapter 26) by adding to it a new node  $\vec{m}$  called the **missingness variable**. Recall that node  $\theta$  represents the **unknown parameters**, node  $\vec{x}$  represents the **observed variables**, and node  $\vec{h}$  represents the **hidden variables**. Both  $\theta$  and  $\vec{h}$  are hidden (i.e., unobserved). Fig.59.1 shows 3 popular ways of connecting node  $\vec{m}$  to the other nodes in the graph Fig.26.1.

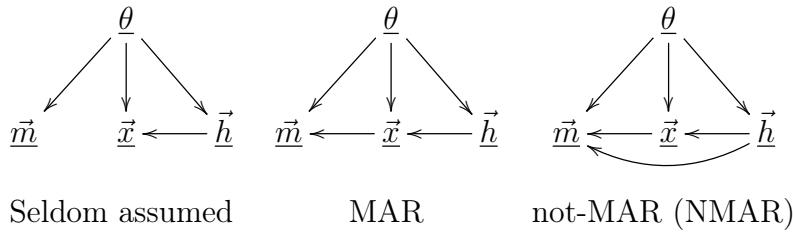


Figure 59.1: The left bnet is seldom assumed. The middle bnet is referred to as the MAR (missing at random) assumption. The right bnet is referred to as the not-MAR (NMAR) assumption.

From Fig.59.1, we have

$$P(\vec{m}|\vec{x}, \vec{h}, \theta) = \begin{cases} P(\vec{m}|\theta) & \text{Seldom assumed. Called missing-CAR (MCAR)} \\ P(\vec{m}|\vec{x}, \theta) & \text{MAR} \\ P(\vec{m}|\vec{x}, \vec{h}, \theta) & \text{not-MAR (NMAR)} \end{cases}. \quad (59.1)$$

For doing imputation via EM, we connect node  $\vec{m}$  as shown in the middle bnet (called MAR) of Fig.59.1.

For the example of Table 59.1, we have variables  $\vec{m}$ ,  $\vec{x}$  and  $\vec{h}$  whose values range over the following sets:

$$\begin{aligned} \vec{x} &= (\vec{x}_0, \vec{x}_1, \vec{x}_2) \\ \vec{h} &= (\vec{h}_0) \end{aligned}$$

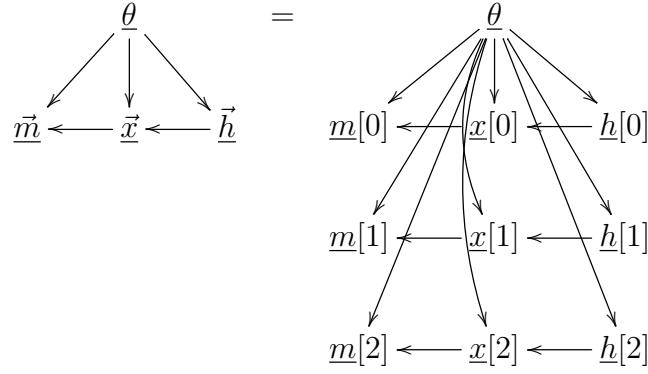


Figure 59.2: MAR bnet with  $nsam = 3$ .

$$\begin{aligned} h_0[\sigma] &\in \{0, 1\}, \\ \underline{x}_i[\sigma] &\in \{0, 1\} \text{ for } i = 0, 1, 2, \\ \underline{m}_i[\sigma] &\in \{0, 1\} \text{ for } i = 0, 1, 2. \end{aligned}$$

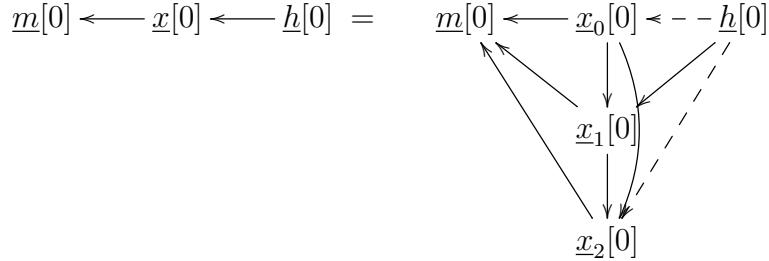


Figure 59.3: Our example for imputation via EM assumes this bnet between nodes  $\underline{m}[\sigma], \underline{x}[\sigma], \underline{h}[\sigma]$ .

For concreteness, we will assume that the Markov chain  $\underline{m}[\sigma] \leftarrow \underline{x}[\sigma] \leftarrow \underline{h}[\sigma]$  has a finer grained DAG structure given by Fig.59.3. where we will omit the dashed arrows. If one doesn't want to assume that the data can be fitted well by the bnet of Fig.59.3 without the dashed arrows, one can include those arrows too, at the expense of more unknown parameters (i.e., degrees of freedom) to be lumped into  $\theta$ . We will parameterize the TPMs corresponding to Fig.59.3 using a Categorical Distribution for each column of the TPMs. We will thus assume that the TPMs, printed in blue, for bnet Fig.59.3, are as follows.

$$P(h_0^\sigma | \theta) = \frac{1}{\theta_0} \begin{array}{c|c} & 1 - \theta_0 \\ \hline 1 & \theta_0 \end{array} \quad (59.2)$$

$$P(x_0^\sigma | \theta) = \begin{array}{c|cc} & 0 & 1 - \theta_1 \\ \hline 0 & & \theta_1 \\ 1 & & \end{array} \quad (59.3)$$

$$P(x_1^\sigma | x_0^\sigma, h^\sigma, \theta) = \begin{array}{c|ccccc} & 00 & 01 & 10 & 11 \\ \hline 0 & 1 - \theta_2 & 1 - \theta_3 & 1 - \theta_4 & 1 - \theta_5 \\ 1 & \theta_2 & \theta_3 & \theta_4 & \theta_5 \end{array} \quad (59.4)$$

$$P(x_2^\sigma | x_1^\sigma, x_0^\sigma, \theta) = \begin{array}{c|ccccc} & 00 & 01 & 10 & 11 \\ \hline 0 & 1 - \theta_6 & 1 - \theta_7 & 1 - \theta_8 & 1 - \theta_9 \\ 1 & \theta_6 & \theta_7 & \theta_8 & \theta_9 \end{array} \quad (59.5)$$

$$P(m^\sigma | x^\sigma, \theta) = \frac{1}{nsam} P((x_i)_{\forall i \ni m_i=1} | (x_i)_{\forall i \ni m_i=0}, \theta) \quad (59.6)$$

Eq.(59.6) can be illustrated as follows. In Table 59.2, we added a  $P(m)$  column to Table 59.1.

	$h_0$	$x_0$	$x_1$	$x_2$	$m$	$P(m)$
1	NA	0	1	1	(0,0,0)	$\frac{1}{nsam}$
2	NA	0	0	0	(0,0,0)	$\frac{1}{nsam}$
3	NA	1	1	0	(0,0,0)	$\frac{1}{nsam}$
4	NA	0		0		$\frac{1}{nsam} P(x_0 = 0, x_2 = 0   x_1 = 1, \theta)$
		0		1		$\frac{1}{nsam} P(x_0 = 0, x_2 = 1   x_1 = 1, \theta)$
		1	1	0	(1,0,1)	$\frac{1}{nsam} P(x_0 = 1, x_2 = 0   x_1 = 1, \theta)$
		1		1		$\frac{1}{nsam} P(x_0 = 1, x_2 = 1   x_1 = 1, \theta)$
5	NA	0	0	1	(0,1,0)	$\frac{1}{nsam} P(x_1 = 0   x_0 = 0, x_2 = 1, \theta)$
		1				$\frac{1}{nsam} P(x_1 = 1   x_0 = 0, x_2 = 1, \theta)$
6	NA	0	0	1	(0,0,0)	$\frac{1}{nsam}$

Table 59.2:  $P(m)$  column added to Table 59.1. Note that  $\sum_m P(m) = 1$ .

$$\theta = (\theta_i)_{i=0,1,\dots,9} \quad (59.7)$$

$$P(m^\sigma, x^\sigma, h^\sigma | \theta) = P(m^\sigma | x^\sigma, \theta) P(x^\sigma | h^\sigma, \theta) P(h^\sigma | \theta) \quad (59.8)$$

$$P(x^\sigma | h^\sigma, \theta) = P(x_2^\sigma | x_1^\sigma, x_0^\sigma, \theta) P(x_1^\sigma | x_0^\sigma, h^\sigma, \theta) P(x_0^\sigma | \theta) \quad (59.9)$$

$$P(x_1^\sigma | x_0^\sigma, \theta) = \sum_h P(x_1^\sigma | x_0^\sigma, h^\sigma, \theta) P(h^\sigma | \theta) \quad (59.10)$$

$$P(x^\sigma | \theta) = P(x_2^\sigma | x_1^\sigma, x_0^\sigma, \theta) P(x_1^\sigma | x_0^\sigma, \theta) P(x_0^\sigma | \theta) \quad (59.11)$$

$$Q(\theta | \theta^{(t)}) = \sum_{\vec{m}, \vec{h}} P(\vec{m}, \vec{h} | \vec{x}, \theta^{(t)}) \ln P(\vec{m}, \vec{x}, \vec{h} | \theta) \quad (59.12)$$

$$= \sum_{\vec{m}, \vec{h}} \left[ \prod_\sigma P(m^\sigma, h^\sigma | x^\sigma, \theta^{(t)}) \right] \ln \left[ \prod_\sigma P(m^\sigma, x^\sigma, h^\sigma | \theta) \right] \quad (59.13)$$

$$= \sum_\sigma \sum_{m^\sigma, h^\sigma} P(m^\sigma, h^\sigma | x^\sigma, \theta^{(t)}) \ln P(m^\sigma, x^\sigma, h^\sigma | \theta) \quad (59.14)$$

$$= \sum_\sigma \sum_{m^\sigma, h^\sigma} \frac{P(m^\sigma, h^\sigma, x^\sigma | \theta^{(t)})}{P(x^\sigma | \theta^{(t)})} \ln P(m^\sigma, x^\sigma, h^\sigma | \theta) \quad (59.15)$$

Once you find optimal parameters  $\theta^*$  by recursing this  $Q(\theta | \theta^{(t)})$ , you can evaluate numerically the  $P(m)$  column of Table 59.2. In Table 59.2, out of the 4 sub-rows for row 4, choose the one with the highest probability. Similarly, out of the 2 sub-rows for row 5, choose the one with the highest probability.

## 59.2 Imputation via MCMC

A simple and popular way to do imputation via MCMC is described in Ref.[67]. It goes as follows.

Let

$$\underline{H}[\sigma] = (\underline{h}[\sigma], \underline{m}[\sigma]) \quad (59.16)$$

for  $\sigma = 0, 1, \dots, nsam - 1$ . Initialize  $\theta^{(0)}$  to a random value within the allowed ranges. Do the following 2 steps, for  $t = 0, 1, \dots, T - 1$ , where  $T$  is large enough that  $\theta^{(t)}$  has reached a steady value that is independent of  $\theta^{(0)}$ . To do the sampling, use a standard sampling technique such as Gibbs sampling.

- **STEP 1:** For  $\sigma = 0, 1, \dots, nsam - 1$ , find a sample

$$(H^\sigma)^{(t+1)} \sim P(H^\sigma | x^\sigma, \theta^{(t)}) . \quad (59.17a)$$

- **STEP 2:** Find a sample

$$\theta^{(t+1)} \sim P^{(t+1)}(\theta) \quad (59.17b)$$

where

$$P^{(t+1)}(\theta) = \mathcal{N}(!\theta) P(\vec{x}, \vec{H}^{(t+1)} | \theta) \quad (59.17c)$$

$$= \mathcal{N}(!\theta) \prod_{\sigma} P(x^{\sigma}, (H^{\sigma})^{(t+1)} | \theta). \quad (59.17d)$$

Fig.59.4 illustrates this two step recursive process using a bnet.

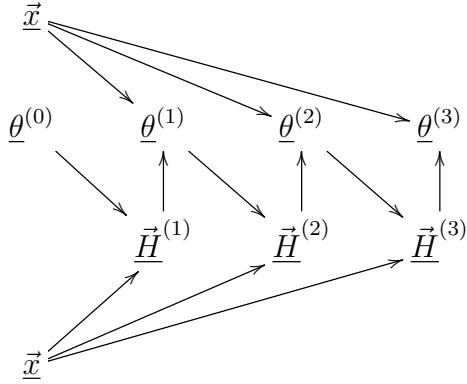


Figure 59.4: bnet illustrating Eqs.(59.17) for doing imputation via MCMC. The **same** node  $\vec{x}$  appears twice to make the graph clearer.

### 59.3 Multiple Imputations

**Multiple imputations** means calculating  $\theta^*$  (i.e., the optimum  $\theta$ ) and the concomitant dataset  $\vec{x}^*, \vec{H}^*$ , via any method (such as EM or MCMC), a large number of times, starting from different, randomly chosen  $\theta^{(0)}$  initial parameters. Then calculating the average and the variance of  $\theta^*, \vec{x}^*, \vec{H}^*$  and functions thereof.

# Chapter 60

## Modified Treatment Policy

This chapter is based primarily on Ref. [21]. Refs. [23] and [24] were also very helpful.

A **Modified Treatment Policy (MTP)** is a generalization of the Potential Outcomes (PO)<sup>1</sup> model so as to modify the original treatment. This is accomplished by adding a modified treatment dose node  $\tilde{x}$  acting as a mediator between the treatment dose node  $x$  and the treatment effect node  $y$  (i.e., by considering  $x \rightarrow \tilde{x} \rightarrow y$ ).

### 60.1 One time MTP

Consider a typical PO bnet  $G$  and its corresponding imagined bnet  $G_{im2}$  (see Fig.60.1)<sup>2</sup>. A MTP adds a Bayesian prior to the node  $\tilde{x}$  in  $G_{im2}$ . The prior depends on the treatment dose variable (a.k.a. exposure variable)  $x$  and its parents  $pa(x) = c$ . This adds to  $G_{im2}$  new arrows  $c \rightarrow \tilde{x}$  and  $x \rightarrow \tilde{x}$  (see Fig.60.2).

The TPM, printed in blue, for node  $\tilde{x}$  of the imagined bnet  $G_{im2}$  in Fig.60.2, is as follows

$$P(\tilde{x} = \tilde{x}; x) = \delta(\tilde{x}, x) \quad (60.1)$$

The TPM, printed in blue, for node  $\tilde{x}$  of the modified imagined bnet  $G_{im2,mod}$  in Fig.60.2, is as follows

$$P(\tilde{x} = \tilde{x}|x = x, c) = \text{prior} \quad (60.2)$$

Hence, node  $\tilde{x}$  has a totally informative, parametric (frequentist) prior in  $G_{im2}$ , and it has a more general (Bayesian) prior in  $G_{im2,mod}$ .

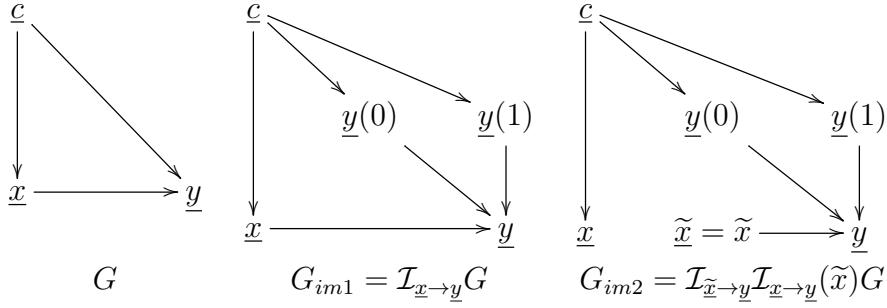
The following assumptions will be made about bnet  $G_{im2,mod}$ :

#### 1. Consistency (a.k.a. SUTVA)

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<sup>1</sup>PO theory is discussed in Chapter 72.

<sup>2</sup>Ref.[21] uses the notation  $L = c$ ,  $A = x$ ,  $Y = y$ ,  $Q = \tilde{x}$ ,  $Y_q = y(\tilde{x})$ . Furthermore, it does not display a DAG.



( As usual in this book,  $S_{\underline{a}}$  denotes the set of values that a random variable  $\underline{a}$  can assume. Imagine operators such as  $I_{\underline{x} \rightarrow y}$  and  $I_{\underline{x} \rightarrow y}(\tilde{x})$  are discussed in Chapter 12. )

Figure 60.1:  $G$  is one of the simplest possible bnets considered in PO theory. In the usual PO theory, one only considers the bnet  $G_{im1}$ . In MTP theory, one considers the bnet  $G_{im2}$ . For  $G_{im2}$ ,  $\tilde{x} \in S_{\tilde{x}} = S_x = \{0, 1\}$ .

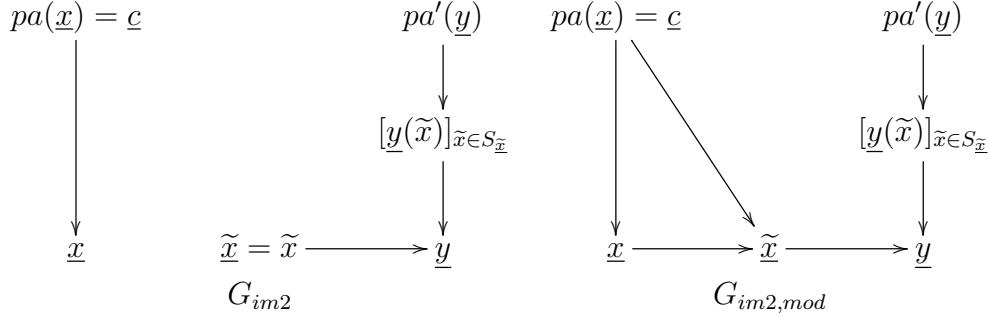


Figure 60.2: In this figure,  $G_{im2}$  is the generalization of the  $G_{im2}$  in Fig.60.1. Note that  $pa'(y)$  are the parents in  $G$  of  $y$ , excluding  $\underline{x}$ . Note that  $S_{\tilde{x}} \subset S_x$ .

The TPM, printed in blue, for node  $\underline{y}$  of the modified imagined bnet  $G_{im2,mod}$  in Fig.60.2, is as follows

$$P(y | \tilde{x}, \{y(\tilde{x}')\}_{\tilde{x}' \in S_{\tilde{x}}}) = \mathbb{1}(\quad y = \sum_{\tilde{x}' \in S_{\tilde{x}}} y(\tilde{x}') \mathbb{1}(\tilde{x}' = \tilde{x}) \quad) \quad (60.3)$$

When  $S_{\tilde{x}} = \{0, 1\}$ , this becomes the more familiar statement from standard PO theory:

$$P(y | \tilde{x}, \{y(0), y(1)\}) = \mathbb{1}(\quad y = y(0)(1 - \tilde{x}) + y(1)\tilde{x} \quad) \quad (60.4)$$

An immediate consequence of this deterministic TPM for node  $\underline{y}$  is that

$$P(\underline{y} = \underline{y} | \tilde{\underline{x}}, pa'(\underline{y}) = \xi) = P(\underline{y}(\tilde{\underline{x}}) = \underline{y} | \tilde{\underline{x}}, pa'(\underline{y}) = \xi) \quad (60.5)$$

## 2. Ignorability (a.k.a. conditional independence assumption (CIA))

$$P(\underline{y}(\tilde{\underline{x}}') = \underline{y} | \tilde{\underline{x}}, pa'(\underline{y}) = \xi) = P(\underline{y}(\tilde{\underline{x}}') = \underline{y} | pa'(\underline{y}) = \xi) \quad (60.6)$$

CIA follows from the structure of the DAG  $G_{im2,mod}$ , because in that DAG, fixing the value of  $pa'(\underline{y})$  blocks messages from  $\tilde{\underline{x}}$  to  $\underline{y}(\tilde{\underline{x}})$  (i.e., for all  $\tilde{\underline{x}} \in S_{\tilde{\underline{x}}}$ , we have  $\tilde{\underline{x}} \perp \underline{y}(\tilde{\underline{x}}) | pa'(\underline{y})$ .)

## 3. Identifiability

We must have

$$S_{\tilde{\underline{x}}} \subset S_{\underline{x}} \quad (60.7)$$

in  $G_{im2,mod}$  or else queries of the type  $P(\underline{y}(\tilde{\underline{x}}) = \underline{y} | pa'(\underline{y}) = \xi)$  are not identifiable. This is clear because if  $\tilde{\underline{x}} \notin S_{\underline{x}}$ , then we have no information of the type

$$P(\underline{y} = \underline{y} | \tilde{\underline{x}}, pa'(\underline{y}) = \xi) = P(\underline{y}(\tilde{\underline{x}}) = \underline{y} | pa'(\underline{y}) = \xi). \quad (60.8)$$

## 4. Positivity

Define the following 2 propensities for  $x \in S_{\underline{x}}$  and  $\tilde{x} \in S_{\tilde{\underline{x}}}$ :

$$g_{x|c} = P(\underline{x} = x | c) \quad (60.9)$$

$$\tilde{g}_{\tilde{x}|c} = P(\tilde{\underline{x}} = \tilde{x} | c) \quad (60.10)$$

Positivity for  $G_{im2,mod}$  is the requirement that

$$0 < g_{\tilde{x}|c} < 1 \text{ for all } \tilde{x} \in S_{\tilde{\underline{x}}} \text{ and } c \in S_c \quad (60.11)$$

If  $g_{\tilde{x}|c}$  is deterministic, then this requirement is not satisfied, and we cannot do IPW (i.e., inverse propensity weighing).

Note that using a MTP can allow IPW to be performed in cases when the propensity  $g_{x|c}$  is anomalous (i.e., is either not defined or violates positivity) for some  $x \in S_{\underline{x}}$ , but is not anomalous for all  $\tilde{x} \in S_{\tilde{\underline{x}}}$ , where  $S_{\tilde{\underline{x}}}$  is some proper subset of  $S_{\underline{x}}$ .

The probability distribution  $P(\tilde{x}|x, c)$  (i.e., the  $\tilde{x}$  prior for  $G_{im2,mod}$ ) is called the **MTP**. An MTP can be either deterministic or probabilistic. An MTP that depends (resp., does not depend) on  $x$  is said to be **dynamic** (resp., **static**), because  $\tilde{x}$  depends (resp., does not depend) on the previous value of  $x$ .

### 1. Deterministic MTP

Suppose  $S_{\tilde{x}} \subset S_x$  and we are given a function  $\tilde{x}_c(\cdot) : S_x \rightarrow S_{\tilde{x}}$ . Then let the TPM, printed in blue, for node  $\tilde{x}$ , be as follows:

$$P(\tilde{x} = \tilde{x}|x = x, c) = \delta(\tilde{x}, \tilde{x}_c(x)) \quad (60.12)$$

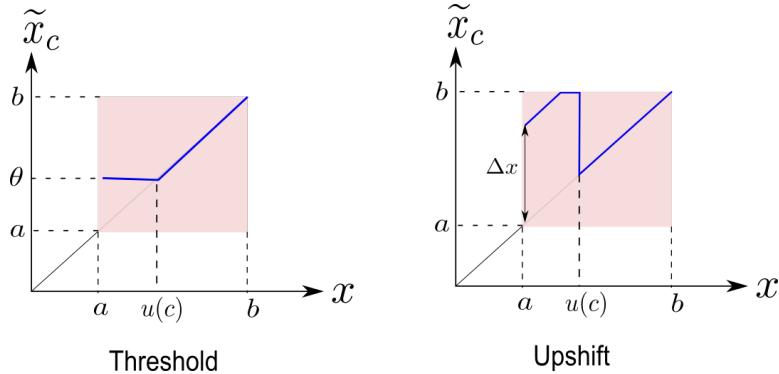


Figure 60.3: Two possible maps  $\tilde{x}_c : [a, b] \rightarrow [a, b]$  for a deterministic MTP.

Examples of  $\tilde{x}_c(x)$ :

- threshold in the value of  $x$  for small values of  $x$ . (See Fig.60.3)

Let  $S_x = [a, b]$  where  $a < b$ . For some  $\theta \in [a, b]$  and  $u(c) \in [a, b]$ , set

$$\tilde{x}_c(x) = \begin{cases} \theta & \text{if } x \leq u(c) \\ x & \text{if } x > u(c) \end{cases} \quad (60.13)$$

- upshift in the value of  $x$  for small values of  $x$ . (See Fig.60.3)

Let  $S_x = [a, b]$  where  $a < b$ . For some  $\Delta x > 0$ , and  $u(c) \in [a, b]$ , set

$$\tilde{x}_c(x) = \begin{cases} (x + \Delta x) & \text{if } x < u(c) \text{ and } (x + \Delta x) \in [a, b] \\ x & \text{if } x > u(c) \\ b & \text{if } (x + \Delta x) > b \end{cases} \quad (60.14)$$

### 2. Stochastic MTP

For some convenient, user specified, probability distribution  $P(\tilde{x}|x', x, c)$ , where  $\tilde{x} \in S_{\tilde{x}}$ ,  $x, x' \in S_x$ , and  $c \in S_c$ , let the TPM, printed in blue, for node  $\tilde{x}$ , be as follows:

$$P(\tilde{x}|x, c) = \sum_{x' \in S_{\underline{x}}} P(\tilde{x}|x', x, c) \underbrace{P(\underline{x} = x'|c)}_{\text{unmodified propensity}} \quad (60.15)$$

Examples

- Suppose we are given a function  $x_c : S_{\tilde{x}} \rightarrow S_{\underline{x}}$ . ( $x_c(\tilde{x})$  could be the inverse, if it exists, of the function  $\tilde{x}_c(x)$  defined in the deterministic TMP case.)

$$P(\tilde{x}|x, c) = \frac{P(\underline{x} = x_c(\tilde{x})|c)}{\sum_{\tilde{x}} \text{numerator}} \quad (60.16)$$

- Suppose  $S_{\underline{x}} = S_{\tilde{x}} = \{0, 1\}$ ,  $\theta \in \mathbb{R}$ , and let

$$P(\tilde{x}|x, c) = [\pi(x|c)]^{\tilde{x}}[1 - \pi(x|c)]^{1-\tilde{x}} \quad (60.17)$$

where

$$\pi(x|c) = \frac{\theta^x P(\underline{x} = x|c)}{\sum_x \text{numerator}} \quad (60.18)$$

## 60.2 $\Delta_{|c}$ estimand

Let

$$\mathcal{Y}_{|x,c} = \sum_y y P(\underline{y}(x) = y | x, c) \quad (60.19)$$

$$= \sum_y y P(\underline{y} = y | x, c) \quad (60.20)$$

$$\tilde{\mathcal{Y}}_{|\tilde{x}=\tilde{x}, c} = \sum_y y P(\underline{y}(\tilde{x}) = y | \tilde{x}, c) \quad (60.21)$$

$$= \sum_y y P(\underline{y} = y | \tilde{x}, c) \quad (60.22)$$

$$\tilde{\mathcal{Y}}_{|\underline{x}=x, c} = \sum_{\tilde{x}} \tilde{\mathcal{Y}}_{|\tilde{x}=\tilde{x}, c} P(\tilde{x}|x, c) \quad (60.23)$$

$$\mathcal{Y}_{|c} = \sum_x \mathcal{Y}_{|x,c} P(x|c), \quad \mathcal{Y} = \sum_c P(c) \mathcal{Y}_{|c} \quad (60.24)$$

$$\tilde{\mathcal{Y}}_{|c} = \sum_x \tilde{\mathcal{Y}}_{|\underline{x}=x,c} P(x|c), \quad \tilde{\mathcal{Y}} = \sum_c P(c) \tilde{\mathcal{Y}}_{|c} \quad (60.25)$$

Note that there are two  $\tilde{\mathcal{Y}}$ , namely  $\tilde{\mathcal{Y}}_{|\underline{x}=x,c}$  and  $\tilde{\mathcal{Y}}_{|\tilde{x}=\tilde{x},c}$ . Define the  $\Delta_{|c}$  estimand by:

$$\Delta_{|c} = \mathcal{Y}_{|c} - \tilde{\mathcal{Y}}_{|c}, \quad \Delta = \sum_c P(c) \Delta_{|c} \quad (60.26)$$

$\Delta_{|c}$  measures the difference between the real world represented by  $\mathcal{Y}_{|c}$  and a modified world represented by  $\tilde{\mathcal{Y}}_{|c}$ .

**Claim 87** Consider the deterministic MTP case  $P(\tilde{x}|x,c) = \delta(\tilde{x}, \tilde{x}_c(x))$ , where the function  $\tilde{x} = \tilde{x}_c(x)$  is invertible with inverse  $x = x_c(\tilde{x})$  for some  $x \in \mathbb{X} \subset \mathbb{R}$ . Then,

$$\tilde{\mathcal{Y}}_{|\underline{x}=x,c} = \mathcal{Y}_{|x_c(\tilde{x}),c} \quad (60.27)$$

**proof:**

$$\tilde{\mathcal{Y}}_{|\underline{x}=x,c} = \sum_{\tilde{x}} \sum_y y P(y = y | \tilde{x} = \tilde{x}, c) \delta(\tilde{x}, \tilde{x}_c(x)) \quad (60.28)$$

$$= \sum_y y P(y = y | \tilde{x} = \tilde{x}_c(x), c) \quad (60.29)$$

$$= \sum_y y P(y = y | \underline{x} = x_c(\tilde{x}), c) \quad (60.30)$$

$$= \mathcal{Y}_{|x_c(\tilde{x}),c} \quad (60.31)$$

**QED**

Henceforth in this chapter, we will restrict our attention to the deterministic MTP case in which  $P(\tilde{x}|x,c) = \delta(\tilde{x}, \tilde{x}_c(x))$ . We will also assume that the domain  $\mathbb{X}_c$  of  $\tilde{x}_c(x)$  is a union of disjoint sets  $\mathbb{X}_c^j$  for  $j = 1, 2, \dots, nj(c)$ , and that on each set  $\mathbb{X}_c^j$ ,  $\tilde{x}_c(x)$  is invertible and differentiable.

$$\begin{cases} \mathbb{X} = S_x \\ \mathbb{X}_c^j \cap \mathbb{X}_c^{j'} = \emptyset \text{ for } j \neq j' \\ \mathbb{X}_c = \cup_{j=1}^{nj(c)} \mathbb{X}_c^j \subset \mathbb{X} \end{cases} \quad (60.32)$$

$$\tilde{x}_c(x) = \sum_{j=1}^{nj(c)} \mathbb{1}(x \in \mathbb{X}_c^j) \tilde{x}_c^j(x) \quad (60.33)$$

$$P(\tilde{x}|x,c) = \delta(\tilde{x}, \tilde{x}_c(x)) = \sum_j \mathbb{1}(x \in \mathbb{X}_c^j) \delta(\tilde{x}, \tilde{x}_c^j(x)) \quad (60.34)$$

$$(\tilde{x}_c^j)^{-1}(\tilde{x}) = x^j(\tilde{x}) \quad (60.35)$$

$$\tilde{\mathbb{X}}_c^j = \tilde{x}_c^j(\mathbb{X}_c^j) = \{\tilde{x}_c^j(x) : x \in \mathbb{X}_c^j\} \quad (60.36)$$

$$P_{\mathbb{X}_c} = P(\underline{x} \in \mathbb{X}_c) \quad (60.37)$$

**Claim 88**

$$\tilde{\mathcal{Y}}_{|c} = \frac{1}{P_{\mathbb{X}_c}} E_{\tilde{x}|c} [\lambda_c(\tilde{x}) \mathcal{Y}_{|x_c(\tilde{x}), c}] , \quad (60.38)$$

$$\mathcal{Y}_{|c} = \frac{1}{P_{\mathbb{X}_c}} E_{\tilde{x}|c} [\lambda_c(\tilde{x}) \mathcal{Y}_{|\tilde{x}, c}] \quad (60.39)$$

and

$$P_{\mathbb{X}_c} = E_{\tilde{x}|c} [\lambda_c(\tilde{x})] \quad (60.40)$$

where<sup>3</sup>

$$\lambda_c(\tilde{x}) = \sum_j \mathbb{1}(\tilde{x} \in \tilde{\mathbb{X}}_c^j) \frac{dx_c^j(\tilde{x})}{d\tilde{x}} \underbrace{\frac{P(\underline{x} = x_c^j(\tilde{x})|c)}{P(\underline{x} = \tilde{x}|c)}}_{=1} \quad (60.41)$$

**proof:**

$$\tilde{\mathcal{Y}}_{|c} = \frac{1}{P_{\mathbb{X}_c}} \int_{x \in \mathbb{X}_c} dx P(x|c) \sum_y y P(y|\underline{x} = \tilde{x}_c(x), c) \quad (60.42)$$

$$= \frac{1}{P_{\mathbb{X}_c}} \sum_j \int_{x \in \mathbb{X}_c^j} dx P(x|c) \sum_y y P(y|\underline{x} = \tilde{x}_c^j(x), c) \quad (60.43)$$

$$= \frac{1}{P_{\mathbb{X}_c}} \sum_j \int_{\tilde{x} \in \tilde{\mathbb{X}}_c^j} d\tilde{x} \frac{dx_c^j(\tilde{x})}{d\tilde{x}} P(\tilde{x}|c) \underbrace{\frac{P(\underline{x} = x_c^j(\tilde{x})|c)}{P(\tilde{x}|c)}}_{\mathcal{Y}_{|x_c^j(\tilde{x}), c}} \sum_y y P(y|\underline{x} = x_c^j(\tilde{x}), c) \quad (60.44)$$

$$= \frac{1}{P_{\mathbb{X}_c}} \int_{\tilde{x} \in \tilde{\mathbb{X}}_c} d\tilde{x} P(\tilde{x}|c) \lambda_c(\tilde{x}) \mathcal{Y}_{|x_c(\tilde{x}), c} \quad (\text{see Eq(60.41)}) \quad (60.45)$$

$$= \frac{1}{P_{\mathbb{X}_c}} E_{\tilde{x}|c} [\lambda_c(\tilde{x}) \mathcal{Y}_{|x_c(\tilde{x}), c}] \quad (60.46)$$

To get Eq.(60.39), replace  $\mathcal{Y}_{|x_c(\tilde{x}), c}$  by  $\mathcal{Y}_{|\tilde{x}, c}$  in Eq.(60.38).

To get Eq.(60.40), replace  $\mathcal{Y}_{|x_c(\tilde{x}), c}$  by 1 in Eq.(60.38).

**QED**

From the last claim, it follows that

$$\Delta_{|c} = \frac{E_{y, \tilde{x}|c} [\lambda_c(\tilde{x})(y - \mathcal{Y}_{|x_c(\tilde{x}), c})]}{E_{\tilde{x}|c} [\lambda_c(\tilde{x})]} \quad (60.47)$$

---

<sup>3</sup> $\lambda_c(\tilde{x})$  is just a piecewise Jacobian. In Ref.[21], the part of Eq.(60.41) which is marked as being equal to 1 is incorrectly assumed to be different from 1.

## 60.3 Estimates of $\Delta_{|c}$

### 60.3.1 Empirical estimate of $\Delta_{|c}$

Consider a population  $\Sigma$  of individuals  $\sigma \in \Sigma$ , with  $|\Sigma| = N$ .

Let

$$N_c = \sum_{\sigma} \delta(c_{\sigma}, c) , \quad (60.48)$$

$$P(\sigma|c) = \frac{\delta(c_{\sigma}, c)}{N_c} , \quad (60.49)$$

and

$$E_{\sigma|c}[\xi_{\sigma}] = \sum_{\sigma} P(\sigma|c) \xi_{\sigma} . \quad (60.50)$$

Then set

$$\widehat{\Delta}_{|c} = \frac{E_{\sigma|c} [\lambda_c(\tilde{x}_{\sigma})(y_{\sigma} - \mathcal{Y}_{|x_c(\tilde{x}_{\sigma}), c})]}{E_{\sigma|c} [\lambda_c(\tilde{x}_{\sigma})]} \quad (60.51)$$

### 60.3.2 OR estimate of $\Delta_{|c}$

**Outcome Regression (OR)** estimate of  $\Delta_{|c}$ .

Calculate the following estimates in this order:  $\widehat{\tau} \rightarrow \widehat{\Delta}_{|c}$ .

Steps:

1. Calculate  $\widehat{\tau}$

Let

$$X^T = [1, \tilde{x}, c], \quad X_{\sigma}^T = [1, \tilde{x}_{\sigma}, c_{\sigma}] . \quad (60.52)$$

Use Generalized Linear Modeling (GLM)<sup>4</sup> to approximate  $y_{\sigma}$ :

$$y_{\sigma} \approx \widehat{y}(X_{\sigma}^T \widehat{\tau}) \quad (60.53)$$

$$\widehat{y}(X_{\sigma}^T \widehat{\tau}) = g^{-1}(X_{\sigma}^T \widehat{\tau}) \quad (60.54)$$

where  $g()$  is the link function.

2. Calculate  $\widehat{\Delta}_{|c}$

$$\widehat{\Delta}_{|c} = \frac{E_{\sigma|c} [\lambda_c(\tilde{x}_{\sigma})(y_{\sigma} - \widehat{y}(X_{\sigma}^T \widehat{\tau}))]}{E_{\sigma|c} [\lambda_c(\tilde{x}_{\sigma})]} \quad (60.55)$$

---

<sup>4</sup>GLM is discussed in Chapter 32.

**Claim 89** (*Asymptotic behavior of OR estimate*)

As  $N \rightarrow \infty$ ,

$$\sqrt{N_c}(\widehat{\Delta}_{|c} - \Delta_{|c}^*) \rightarrow \mathcal{N}(0, \mathcal{V}) \quad (60.56)$$

where

$$\mathcal{V} = E_{\sigma|c}[(IF_\sigma)^2] \quad (60.57)$$

$$IF_\sigma = \frac{R_\sigma(\widehat{\tau}, \widehat{\Delta}_{|c}) + B(\widehat{\tau})}{C} \quad (60.58)$$

$$R_\sigma(\tau, \Delta_{|c}) = \lambda_c(\tilde{x}_\sigma)(y_\sigma - \widehat{y}(X_\sigma^T \tau) - \Delta_{|c}) \quad (60.59)$$

$$C = -E_{\sigma|c}[\lambda_c(\tilde{x}_\sigma)] \quad (60.60)$$

$$B(\tau) = \sum_i E_{\sigma|c} \left[ \lambda_c(\tilde{x}_\sigma) \frac{\partial \widehat{y}(X_\sigma^T \tau)}{\partial \tau_i} \right] \frac{E_{\sigma|c}[S_{i,\sigma}(\tau)]}{E_{\sigma|c} \left[ \frac{\partial S_{i,\sigma}(\tau)}{\partial \tau_i} \right]} \quad (60.61)$$

(Note that index  $i$  labels the components of the column vector  $\tau$ )

**proof:**

Eq.(60.55) that defines the OR estimate can be rewritten as

$$0 = E_{\sigma|c}[\underbrace{\lambda_c(\tilde{x}_\sigma)(y_\sigma - \widehat{y}(X_\sigma^T \widehat{\tau}) - \widehat{\Delta}_{|c})}_{R_\sigma(\widehat{\tau}, \widehat{\Delta}_{|c})}] \quad (60.62)$$

If we Taylor expand  $R_\sigma(\widehat{\tau}, \widehat{\Delta}_{|c})$  to first order in each of its 2 estimator arguments, we get

$$E_{\sigma|c}[R_\sigma(\widehat{\tau}, \widehat{\Delta}_{|c})] = \begin{cases} \underbrace{E_{\sigma|c}[R_\sigma(\tau^*, \Delta_{|c}^*)]}_A \\ + \sum_i \underbrace{E_{\sigma|c} \left[ \frac{\partial R_\sigma(\tau^*, \Delta_{|c}^*)}{\partial \tau_i} \right]}_{B_i} (\widehat{\tau}_i - \tau_i^*) \\ + \underbrace{E_{\sigma|c} \left[ \frac{\partial R_\sigma(\tau^*, \Delta_{|c}^*)}{\partial \Delta_{|c}^*} \right]}_{-C} (\widehat{\Delta}_{|c} - \Delta_{|c}^*) \end{cases} \quad (60.63)$$

Solving the last equation for  $\widehat{\Delta}_{|c} - \Delta_{|c}^*$  yields

$$\widehat{\Delta}_{|c} - \Delta_{|c}^* = \frac{A + \overbrace{\sum_i^B B_i(\widehat{\tau}_i - \tau_i^*)}^{C}}{C} \quad (60.64)$$

Assuming  $y_\sigma \in \{0, 1\}$ , define the Cross Entropy and its first derivative with respect to  $\tau_i$  by

$$CE_\sigma = \sum_{y_\sigma=0,1} y_\sigma \ln \widehat{y}(X_\sigma^T \tau) \quad (60.65)$$

$$S_{i,\sigma}(\tau) = \frac{\partial CE_\sigma}{\partial \tau_i} \quad (60.66)$$

In this notation, according to the maximum likelihood principle, the best choice of parameters  $\tau_i$  must satisfy

$$0 = E_{\sigma|c}[S_{i,\sigma}(\widehat{\tau})] \quad (60.67)$$

If we Taylor expand  $S_{i,\sigma}(\widehat{\tau})$  to first order in its estimator argument, we get

$$E_{\sigma|c}[S_{i,\sigma}(\widehat{\tau})] = E_{\sigma|c}[S_{i,\sigma}(\tau^*)] + E_{\sigma|c} \left[ \frac{\partial S_{i,\sigma}(\tau^*)}{\partial \tau_i} \right] (\widehat{\tau}_i - \tau_i^*) \quad (60.68)$$

Hence,

$$\widehat{\tau}_i - \tau_i^* = - \frac{E_{\sigma|c}[S_{i,\sigma}(\tau^*)]}{E_{\sigma|c} \left[ \frac{\partial S_{i,\sigma}(\tau^*)}{\partial \tau_i} \right]} . \quad (60.69)$$

Now putting our previous results together, we get

$$A = E_{\sigma|c}[R_\sigma(\tau^*, \Delta_{|c}^*)] \quad (60.70)$$

$$= E_{\sigma|c}[\lambda_c(\tilde{x}_\sigma)(y_\sigma - \widehat{y}(X_\sigma^T \tau^*) - \Delta_{|c}^*)] \quad (60.71)$$

$$B_i = -E_{\sigma|c} \left[ \lambda_c(\tilde{x}_\sigma) \frac{\partial \widehat{y}(X_\sigma^T \tau^*)}{\partial \tau_i^*} \right] \quad (60.72)$$

$$B(\tau^*) = \sum_i B_i(\widehat{\tau}_i - \tau_i^*) \quad (60.73)$$

$$= \sum_i E_{\sigma|c} \left[ \lambda_c(\tilde{x}_\sigma) \frac{\partial \widehat{y}(X_\sigma^T \tau^*)}{\partial \tau_i^*} \right] \frac{E_{\sigma|c}[S_{i,\sigma}(\tau^*)]}{E_{\sigma|c} \left[ \frac{\partial S_{i,\sigma}(\tau^*)}{\partial \tau_i} \right]} \quad (60.74)$$

$$C = -E_{\sigma|c}[\lambda_c(\tilde{x}_\sigma)] \quad (60.75)$$

$$IF_\sigma = \frac{R_\sigma(\hat{\tau}, \hat{\Delta}_{|c}) + B(\hat{\tau})}{C} \quad (60.76)$$

$$\mathcal{V} = E_{\sigma|c}[(IF_\sigma)^2] \quad (60.77)$$

**QED**

## 60.4 Other Estimands besides $\Delta_{|c}$

Suppose  $\tilde{x}_0, \tilde{x}_1 \in S_{\tilde{x}}$ . Define the **Modified ATE (MATE)** by

$$MATE_{|c} = \tilde{\mathcal{Y}}_{|\tilde{x}=\tilde{x}_1, c} - \tilde{\mathcal{Y}}_{|\tilde{x}=\tilde{x}_0, c} \quad (60.78)$$

$$MATE = \sum_c P(c) MATE_{|c} \quad (60.79)$$

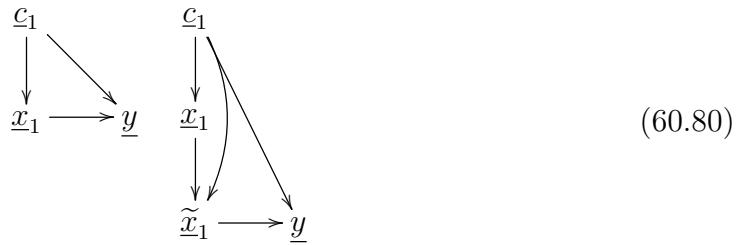
## 60.5 Multi-time MTP

A g-formula is any formula that defines recursively the full probability distribution of a bnet. In other words, it's a recursive definition of a Dynamical Bayesian Network.<sup>5</sup>

Let's define a g-formula<sup>6</sup> for Multi-time (a.k.a. longitudinal) MTP (LMTP).

Consider  $t = 1, 2, \dots, nt$ ,

For  $nt = 1$ ,



$$P(y, x_1, c_1) = P(y|x_1, c_1)P(x_1|c_1)P(c_1) \quad (60.81)$$

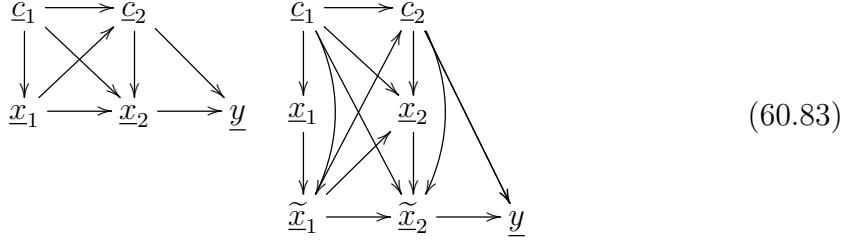
$$P(y, \tilde{x}_1, x_1, c_1) = P(y|\tilde{x}_1, c_1)P(x_1|c_1)P(\tilde{x}_1|x_1, c_1)P(c_1) \quad (60.82)$$

For  $nt = 2$ ,

---

<sup>5</sup>Dynamical Bayesian Networks are discussed in Chapter 25.

<sup>6</sup>Chapter 30 defines a different g-formula that we call a sequential backdoor g-formula.

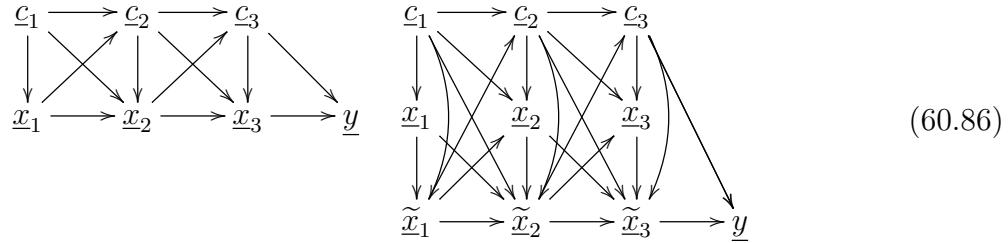


(60.83)

$$P(y, x_{\leq 2}, c_{\leq 2}) = \begin{cases} P(x_1|c_1)P(c_1) \\ *P(x_2|x_1, c_{2,1})P(c_2|x_1, c_1) \\ *P(y|x_2, c_2) \end{cases} \quad (60.84)$$

$$P(y, \tilde{x}_{\leq 2}, x_{\leq 2}, c_{\leq 2}) = \begin{cases} P(x_1|c_1)P(\tilde{x}_1|x_1, c_1)P(c_1) \\ *P(x_2|\tilde{x}_1, c_{2,1})P(\tilde{x}_2|x_2, c_{2,1})P(c_2|\tilde{x}_1, c_1) \\ *P(y|\tilde{x}_2, c_2) \end{cases} \quad (60.85)$$

For  $nt = 3$ ,



(60.86)

$$P(y, x_{\leq 3}, c_{\leq 3}) = \begin{cases} P(x_1|c_1)P(c_1) \\ *P(x_2|x_1, c_{2,1})P(c_2|x_1, c_1) \\ *P(x_3|x_2, c_{3,2})P(c_3|x_2, c_2) \\ *P(y|x_3, c_3) \end{cases} \quad (60.87)$$

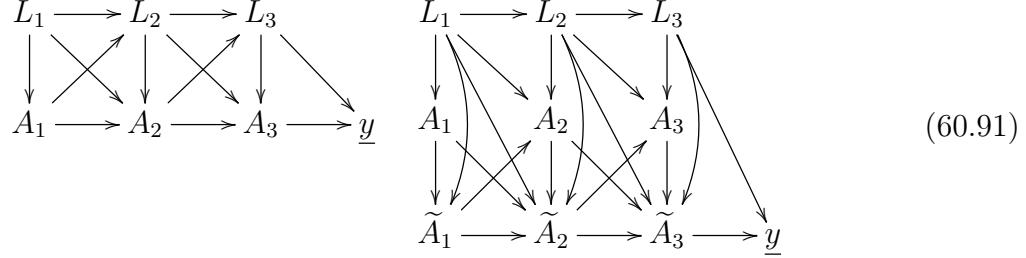
$$P(y, \tilde{x}_{\leq 3}, x_{\leq 3}, c_{\leq 3}) = \begin{cases} P(x_1|c_1)P(\tilde{x}_1|x_1, c_1)P(c_1) \\ *P(x_2|\tilde{x}_1, c_{2,1})P(\tilde{x}_2|\tilde{x}_1, x_{2,1}, c_{2,1})P(c_2|\tilde{x}_1, c_1) \\ *P(x_3|\tilde{x}_2, c_{3,2})P(\tilde{x}_3|\tilde{x}_2, x_{3,2}, c_{3,2})P(c_3|\tilde{x}_2, c_2) \\ *P(y|\tilde{x}_3, c_3) \end{cases} \quad (60.88)$$

In general,

$$P(y, x_{\leq nt}, c_{\leq nt}) = \begin{cases} \prod_{t=1}^{nt} \{P(x_t|x_{t-1}, c_{t,t-1})P(c_t|x_{t-1}, c_{t-1})\} \\ *P(y|x_{nt}, c_{nt}) \end{cases} \quad (60.89)$$

$$P(y, \tilde{x}_{\leq nt}, x_{\leq nt}, c_{\leq nt}) = \begin{cases} \prod_{t=1}^{nt} P(x_t|\tilde{x}_{t-1}, c_{t,t-1})P(\tilde{x}_t|\tilde{x}_{t-1}, x_{t,t-1}, c_{t,t-1})P(c_t|\tilde{x}_{t-1}, c_{t-1}) \\ *P(y|\tilde{x}_{nt}, x_{nt}, c_{nt}) \end{cases} \quad (60.90)$$

Note that Ref.[23] by Hernán and Robins (HR) uses the notation  $L_t = \underline{c}_t$ ,  $A_t = \underline{x}_t$  for  $t = 1, 2, \dots, nt$ . Hence, the  $nt = 3$  bnet Eq.(60.86), written in the HR notation, is as follows (before and after adding the  $\tilde{A}$  nodes):



HR doesn't actually display the  $\tilde{A}$  nodes in its DAGs. Furthermore, in HR, nodes  $A_t$  and  $L_t$  have parent nodes that are time steps  $0, 1, 2, 3, \dots$  in the past. I, on the other hand, do not draw or consider parents that are more than one time steps in the past, because I assume the effect of those parents is negligible to first approximation.

# Chapter 61

## Monty Hall Problem

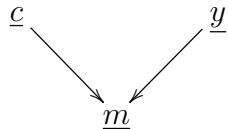


Figure 61.1: Monty Hall Problem.

Mr. Monty Hall, host of the game show "Let's Make a Deal", hides a car behind one of three doors and a goat behind each of the other two. The contestant picks Door No. 1, but before opening it, Mr. Hall opens Door No. 2 to reveal a goat. Should the contestant stick with No. 1 or switch to No. 3?

The Monty Hall problem can be modeled by the bnet Fig.61.1, where

- $\underline{c}$  = the door behind which the car actually is.
- $\underline{y}$  = the door opened by you (the contestant), on your first selection.
- $\underline{m}$  = the door opened by Monty (game host)

We label the doors 1,2,3 so  $S_c = S_y = S_m = \{1, 2, 3\}$ .

The TPMs, printed in blue, for this bnet, are as follows:

$$P(c) = \frac{1}{3} \text{ for all } c \quad (61.1)$$

$$P(y) = \frac{1}{3} \text{ for all } y \quad (61.2)$$

$$P(m|c, y) = \mathbb{1}(m \neq c) \left[ \frac{1}{2} \mathbb{1}(y = c) + \mathbb{1}(y \neq c) \mathbb{1}(m \neq y) \right] \quad (61.3)$$

It's easy to show that the above node probabilities imply that

$$P(c = 1|m = 2, y = 1) = \frac{1}{3} \quad (61.4)$$

$$P(c = 3|m = 2, y = 1) = \frac{2}{3} \quad (61.5)$$

So you are twice as likely to win if you switch your final selection to be the door which is neither your first choice nor Monty's choice.

The way I justify this to myself is: Monty gives you a piece of information. If you don't switch your choice, you are wasting that info, whereas if you switch, you are using the info.

# Chapter 62

## Multi-armed Bandits

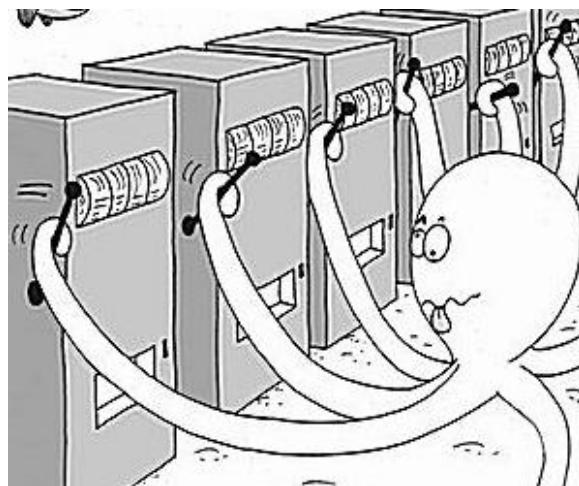


Figure 62.1: Multi-armed bandit (MAB).

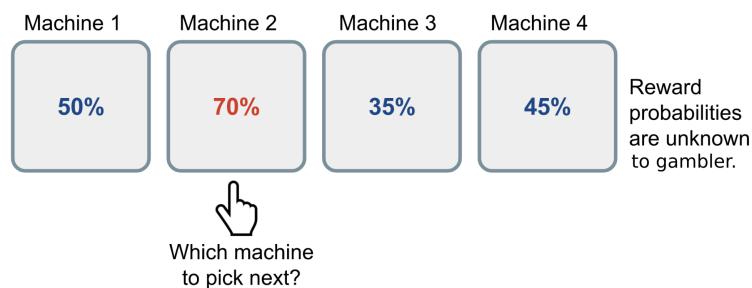


Figure 62.2: Bernoulli MAB (Bern-MAB) with 4 arms. For a Bern-MAB, the conditional probability distribution  $P(r|a)$  for reward  $r$ , given arm  $a$ , is initially totally unknown to the gambler (agent), but it is known by the environment to be a Bernoulli distribution  $P(r|a) = \mu_a^r(1 - \mu_a)^{1-r}$  for  $r \in \{0, 1\}$ , where  $0 < \mu_a < 1$  for each  $a$ . The percentages shown are  $\mu_a$  for each arm  $a$ .

This chapter is mostly based on Refs. [58] and [84].

Multi-armed Bandits (MABs) are a simple version of Reinforcement Learning (RL). RL is discussed in Chapter 78.

The term “one-armed-bandit” is a humorous term for what is also called a slot machine. A slot machine is a gambling device which has a slot into which you put coins or tokens for the privilege of being allowed to pull down a lever (arm) on one side of the device. This action generates a random combination of three shapes, which may or may not, depending on their combination, entitle the player to a money award.

Multi-armed bandit (MAB) is the name given to the optimization problem that considers an agent (gambler) that is playing multiple one-armed-bandits, each with a possibly different odds of winning. The optimization problem is to determine an efficient schedule whereby the gambler can converge on the device with the highest odds of winning.

MABs are often used in marketing as an alternative to A/B testing. These 2 methods yield different information but overlap in that they both can discover consumer preferences.

The MAB problem is an optimization problem (i.e., finding the maximum of a reward function or the minimum of a cost function). As with any minimization problem, an algorithm to solve it runs the danger of converging to a local minimum that isn’t the global (i.e., the overall) minimum. This danger can be diminished by doing both **exploration and exploitation**. Algorithms that do no exploration, only exploitation, are said to be **greedy**, and they are at the highest risk of converging to a non-global minimum.

## 62.1 Bnet for MAB

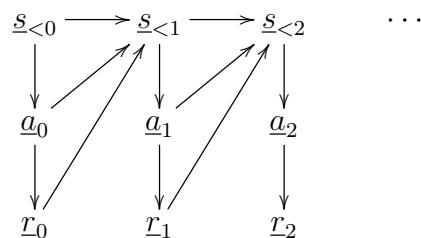


Figure 62.3: Bnet for a multi-armed bandit (MAB).

Let

$t \in \{0, 1, 2, \dots\}$  be the **time** slice (step),

$\underline{a}_t \in \{0, 1, \dots, N_a - 1\} = S_a$  be the **arm** of bandit that is pulled at time  $t$ , out of  $N_a$  arms. In RL language, it's also the **action** taken.

$\underline{r}_t \in \mathbb{R}$  be the **reward** at time  $t$ ,

$s_{<t} = \underbrace{[(a_\tau, r_\tau) : \tau < t]}_{s_\tau}$  be the **state** at time  $t$ .

Fig.62.3 shows a bnet for a MAB. The TPMs, printed in blue, for this bnet, are as follows.

$$P(s_{<t}|s_{<t-1}, a_{t-1}, r_{t-1}) = \mathbb{1}(s_{<t} = s_{<t-1} \cup (a_{t-1}, r_{t-1})) \quad (62.1)$$

For  $t = 0$ ,  $s_{<0} = \emptyset$ , so choose a random  $a_0$ .

$$P(a_t|s_{<t}) = \mathbb{1}(a_t = a_t^*) \text{ (agent's response)} , \quad (62.2)$$

where  $a_t^*$  depends on the **strategy (a.k.a. policy)** being used by the **gambler (agent)**. We consider various strategies below.  $a_t^*$  is defined solely in terms of empirical data (i.e.,  $a_t, r_t$  values) collected from previous time-slices. That is the only type of information that the gambler is privy to.  $a_0^*$  is chosen at random. The formulae for  $a_t^*$  that we give below for various strategies should only be used for  $t > 0$ .

$$P(r_t|a_t) = P_{r|a}(r_t|a_t) \text{ (environment's response)} . \quad (62.3)$$

$P_{r|a}$  is a probabilistic model that models the **environment** in which the agent lives. This assumes that the  $a_t$  (and the  $r_t$ ) are i.i.d.  $P_{r|a}$  depends on parameters whose values are known by the environment, but are not known a priori by the gambler. In fact, the goal of this exercise is for the gambler to find ever more accurate estimates of those parameters, using only the empirical data he/she can collect from the past, starting from total ignorance about those parameters.

For a **Bernoulli MAB (Bern-MAB)**, the conditional probability distribution  $P_{r|a}$  is a Bernoulli distribution

$$P(r|a) = \mu_a^r (1 - \mu_a)^{1-r} \quad (62.4)$$

for  $r \in \{0, 1\}$ , where  $0 < \mu_a < 1$  for each  $a$ . The parameters  $\mu_a$  are initially unknown to the gambler. Note that  $E[r|a] = \sum_r r P(r|a) = P(r=1|a) = \mu_a$ .

For a **Gaussian MAB**, the conditional probability distribution  $P_{r|a}$  is a Normal (Gaussian) distribution

$$P(r|a) = \mathcal{N}(r; \mu_a, \sigma_a^2) . \quad (62.5)$$

for  $r \in \mathbb{R}$ . The parameters  $\mu_a, \sigma_a^2$  are initially unknown to the gambler.

## 62.2 Reward functions

For  $a \in S_{\underline{a}}$ , define the **Long term Average Reward** for action  $a$  by

$$\mu_a = Q(a) = E_{|a}[\underline{r}] = \sum_r r P(r|a) . \quad (62.6)$$

Let

$$a^* = \operatorname{argmax}_a Q(a) \quad (62.7)$$

$$\mu^* = \max_a Q(a) = Q(a^*) \quad (62.8)$$

$$\Delta_a = \mu^* - Q(a) \quad (62.9)$$

$\mu_a, a^*, \mu^*$  and  $\Delta_a$  are not known to the gambler.

Define the **Instantaneous (at time  $t$ ) Average Reward** for action  $a$  by

$$Q_t(a) = \frac{1}{N_t(a)} \sum_{\tau=0}^t r_\tau \mathbb{1}(a_\tau = a) \quad (62.10a)$$

where

$$N_t(a) = N_{in} + \sum_{\tau=0}^t \mathbb{1}(a_\tau = a) \quad (62.10b)$$

$N_{in} > 0$  insures that we never divide by zero. Note that Eqs.(62.10) can be stated recursively as

$$N_t(a)Q_t(a) = N_{t-1}(a)Q_{t-1}(a) + r_t \mathbb{1}(a_t = a) \quad (62.11a)$$

$$N_t(a) = N_{t-1}(a) + \mathbb{1}(a_t = a) \quad (62.11b)$$

with  $Q_{-1}(a) = 0$  and  $N_{-1}(a) = N_{in}$  for all  $a$ . We assume that at large  $t$ ,  $N_{in} \ll N_t(a)$  for all  $a$ . For instance, one can use  $N_{in} = 1$ .

$Q(a)$  is not known to the gambler but  $N_t(a)$  and  $Q_t(a)$  are because they are empirical.

We will write a hat over random variables that are defined by an empirical probability distribution.<sup>1</sup> Whereas we assume that  $\underline{a}_t$  and  $\underline{r}_t$  are i.i.d., we will not assume that  $\widehat{a}_t$  and  $\widehat{r}_t$  are i.i.d. for finite times  $t$ . What we will assume is that as  $t \rightarrow \infty$ ,

---

<sup>1</sup>An alternative convention is to not distinguish between  $\widehat{a}_t$  and  $\underline{a}_t$ , or between  $\widehat{r}_t$  and  $\underline{r}_t$ , but to distinguish between  $P(r_t|a_t)$  and  $\widehat{P}(r_t|a_t)$ , where  $\widehat{P}()$  is an empirical estimate of  $P()$ .

$$\widehat{a}_t \rightarrow \underline{a}, \quad \widehat{r}_t \rightarrow \underline{r} \quad (62.12)$$

Note that

$$\sum_a \frac{N_t(a)}{t+1} = 1 \quad (62.13)$$

so define

$$P(\widehat{a}_t = a) = \frac{N_t(a)}{t+1}. \quad (62.14)$$

Thus

$$E[Q(\widehat{a}_t)] = \sum_a P(\widehat{a}_t = a) Q(a). \quad (62.15)$$

**Claim 90**

$$Q_t(a) = E_{|\widehat{a}_t=a}[\widehat{r}_t] \quad (62.16)$$

**proof:**

Note that

$$\sum_r \sum_{\tau=0}^t \frac{\mathbb{1}(a_\tau = a, r_\tau = r)}{N_t(a)} = 1. \quad (62.17)$$

so define

$$P(\widehat{r}_t = r | \widehat{a}_t = a) = \sum_{\tau=0}^t \frac{\mathbb{1}(a_\tau = a, r_\tau = r)}{N_t(a)}. \quad (62.18)$$

Thus

$$Q_t(a) = \sum_r r \sum_{\tau=0}^t \frac{\mathbb{1}(a_\tau = a, r_\tau = r)}{N_t(a)} \quad (62.19)$$

$$= \sum_r r P(\widehat{r}_t = r | \widehat{a}_t = a) \quad (62.20)$$

$$= E_{|\widehat{a}_t=a}[\widehat{r}_t] \quad (62.21)$$

**QED**

**Claim 91** As  $t \rightarrow \infty$ ,

$$Q_t(a) \rightarrow E_{a=a}[\underline{r}] = Q(a) \quad (62.22)$$

$$E[Q(\widehat{a}_t)] \rightarrow E[Q(\underline{a})] \quad (62.23)$$

**proof:** This is clear from  $\hat{a}_t \rightarrow a$  and  $\hat{r}_t \rightarrow r$  and Claim 90.

**QED**

## 62.3 Regret functions

Define the **Instantaneous (at time  $t$ ) Average Regret (I-Regret)** by

$$IReg_t = \mu^* - E[Q(\hat{a}_t)] = E[\Delta_{\hat{a}_t}] \quad (62.24)$$

and the **Cumulative (for times  $\leq t$ ) Average Regret (C-Regret)** by

$$CReg_t = \sum_{\tau=0}^t IReg_\tau . \quad (62.25)$$

Note that

$$CReg_t = \sum_{\tau=0}^t E[\Delta_{\hat{a}_\tau}] \quad (62.26)$$

$$= \sum_a \Delta_a \sum_{\tau=0}^t \frac{N_\tau(a)}{\tau + 1} \quad (62.27)$$

Let

$$\rho_t = \frac{1}{t+1} \sum_{t=0}^t r_t . \quad (62.28)$$

Define the **Cumulative Average Reward (C-Reward)** by

$$CRew_t = E_{|\hat{a}_t=a}[(t+1)\hat{\rho}_t] . \quad (62.29)$$

It can be shown that minimizing the C-Regret is equivalent to maximizing the C-Reward.

**Claim 92** As  $t \rightarrow \infty$ ,

$$IReg_t \rightarrow E[\Delta_a] \quad (62.30)$$

**proof:** This is clear from  $\hat{a}_t \rightarrow a$  and  $\hat{r}_t \rightarrow r$ .

**QED**

## 62.4 Strategies with random exploration

In this section, we consider MAB algorithms that explore all values of the action  $a$  at random. In the section following this one, we consider MAB algorithm that do a more deliberate search of the action space.

### 62.4.1 $\epsilon$ -greedy algorithm

Recall that  $\underline{a}_t \in \{0, 1, \dots, N_a - 1\} = S_a$ . The user of the algorithm specifies an  $\epsilon \in [0, 1]$  which measures the amount of exploration to be conducted.

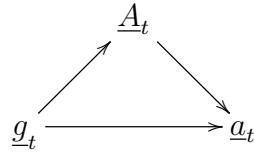


Figure 62.4: Extra structure added to MAB Bnet Fig.62.3 for  $\epsilon$ -greedy algorithm.

For each  $t$ , add extra the structure shown in Fig.62.4 to the MAB bnet Fig.62.3.  $g_t \in \{0, 1\}$  and  $a_t, A_t \in S_a$ . ("g" stands for greedy). The TPMs, printed in blue, for the new nodes, are as follows

$$P(g_t) = \begin{cases} \epsilon & (\text{exploration}) & \text{if } g_t = 0 \\ 1 - \epsilon & (\text{exploitation}) & \text{if } g_t = 1 \end{cases}. \quad (62.31)$$

$$P(A_t|g_t) = \begin{cases} \frac{1}{N_a} & (\text{exploration}) & \text{if } g_t = 0 \\ \mathbb{1}(A_t = 0) & (\text{exploitation}) & \text{if } g_t = 1 \end{cases} \quad (62.32)$$

$$P(a_t|A_t, g_t) = \begin{cases} \mathbb{1}(a_t = A_t) & (\text{exploration}) & \text{if } g_t = 0 \\ \mathbb{1}(a_t = a_t^*) & (\text{exploitation}) & \text{if } g_t = 1 \end{cases} \quad (62.33)$$

where  $a_t^*$  is defined as follows:

$$a_t^* = \underset{a}{\operatorname{argmax}} Q_{t-1}(a).$$

(62.34)

As  $t \rightarrow \infty$ ,

$$\frac{N_t(a)}{t+1} = P(\hat{a}_t = a) \quad (62.35)$$

$$\rightarrow P(a, g_t = 0)\epsilon + P(a, g_t = 1)(1 - \epsilon) \quad (62.36)$$

$$\geq P(a, g_t = 0)\epsilon \quad (62.37)$$

$$= \frac{\epsilon}{N_{\underline{a}}} \quad (62.38)$$

Hence

$$IReg_t = \sum_a \Delta_a \sum_{\tau=0}^t \frac{N_\tau(a)}{\tau+1} \quad (62.39)$$

$$\geq \frac{\epsilon}{N_{\underline{a}}} \sum_a \Delta_a \quad (62.40)$$

and  $CReg_t \geq \mathcal{N}(!t)(t+1)$ .

### 62.4.2 $\epsilon_t$ -greedy algorithm

Replace time-independent constant  $\epsilon$  in the  $\epsilon$ -greedy algorithm by a time dependent function  $\epsilon_t$ .

## 62.5 Strategies with nonrandom exploration

### 62.5.1 Upper Confidence Bounds (UCB) algorithms

A MAB algorithm that maximizes merely  $Q_t(a)$  to get  $a_t^*$  is totally greedy (i.e., does no exploration, only exploitation). This doesn't work too well because once the algo finds a particular  $a_t^*$ , it sticks with it. For times  $t$  after that, the  $Q_t(a)$  for all  $a$  stay more or less the same. The  $N_t(a)$  for  $a \neq a_t^*$  also stay the same. Only  $N_t(a_t^*)$  increases. To avoid this problem, **Upper Confidence Bounds (UCB) algorithms** maximize an effective  $Q_t(a)_{\text{eff}} = Q_t(a) + U_t(a)$ , where  $U_t(a) > 0$ , instead of maximizing merely  $Q_t(a)$  to get  $a_t^*$ .  $U_t(a)$  is proportional to  $1/\sqrt{N_t(a)}$  (that's a property of UCBs). Adding  $U_t(a)$  to  $Q_t(a)$  gives those  $a$  with low  $N_t(a)$  a  $Q_t(a)_{\text{eff}} \gg Q_t(a)$ . This encourages exploration of  $a$  different from  $a_t^* = \operatorname{argmax}_a Q_t(a)$ . In conclusion, for all UCB algorithms, we have

$$a_t^* = \operatorname{argmax}_a [Q_{t-1}(a) + U_{t-1}(a)] \quad (62.41)$$

Different UCB algos differ only in the definition of  $U_t(a)$ .

Next, we consider two UCB algorithms, frequentist UCB (UCB1), and Bayesian UCB.

## Frequentist UCB (UCB1) algorithm

**Claim 93** (*Hoeffding's Inequality- HI*) Let  $\underline{x}_0, \underline{x}_1, \dots, \underline{x}_{T-1}$  be i.i.d. random variables such that  $0 \leq \underline{x}_t \leq 1$  for all  $t$ . Let  $\underline{m}_{T-1} = \frac{1}{T} \sum_{t=0}^{T-1} \underline{x}_t$  denote the sample mean. Then for  $u > 0$ , we have:

$$P(E[\underline{x}] > \underline{m}_{T-1} + u) \leq e^{-2Tu^2}. \quad (62.42)$$

**proof:** See Ref.[120].

**QED**

Let<sup>2</sup>

$$\underline{x}^T = \{\underline{x}_t : t \in \mathbb{Z}_{[0, T-1]}\} \quad (62.43)$$

and

$$\underline{r}_{\leq t-1}(a) = \{\underline{r}_\tau : \underline{a}_\tau = a, \tau \in \mathbb{Z}_{[0, t-1]}\}. \quad (62.44)$$

Note that  $\underline{x}^T$  has  $T$  components and  $\underline{r}_{\leq t-1}(a)$  has  $N_{t-1}(a)$  components. If we apply the HI with  $\underline{x}^T$  replaced by  $\underline{r}_{\leq t-1}(a)$ , we get

$$P(Q(a) > Q_{t-1}(a) + U_{t-1}(a)) \leq e^{-2N_{t-1}(a)[U_{t-1}(a)]^2} \quad (62.45)$$

If we define a threshold probability  $p$  by

$$p = e^{-2N_{t-1}(a)[U_{t-1}(a)]^2}, \quad (62.46)$$

then

$$U_{t-1}(a) = \sqrt{\frac{-\ln p}{2N_{t-1}(a)}} \quad (62.47)$$

If we choose  $p = (t-1)^{-\alpha}$ ,

$$a_t^* = \underset{a}{\operatorname{argmax}} \left[ Q_{t-1}(a) + \sqrt{\frac{\alpha(t-1)}{2N_{t-1}(a)}} \right]$$

(62.48)

## Bayesian UCB algorithm

**Claim 94**<sup>3 4</sup> (*Bayesian updating of mean and deviation. See Fig.62.5.*)  
Suppose

<sup>2</sup>As usual, we define  $\mathbb{Z}_{[a,b]} = \{a, a+1, a+2, \dots, b\}$  for  $a < b$ .

<sup>3</sup>For a **standard deviation**  $\sigma$ , the **precision**  $\tau$  is defined as  $\tau = \frac{1}{\sigma^2}$ .

<sup>4</sup> $\underline{x}|\lambda \sim \mathcal{D}(\lambda)$  means that  $P(x|\lambda) = \mathcal{D}(x; \lambda)$ .  $\mathcal{N}()$  stands for the Normal distribution and  $\text{Gamma}()$  for the Gamma distribution. See Ref.[114] for a discussion of the Gamma distribution.

$$x^n = [x_i] , \quad x_i \text{ are i.i.d. with } \underline{x}_i | \mu, \tau \sim \mathcal{N}(\mu, \tau) \quad (62.49)$$

$$\underline{\mu} | \tau \sim \mathcal{N}(\mu_0, n_0 \tau) \quad (62.50)$$

$$\underline{\tau} \sim \text{Gamma}(\alpha, \beta) . \quad (62.51)$$

Then the posterior is

$$\underline{\mu} | \tau, x^n \sim \mathcal{N} \left( \frac{n \bar{x} + n_0 \mu_0}{n + n_0} , (n + n_0) \tau \right) \quad (62.52)$$

$$\underline{\tau} | x^n \sim \text{Gamma} \left( \alpha + \frac{n}{2} , \beta + \frac{1}{2} \sum_i (x_i - \bar{x})^2 + \frac{n n_0}{2(n + n_0)} (\bar{x} - \mu_0)^2 \right) \quad (62.53)$$

**proof:** See Ref.[28].

**QED**

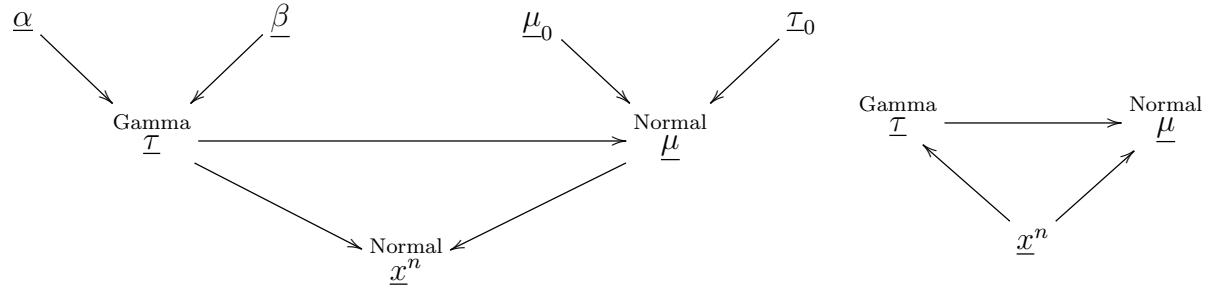


Figure 62.5: Prior and Posterior BNets in Claim 94.

In the Bayesian UCB algorithm, we use

$$a_t^* = \underset{a}{\operatorname{argmax}} E_{\mu_a, \sigma_a | s_{<t}} \left[ \mu_a + c \frac{\sigma_a}{\sqrt{N_{t-1}(a)}} \right] \quad (62.54)$$

for some  $c > 0$ .

Eq.62.54 requires that we know  $P(\mu_a, \sigma_a | s_{<t})$ ; i.e., the posterior distribution of  $\mu_a, \sigma_a$  assuming the prior history  $s_{<t}$ . This follows from Bayes theorem if we assume a Normal distribution for the likelihood  $P(s_{<t} | \mu_a, \sigma_a)$  and we assume conjugate priors for  $P(\mu_a, \sigma_a)$ . More precisely, if we replace  $\underline{x}^n$  by  $\underline{s}_{<t}$  in Claim 94, then

$$P(\mu_a, \tau_a | s_{<t}) = P(\mu_a | \tau_a, s_{<t}) P(\tau_a | s_{<t}) \quad (62.55)$$

where  $P(\mu_a | \tau_a, s_{<t})$  and  $P(\tau_a | s_{<t})$  are given by Claim 94.

### 62.5.2 Thompson Sampling MAB (TS-MAB) algorithm

Bnet for general TS-MAB algorithm

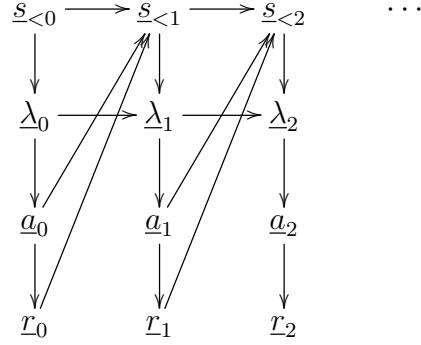


Figure 62.6: Bnet for TS-MAB algorithm.

The Thompson Sampling MAB (TS-MAB) algorithm is described by the bnet Fig.62.6. This bnet differs from the bnet Fig.62.3 in that it includes new nodes  $\lambda_t$ . The TPMs, printed in blue, for bnet Fig.62.6, are as follows.

$$P(s_{<t}|s_{<t-1}, a_{t-1}, r_{t-1}) = \text{ same as for Fig.62.3} \quad (62.56)$$

$$P(\lambda_t|s_{<t}, \lambda_{t-1}) = \mathbb{1}(\lambda_t = \lambda_t^*(s_{<t}, \lambda_{t-1})) \quad (62.57)$$

where  $\lambda_t^*$  is a function to be defined below.

$$P(a_t|\lambda_t) = \mathbb{1}[a_t = a_t(\lambda_t)] \quad (\text{Agent's response}) \quad (62.58)$$

where  $a_t(\lambda_t)$  is a function to be described below.

$$P(r_t|a_t) = \text{ same as for Fig.62.3. } (\text{Environment's response}) \quad (62.59)$$

Let

$$Q_t(a, \lambda_t) = \sum_r r P(\hat{r}_t = r | \hat{a}_t = a, \lambda_t) \quad (62.60)$$

$$= E_{|\hat{a}_t=a, \lambda_t}[\hat{r}_t]. \quad (62.61)$$

Define

$$a_t(\lambda_t) = \operatorname{argmax}_a Q_t(a, \lambda_t) . \quad (62.62)$$

Note that

$$P(a_t | s_{<t}) = \sum_{\lambda_t} P(\lambda_t | s_{<t}) \mathbb{1}[Q_t(a_t, \lambda_t) = \max_a Q_t(a, \lambda_t)] \quad (62.63a)$$

$$= \sum_{\lambda_t} P(\lambda_t | s_{<t}) \mathbb{1}[a_t = a_t(\lambda_t)] \quad (62.63b)$$

$$= E_{\lambda_t | s_{<t}} \{ \mathbb{1}[a_t = a_t(\lambda_t)] \} . \quad (62.63c)$$

If we further assume that  $P(\lambda_t | s_{<t})$  is a delta function, then Eqs.(62.63) reduce to

$$P(a_t | s_{<t}) = \mathbb{1}[a_t = a_t(\lambda_t^*)] \quad (62.64)$$

### TS-MAB algorithm with Beta agent and Bernoulli environment

The Beta distribution  $\text{Beta}(x; \alpha, \beta)$  (see Ref.[94]) is defined for  $\alpha > 0, \beta > 0$  and  $x \in [0, 1]$ . Since  $x \in [0, 1]$ ,  $x$  can be interpreted as a probability. The mean and variance of the Beta distribution are

$$E[\underline{x}] = \frac{\alpha}{\alpha + \beta} , \quad (62.65)$$

$$\langle \underline{x}, \underline{x} \rangle = \frac{\alpha\beta}{(\alpha + \beta)^2(\alpha + \beta + 1)} . \quad (62.66)$$

From this mean and variance, we see that if we increase  $\alpha$  by one and leave  $\beta$  the same, the mean moves towards 1 and the variance decreases. Likewise, if we increase  $\beta$  by 1 and leave  $\alpha$  the same, the mean moves towards 0 and the variance decreases.

Let

$$\alpha_t^a = \sum_{\tau=0}^t \mathbb{1}(r_\tau = 1, a_\tau = a) \quad (62.67)$$

$$\beta_t^a = \sum_{\tau=0}^t \mathbb{1}(r_\tau = 0, a_\tau = a) \quad (62.68)$$

$$\lambda_t^a = (\alpha_{t-1}^a, \beta_{t-1}^a) \quad (62.69)$$

$$\lambda_t = [(\alpha_{t-1}^a, \beta_{t-1}^a) : a \in S_{\underline{a}}] \quad (62.70)$$

$$Q_t(a, \lambda_t) = \sum_r r \text{Beta}(r; \alpha_{t-1}^a, \beta_{t-1}^a) \quad (62.71\text{a})$$

$$= \frac{\alpha_{t-1}^a}{\alpha_{t-1}^a + \beta_{t-1}^a} \quad (62.71\text{b})$$

The TS-MAB algorithm for a Beta agent and Bernoulli environment can be described by the bnet Fig.62.6. For this special case of bnet Fig.62.6, the TPMs, printed in blue, are as follows.

$$P(s_{<t}|s_{<t-1}, a_{t-1}, r_{t-1}) = \text{ same as for Fig.62.6} \quad (62.72)$$

$$P(\lambda_t^a|s_{<t}, \lambda_{t-1}) = \mathbb{1}(\lambda_t^a = \lambda_t^{*a}) = \begin{cases} \mathbb{1}(\lambda_t^a = \lambda_{t-1}^a) & \text{if } a \neq a_{t-1} \\ \mathbb{1}(\lambda_t^a = (\alpha_{t-2}^a + 1, \beta_{t-2}^a)) & \text{if } a_{t-1} = a \text{ and } r_{t-1} = 1 \\ \mathbb{1}(\lambda_t^a = (\alpha_{t-2}^a, \beta_{t-2}^a + 1)) & \text{if } a_{t-1} = a \text{ and } r_{t-1} = 0 \end{cases} \quad (62.73)$$

$$P(\underline{a}_t|\lambda_t) = \mathbb{1}(a_t = a_t(\lambda_t)) \quad (62.74)$$

$$= \mathbb{1}(a_t = \underset{a}{\operatorname{argmax}} \underbrace{Q_t(a, \lambda_t)}_{\text{see Eq.(62.71)}}) \quad (\text{Beta agent response}) \quad (62.75)$$

$$P(r_t|a_t) = \mu_{at}^{rt} (1 - \mu_{at})^{rt} \quad (\text{Bernoulli environment response}) . \quad (62.76)$$

$\mu_a$  known to environment but unknown to agent.

### TS-MAB algorithm, skeletal reprise

The TS-MAB algorithm is not very complicated but explaining it with precision requires nightmarishly many indices. Here is a pedagogical reprise of what we have said so far, where we have stripped out some of the inessential indices.

$$P(\lambda) = \mathbb{1}(\lambda, \lambda^*) \quad (62.77)$$

$$P(a|\lambda) = \mathbb{1}(a = a(\lambda)) \quad (62.78)$$

$$= \mathbb{1}(a = \underset{a}{\operatorname{argmax}} \sum_r r P(\hat{r} = r | \hat{a} = a, \lambda)) \quad (62.79)$$

$$= \mathbb{1}(a = \underset{a}{\operatorname{argmax}} \sum_r r \text{Beta}(r; \lambda^a)) \quad (\text{Beta agent response}) \quad (62.80)$$

Define  $q()$  by

$$q(r; \lambda^a) = P(\hat{r} = r | \hat{a} = a, \lambda) \quad (62.81)$$

- PRIOR:

$$P(a) = \sum_{\lambda} P(\lambda) P(a|\lambda) \quad (62.82)$$

$$= P(a|\lambda^*) \quad (62.83)$$

$$= \mathbb{1}(a = \operatorname{argmax}_a \sum_r r q(r; \lambda^{*a})) \quad (62.84)$$

1. Use fact that  $q = \text{Beta}$

$$\sum_r r \text{Beta}(r; \lambda^{*a}) = \frac{\alpha^{*a}}{\alpha^{*a} + \beta^{*a}} \quad (62.85)$$

2. Don't use fact that  $q = \text{Beta}$ .

For each  $a$ , get samples  $r^\sigma \sim q(r; \lambda^{*a})$  for  $\sigma = 0, 1, \dots, nsam - 1$  and estimate

$$\sum_r r q(r; \lambda^{*a}) \approx \frac{1}{nsam} \sum_{\sigma} r^\sigma q(r^\sigma; \lambda^{*a}). \quad (62.86)$$

This sampling is why TS is called a sampling.

- LIKELIHOOD:

$$P(r|a) = \mu_a^r (1 - \mu_a)^{r'} \quad (\text{Bernoulli environment response}) \quad (62.87)$$

### 62.5.3 Grad-MAB algorithm

Let

$$\lambda_{t+1}(a) = \lambda_t(a) + \eta r_t [\mathbb{1}(a_t = a) - \pi_t(a)] \quad (62.88)$$

for some  $\eta > 0$ , where  $\pi_t(a)$  is defined by

$$\pi_t(a) = P(\underline{a}_t = a | \lambda_t) = \frac{e^{\lambda_t(a)}}{\sum_a e^{\lambda_t(a)}} \cdot \underbrace{\sum_a e^{\lambda_t(a)}}_{\text{softmax}(\lambda_t)(a)}. \quad (62.89)$$

The  $\lambda_t(a)$  are called **scores** at time  $t$ . Let

$$a_t^* = \operatorname{argmax}_a \pi_t(a)$$

(62.90)

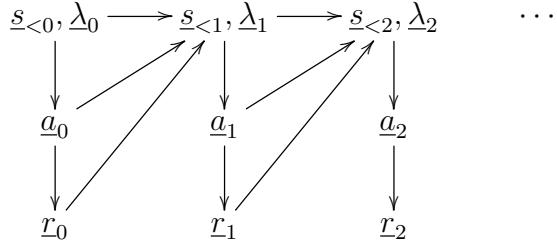


Figure 62.7: Bnet for Grad-MAB algorithm.

The Gradient MAB (Grad-MAB) algorithm is described by the bnet Fig.62.7. This bnet differs from the bnet Fig.62.3 in that it includes new nodes  $\underline{\lambda}_t$ . The TPMs, printed in blue, for bnet Fig.62.7, are as follows.

$$P(\underline{\lambda}_{t+1} = \lambda | a_t, r_t, \lambda_t) = \mathbb{1}(\lambda = \lambda_{t+1} \text{ given by Eq.(62.88)}). \quad (62.91)$$

$$P(a_t | \lambda_t) = \mathbb{1}(a_t = a_t^*) \quad \text{or, alternatively, } = P(\underline{a}_t = a_t | \lambda_t) = \pi_t(a_t) \quad (\text{agent's response}) \quad (62.92)$$

$$P(r_t | a_t) = P_{\underline{r}|\underline{a}}(r_t | a_t) \quad (\text{environment's response}). \quad (62.93)$$

Motivation:

Define the **Instantaneous Average Reward** by

$$\mathcal{R}_t(\lambda_t) = \sum_a P(\underline{a}_t = a | \lambda_t) E_{r_t | a_t = a}[\underline{r}_t] = E_{r_t, a_t | \lambda_t}[\underline{r}_t]. \quad (62.94)$$

We will assume that as  $t \rightarrow \infty$ ,  $\underline{a}_t \rightarrow \underline{a}$ ,  $\underline{r}_t \rightarrow \underline{r}$  and  $\lambda_t \rightarrow \lambda$ . Therefore,  $\mathcal{R}_t(\lambda_t) \rightarrow E_{\underline{r}, \underline{a} | \lambda}[\underline{r}] = E_{\underline{r} | \lambda}[\underline{r}]$ .

Note that if  $E_{r_t | a_t = a}[\underline{r}_t] = B$ , where  $B$  is independent of  $a$ , then  $\mathcal{R}_t(\lambda_t) = B$  and  $\frac{\partial \mathcal{R}_t}{\partial \lambda_t(a)} = 0$ .

**Claim 95** *The gradient of  $\mathcal{R}_t(\lambda_t)$  is*

$$\frac{\partial \mathcal{R}_t}{\partial \lambda_t(a)} = E_{r_t, a_t | \lambda_t}[g(r_t, \underline{a}_t | a, \lambda_t)] \quad (62.95)$$

where

$$g(r_t, \underline{a}_t | a, \lambda_t) = r_t [\mathbb{1}(\underline{a}_t = a) - \pi_t(a)] \quad (62.96)$$

**proof:**

$$\frac{\partial \mathcal{R}_t}{\partial \lambda_t(a)} = \sum_{a'} \frac{\partial \pi_t(a')}{\partial \lambda_t(a)} E_{\underline{r}_t | \underline{a}_t = a'} [\underline{r}_t] \quad (62.97)$$

$$= \sum_{a'} \pi_t(a') \frac{\partial \ln \pi_t(a')}{\partial \lambda_t(a)} E_{\underline{r}_t | \underline{a}_t = a'} [\underline{r}_t] \quad (62.98)$$

$$= \sum_{a'} \pi_t(a') \frac{\partial}{\partial \lambda_t(a)} \left[ \ln \frac{\exp[\lambda_t(a')]}{\sum_a \exp[\lambda_t(a)]} \right] E_{\underline{r}_t | \underline{a}_t = a'} [\underline{r}_t] \quad (62.99)$$

$$= \sum_{a'} \pi_t(a') [\mathbb{1}(a' = a) - \pi_t(a)] E_{\underline{r}_t | \underline{a}_t = a'} [\underline{r}_t] \quad (62.100)$$

$$= \sum_{a'} P(\underline{a}_t = a' | \lambda_t) E_{\underline{r}_t | \underline{a}_t = a'} [\underline{r}_t (\mathbb{1}(a' = a) - \pi_t(a))] \quad (62.101)$$

$$= E_{\underline{r}_t, \underline{a}_t | \lambda_t} [g(\underline{r}_t, \underline{a}_t | a, \lambda_t)] \quad (62.102)$$

**QED**

Eq.(62.88) can be written as

$$\lambda_{t+1}(a) = \lambda_t(a) + \eta g(r_t, a_t | a, \lambda_t) \quad (62.103)$$

# Chapter 63

## Naive Bayes

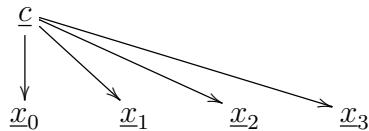


Figure 63.1: bnet for Naive Bayes with 4 features

Class node  $\underline{c} \in S_{\underline{c}}$ .  $|S_{\underline{c}}| = n_{\underline{c}}$ = number of classes.

Feature nodes  $\underline{x}_i \in S_{\underline{x}_i}$  for  $i = 0, 1, 2, \dots, F - 1$ .  $F$ =number of features.

Define

$$x. = [x_0, x_1, \dots, x_{F-1}] . \quad (63.1)$$

For the bnet of Fig.63.1,

$$P(c, x.) = P(c) \prod_{i=0}^{F-1} P(x_i|c) . \quad (63.2)$$

Given  $x.$  values, find most likely class  $c \in S_{\underline{c}}$ .

Maximum a Posteriori (MAP) estimate:

$$c^* = \operatorname{argmax}_c P(c|x.) \quad (63.3)$$

$$= \operatorname{argmax}_c \frac{P(c, x.)}{P(x.)} \quad (63.4)$$

$$= \operatorname{argmax}_c P(c, x.) . \quad (63.5)$$

# Chapter 64

## Neural Networks

In this chapter, we discuss Neural Networks (NNs) of the feedforward kind, which is the most popular kind. In their plain, vanilla form, NNs only have deterministic nodes. But the nodes of a bnet can be deterministic too, because the TPM of a node can reduce to a delta function. Hence, NNs should be expressible as bnets. We will confirm this in this chapter.

Henceforth in this chapter, if we replace an index of an indexed quantity by a dot, it will mean the collection of the indexed quantity for all values of that index. For example,  $x.$  will mean the array of  $x_i$  for all  $i$ .

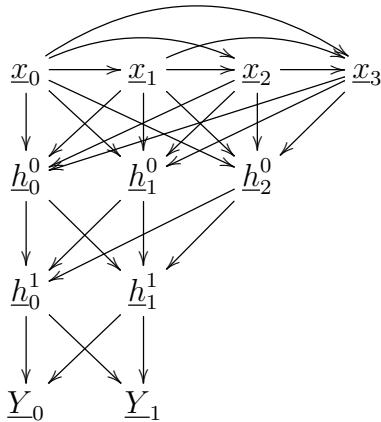


Figure 64.1: Neural Network (feed forward) with 4 layers: input layer  $\underline{x}.$ , 2 hidden layers  $\underline{h}^0.$ ,  $\underline{h}^1.$  and output layer  $\underline{Y}.$

Consider Fig.64.1.

$\underline{x}_i \in \{0, 1\}$  for  $i = 0, 1, 2, \dots, nx - 1$  is the **input layer**.

$\underline{h}_i^\lambda \in \mathbb{R}$  for  $i = 0, 1, 2, \dots, nh(\lambda) - 1$  is the  $\lambda$ -th **hidden layer**.  $\lambda = 0, 1, 2, \dots, \Lambda - 2$ . A NN is said to be **deep** if  $\Lambda > 2$ ; i.e., if it has more than one hidden layer.

$\underline{Y}_i \in \mathbb{R}$  for  $i = 0, 1, 2, \dots, ny - 1$  is the **output layer**. We use a upper case y here because in the training phase, we will use pairs  $(x.[\sigma], y.[\sigma])$  where  $y_i[\sigma] \in \{0, 1\}$

for  $i = 0, 1, \dots, ny - 1$ .  $Y = \hat{y}$  is an estimate of  $y$ . Note that lower case  $y$  is either 0 or 1, but upper case  $Y$  may be any real. Often, the activation functions are chosen so that  $Y \in [0, 1]$ .

The number of nodes in each layer and the number of layers are arbitrary. Fig.64.1 is fully connected (a.k.a. dense), meaning that every node of a layer is impinged arrow coming from every node of the preceding layer. Later on in this chapter, we will discuss non-dense layers.

Let  $w_{i|j}^\lambda, b_i^\lambda \in \mathbb{R}$  be given, for  $i \in \mathbb{Z}_{[0, nh(\lambda)]}$ ,  $j \in \mathbb{Z}_{[0, nh(\lambda-1)]}$ , and  $\lambda \in \mathbb{Z}_{[0, \Lambda]}$ .

The TPMs, printed in blue, for bnet Fig.64.1, are as follows.

$$P(x_i | x_{i-1}, x_{i-2}, \dots, x_0) = \text{given} \quad (64.1)$$

$$P(h_i^\lambda | h_{\cdot}^{\lambda-1}) = \delta \left( h_i^\lambda, \mathcal{A}_i^\lambda \left( \sum_j w_{i|j}^\lambda h_j^{\lambda-1} + b_i^\lambda \right) \right), \quad (64.2)$$

where  $P(h_i^0 | h^{-1}) = P(h_i^0 | x)$ .

$$P(Y_i | h_{\cdot}^{\lambda-2}) = \delta \left( Y_i, \mathcal{A}_i^{\lambda-1} \left( \sum_j w_{i|j}^{\lambda-1} h_j^{\lambda-2} + b_i^{\lambda-1} \right) \right). \quad (64.3)$$

## 64.1 Activation Functions $\mathcal{A}_i^\lambda : \mathbb{R} \rightarrow \mathbb{R}$

Activation functions must be nonlinear. Why? Because if they were all linear, the NN mapping would be a bijection (1-1 onto map), and its domain and range would be the same. That is not what you want for a classifier. For a classifier, you want the range to be much smaller than the domain.

- **Step function (Perceptron)**

$$\mathcal{A}(x) = \mathbb{1}(x > 0) \quad (64.4)$$

Zero for  $x \leq 0$ , one for  $x > 0$ .

- **Sigmoid function**

$$\mathcal{A}(x) = \frac{1}{1 + e^{-x}} = \text{smoid}(x) \quad (64.5)$$

Smooth, monotonically increasing function.  $\text{smoid}(-\infty) = 0, \text{smoid}(0) = 1/2, \text{smoid}(\infty) = 1$ .

- **Hyperbolic tangent**

$$\mathcal{A}(x) = \tanh(x) = \frac{e^x - e^{-x}}{e^x + e^{-x}} \quad (64.6)$$

Smooth, monotonically increasing function.  $\tanh(-\infty) = -1, \tanh(0) = 0, \tanh(\infty) = 1$ .

Odd function:

$$\tanh(-x) = -\tanh(x) \quad (64.7)$$

Whereas smoid( $x$ )  $\in [0, 1]$ ,  $\tanh(x) \in [-1, 1]$ .

- **ReLU (Rectified Linear Unit)**

$$\mathcal{A}(x) = \underbrace{x \mathbb{1}(x > 0)}_{x_+} = \max(0, x) . \quad (64.8)$$

Compare this to the step function  $\mathbb{1}(x > 0)$ .

- **Swish**

$$\mathcal{A}(x) = x \text{ smoid}(x) \quad (64.9)$$

- **Softmax**

$$\mathcal{A}(x_i|x.) = \frac{e^{x_i}}{\sum_i e^{x_i}} = \text{softmax}(x.)(i) \quad (64.10)$$

The softmax definition implies that the bnet nodes within a softmax layer are fully connected by arrows to form a “clique”.

## 64.2 Weight optimization via supervised training and gradient descent

The bnet of Fig.64.1 is used for classification of a single data point  $x..$ . It assumes that the weights  $w_{ij}^\lambda, b_i^\lambda$  are given.

To find the optimum weights via supervised training and gradient descent, one uses the bnet Fig.64.2.

In Fig.64.2, the nodes in Fig.64.1 become sampling space vectors. For example,  $\underline{x}.$  becomes  $\vec{x}.$ , where the components of  $\vec{x}.$  in sampling space are  $\underline{x}.[\sigma] \in \{0, 1\}^{nx}$  for  $\sigma = 0, 1, \dots, nsam(\vec{x}) - 1$ .  $nsam(\vec{x})$  is the number of samples in the whole dataset.

To train a NN bnet with a dataset, the standard procedure is to split the dataset into 3 parts (I like to call them the **ttt datasets**):

1. **training dataset**,

2. **tuning (a.k.a. validation) dataset**, for tuning of hyperparameters like  $nsam(\vec{x})$ ,  $\Lambda$ , and  $nh(i)$  for each  $i$ .

### 3. testing dataset

Weights only change while training on the training dataset. While the model is being trained, its performance is periodically tested on the tuning dataset. Training continues until performance on the tuning dataset no longer improves. After that happens, the model is finally applied to the testing dataset.

The training dataset is split into batches. An **epoch** is a pass through all the batches in the training dataset.

Define

$$W_{i|j}^\lambda = [w_{i|j}^\lambda, b_i^\lambda] . \quad (64.11)$$

The TPMs, printed in blue, for bnet Fig.64.2, are as follows.

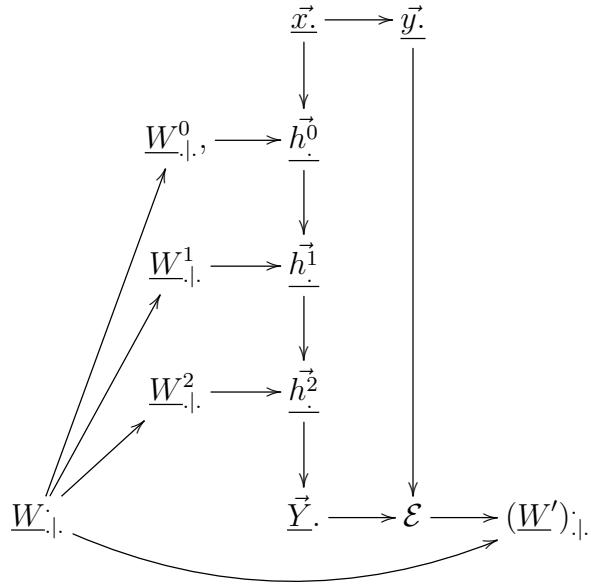


Figure 64.2: bnet for finding optimum weights of the bnet Fig.64.1 via supervised training and gradient descent.

$$P(x.[\sigma]) = \text{given} . \quad (64.12)$$

$$P(y.[\sigma] | x.[\sigma]) = \text{given} . \quad (64.13)$$

$$P(h_i^\lambda[\sigma] | h_i^{\lambda-1}[\sigma]) = \delta\left(h_i^\lambda[\sigma], \mathcal{A}_i^\lambda\left(\sum_j w_{i|j}^\lambda h_j^{\lambda-1}[\sigma] + b_i^\lambda\right)\right) \quad (64.14)$$

$$P(Y_i[\sigma] | h_i^{\Lambda-2}[\sigma]) = \delta\left(Y_i[\sigma], \mathcal{A}_i^{\Lambda-1}\left(\sum_j w_{i|j}^{\Lambda-1} h_j^{\Lambda-2}[\sigma] + b_i^{\Lambda-1}\right)\right) \quad (64.15)$$

$$P(W_{\cdot|\cdot}) = \text{given} \quad (64.16)$$

The first time it is used,  $W_{\cdot|\cdot}$  is arbitrary. After the first time, it is determined by previous stage.

$$P(W_{\cdot|\cdot}^\lambda | W_{\cdot|\cdot}) = \delta(W_{\cdot|\cdot}^\lambda, (W_{\cdot|\cdot}))^\lambda \quad (64.17)$$

$$P(\mathcal{E} | \vec{y}_{\cdot}, \vec{Y}_{\cdot}) = \frac{1}{nsam(\vec{x})} \sum_{\sigma} \sum_i d(y_i[\sigma], Y_i[\sigma]) , \quad (64.18)$$

where

$$d(y, Y) = |y - Y|^2 . \quad (64.19)$$

If  $y, Y \in [0, 1]$ , one can use this instead

$$d(y, Y) = XE(y \rightarrow Y) = -y \ln Y - (1 - y) \ln(1 - Y) . \quad (64.20)$$

$$P((W')_{i|j}^\lambda | \mathcal{E}, W_{\cdot|\cdot}) = \delta((W')_{i|j}^\lambda, W_{i|j}^\lambda - \eta \partial_{W_{i|j}^\lambda} \mathcal{E}) \quad (64.21)$$

$\eta > 0$  is called the learning rate. This method of minimizing the error  $\mathcal{E}$  is called gradient descent.  $W' - W = \Delta W = -\eta \partial_W \mathcal{E}$  so  $\Delta \mathcal{E} = \frac{-1}{\eta} (\Delta W)^2 < 0$ .

### 64.3 Non-dense layers

The TPM for a non-dense layer is of the form:

$$P(h_i^\lambda[\sigma] | h_i^{\lambda-1}[\sigma]) = \delta(h_i^\lambda[\sigma], H_i^\lambda[\sigma]) , \quad (64.22)$$

where  $H_i^\lambda[\sigma]$  will be specified below for each type of non-dense layer.

- **Dropout Layer**

The dropout layer was invented in Ref.[64]. To dropout nodes from a fixed layer  $\lambda$ : For all  $i$  of layer  $\lambda$ , define a new node  $\underline{r}_i^\lambda$  with an arrow  $\underline{r}_i^\lambda \rightarrow \underline{h}_i^\lambda$ . For  $r \in \{0, 1\}$ , and some  $p \in (0, 1)$ , define

$$P(\underline{r}_i^\lambda = r) = [p]^r[1 - p]^{1-r} \text{ (Bernoulli dist.) .} \quad (64.23)$$

Now one has

$$P(\underline{h}_i^\lambda[\sigma] | \underline{h}_{\cdot}^{\lambda-1}[\sigma], \underline{r}_i^\lambda) = \delta(\underline{h}_i^\lambda[\sigma], H_i^\lambda[\sigma]) , \quad (64.24)$$

where

$$H_i^\lambda[\sigma] = \mathcal{A}_i^\lambda(\underline{r}_i^\lambda \sum_j w_{i|j}^\lambda h_j^{\lambda-1}[\sigma] + b_i^\lambda) . \quad (64.25)$$

This reduces overfitting. Overfitting might occur if the weights follow too closely several similar batches. This dropout procedure adds a random component to each batch making groups of similar batches less likely.

The random  $\underline{r}_i^\lambda$  nodes that induce dropout are only used in the training bnet Fig.64.2, not in the classification bnet Fig.64.1. We prefer to remove the  $\underline{r}_i^\lambda$  stochasticity from classification and for Fig.64.1 to act as an average over sampling space of Fig.64.2. Therefore, if weights  $w_{i|j}^\lambda$  are obtained for a dropout layer  $\lambda$  in Fig.64.2, then that layer is used in Fig.64.1 with no  $\underline{r}_i^\lambda$  nodes but with weights  $\langle \underline{r}_i^\lambda \rangle w_{i|j}^\lambda = pw_{i|j}^\lambda$ .

Note that dropout adds non-deterministic nodes to a NN, which in their vanilla form only have deterministic nodes.

- **Convolutional Layer**

- 1-dim

Filter function  $\mathcal{F} : \{0, 1, \dots, nf - 1\} \rightarrow \mathbb{R}$ .

$\sigma$ =stride length

For  $i \in \{0, 1, \dots, nh(\lambda) - 1\}$ , let

$$H_i^\lambda[\sigma] = \sum_{j=0}^{nf-1} h_{j+i\sigma}^{\lambda-1}[\sigma] \mathcal{F}(j) . \quad (64.26)$$

For the indices not to go out of bounds in Eq.(64.26), we must have

$$nh(\lambda - 1) - 1 = nf - 1 + (nh(\lambda) - 1)\sigma \quad (64.27)$$

so

$$nh(\lambda) = \frac{1}{\sigma}[nh(\lambda - 1) - nf] + 1 . \quad (64.28)$$

- 2-dim

$h_i^\lambda[\sigma]$  becomes  $h_{(i,j)}^\lambda[\sigma]$ . Do 1-dim convolution along both  $i$  and  $j$  axes.

### • Pooling Layers (MaxPool, AvgPool)

Here each node  $i$  of layer  $\lambda$  is impinged by arrows from a subset  $Pool(i)$  of the set of all nodes of the previous layer  $\lambda - 1$ . Partition set  $\{0, , 1, \dots, nh(\lambda - 1) - 1\}$  into  $nh(\lambda)$  mutually disjoint, nonempty sets called  $Pool(i)$ , where  $i \in \{0, 1, \dots, nh(\lambda) - 1\}$ .

- AvgPool

$$H_i^\lambda[\sigma] = \frac{1}{|Pool(i)|} \sum_{j \in Pool(i)} h_j^{\lambda-1}[\sigma] \quad (64.29)$$

- MaxPool

$$H_i^\lambda[\sigma] = \max_{j \in Pool(i)} h_j^{\lambda-1}[\sigma] \quad (64.30)$$

## 64.4 Autoencoder NN

If the sequence

$$nx, nh(0), nh(1), \dots, nh(\Lambda - 2), ny \quad (64.31)$$

first decreases monotonically up to layer  $\lambda_{min}$ , then increases monotonically until  $ny = nx$ , then the NN is called an **autoencoder NN**. Autoencoders are useful for unsupervised learning and feature reduction. In this case,  $Y$  estimates  $x$ . The layers before layer  $\lambda_{min}$  are called the **encoder**, and those after  $\lambda_{min}$  are called the **decoder**. Layer  $\lambda_{min}$  is called the **code**.

# Chapter 65

## Noisy-OR gate

The Noisy-OR gate was first proposed by Judea Pearl in his 1988 book Ref.[50].

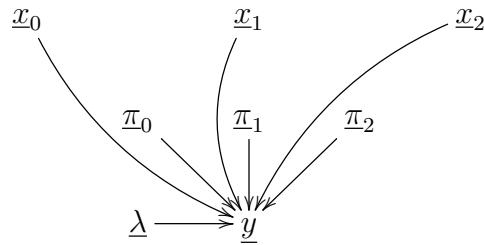


Figure 65.1: Noisy-OR gate  $\underline{y} \in \{0, 1\}$  with  $n = 3$ , Boolean inputs  $(\underline{x}_i)_{i=0,1,2}$  and parameters  $\lambda, (\underline{\pi})_{i=0,1,2}$ .

Let

$\underline{\lambda} \in [0, 1]$  =gate lea.k.a.ge.

$y \in \{0, 1\}$  = gate output

$x^n = (\underline{x}_i)_{i=0,1,\dots,n-1}$ , where  $\underline{x}_i \in \{0, 1\}$  are gate inputs.

$\pi^n = (\underline{\pi}_i)_{i=0,1,\dots,n-1}$ , where  $\underline{\pi}_i \in [0, 1]$  are gate parameters.

The TPM, printed in blue, for the Noisy-OR gate  $\underline{y}$  shown in Fig.65.1, is as follows.

$$P(y = 1|x^n, \lambda, \pi^n) = 1 - (1 - \lambda) \prod_i [1 - \pi_i \underline{x}_i] \quad (65.1)$$

$$P(y = 0|x^n, \lambda, \pi^n) = 1 - P(y = 1|x^n, \lambda, \pi^n) \quad (65.2)$$

Note that if  $\lambda = 0$  and  $\pi_i = 1$  for all  $i$ , then this becomes a deterministic OR-gate. Indeed,

$$P(y = 1|x^n, \lambda = 0, \pi^n = 1^n) = 1 - \prod_i [1 - x_i] = \vee_{i=0}^{n-1} x_i , \quad (65.3)$$

so

$$P(y|x^n, \lambda = 0, \pi^n = 1^n) = \delta(y, \vee_{i=0}^{n-1} x_i) . \quad (65.4)$$

## 65.1 3 ways to interpret the parameters $\pi_i$

1. Note that if  $\lambda = 0$  and  $x^n$  is one hot (i.e.,  $x^n = e_i^n$ , where  $e_i^n$  is the vector with all components zero except for the  $i$ -th component which equals 1), then

$$P(y = 1|x^n = e_i^n, \lambda = 0, \pi^n) = 1 - [1 - \pi_i] = \pi_i . \quad (65.5)$$

This gives an interpretation to the parameters  $\pi_i$ .

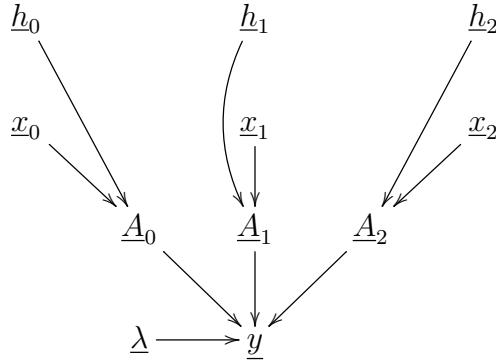


Figure 65.2: Fig.65.1 after replacing parameters  $(\underline{\pi}_i)_{i=0,1,2}$  by hidden nodes  $(\underline{h}_i)_{i=0,1,2}$ .

2. Another way of interpreting the parameters  $\pi_i$  is to associate each of them with a hidden variable  $\underline{h}_i \in \{0, 1\}$  whose average equals  $\pi_i$ . More precisely, consider Fig.65.2.

Let  $\underline{x}_i, \underline{h}_i, \underline{A}_i, \underline{y} \in \{0, 1\}$ .

The TPMs, printed in blue, for the bnet Fig.65.2, are as follows:

$$P(h_i) = \pi_i \delta(h_i, 1) + (1 - \pi_i) \delta(h_i, 0) \quad (65.6)$$

$$P(A_i|h_i, x_i) = \delta(A_i, h_i \wedge x_i) = \delta(A_i, h_i x_i) \quad (65.7)$$

$$P(y = 1|A^n) = 1 - (1 - \lambda) \wedge_{i=0}^{n-1} \bar{A}_i \quad (65.8)$$

$$= 1 - (1 - \lambda) \prod_i (1 - A_i) \quad (65.9)$$

$$P(y = 0|A^n) = 1 - P(y = 1|A^n) \quad (65.10)$$

Note that

$$P(y = 1|x^n, \lambda) = \sum_{h^n} \sum_{A^n} \left[ 1 - (1 - \lambda) \prod_i (1 - A_i) \right] [\prod_i \delta(A_i, h_i x_i)] P(h^n) \quad (65.11)$$

$$= E_{\underline{h}^n} \left[ [1 - (1 - \lambda) \prod_i (1 - h_i x_i)] \right]. \quad (65.12)$$

But

$$E_{\underline{h}_i}[h_i x_i] = \sum_{h_i=0,1} P(h_i) h_i x_i = \pi_i x_i \quad (65.13)$$

so

$$P(y = 1|x^n, \lambda) = 1 - (1 - \lambda) \prod_i (1 - \pi_i x_i). \quad (65.14)$$

3. Another way to interpret the parameters  $\pi_i$  is to associate each of them with a vector of samples  $\vec{\underline{h}}_i$  whose average is  $\pi_i$ . More precisely, consider Fig.65.3.

Suppose  $\underline{h}_i \in \{0, 1\}$  and define

$$P_{\underline{h}_i}(h_i) = \pi_i \delta(h_i, 1) + (1 - \pi_i) \delta(h_i, 0). \quad (65.15)$$

Suppose  $\vec{\underline{h}}_i = (\underline{h}_i[\sigma])_{s=0,1,\dots,nsam-1}$  and the Boolean samples  $\underline{h}_i[\sigma] \in \{0, 1\}$  are i.i.d. with  $\underline{h}_i[\sigma] \sim P_{\underline{h}_i}$  for all  $\sigma$ .

Note that for each  $i$ , an estimate  $\widehat{P}_{\underline{h}_i}(h_i)$  of  $P_{\underline{h}_i}(h_i)$  can be obtained from the vector of samples  $\vec{\underline{h}}_i$  as follows:

$$\widehat{P}_{\underline{h}_i}(h_i) = \frac{1}{nsam} \sum_{\sigma=0}^{nsam-1} \mathbb{1}(\underline{h}_i[\sigma] = h_i). \quad (65.16)$$

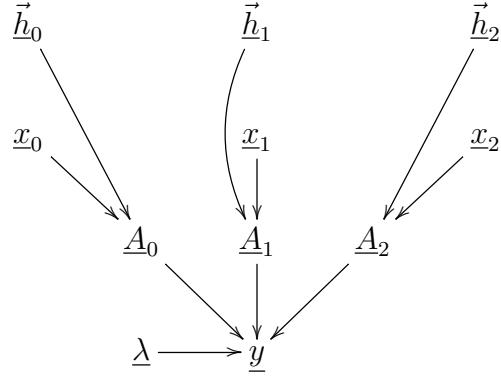


Figure 65.3: Fig.65.2 after replacing the hidden nodes  $(\underline{h}_i)_{i=0,1,2}$  by vectors of samples  $(\vec{h}_i)_{i=0,1,2}$ .

Let  $\underline{x}_i, \underline{h}_i[\sigma], \underline{A}_i, \underline{y} \in \{0, 1\}$ .

The TPMs, printed in blue, for the bnet Fig.65.3, are as follows:

$$P(\vec{h}_i) = \prod_{\sigma=0}^{nsam-1} P_{\underline{h}}(h_i[\sigma]) \quad (65.17)$$

$$P(A_i | \vec{h}_i, x_i) = \delta(A_i, \frac{1}{nsam} \sum_{\sigma} h_i[\sigma] \wedge x_i) \quad (65.18)$$

$$= \delta(A_i, \pi_i x_i) \quad (65.19)$$

$$P(y = 1 | A^n) = 1 - (1 - \lambda) \wedge_{i=0}^{n-1} \overline{A}_i \quad (65.20)$$

$$= 1 - (1 - \lambda) \prod_i (1 - A_i) \quad (65.21)$$

$$P(y = 0 | A^n) = 1 - P(y = 1 | A^n) \quad (65.22)$$

Note that

$$P(y = 1|x^n, \lambda, \vec{h}^n) = \sum_{A^n} \left[ 1 - (1 - \lambda) \prod_i (1 - A_i) \right] \prod_i \delta(A_i, \pi_i x_i) \quad (65.23)$$

$$= 1 - (1 - \lambda) \prod_i (1 - \pi_i x_i) . \quad (65.24)$$

# Chapter 66

## Non-negative Matrix Factorization

Based on Ref.[145].

Given matrix  $V$ , factor it into product of two matrices

$$V = WH , \quad (66.1)$$

where all 3 matrices have non-negative entries.

$V \in \mathbb{R}_{\geq 0}^{nv \times na}$ : visible info matrix

$W \in \mathbb{R}_{\geq 0}^{nv \times nh}$ : weight info matrix

$H \in \mathbb{R}_{\geq 0}^{nh \times na}$ : hidden info matrix

Usually,  $nv > nh < na$  so compression of information (a.k.a. dimensional reduction, clustering)

### 66.1 Bnet interpretation

Express node  $\underline{v}$  as a chain of two nodes.

$$\underline{v} \longleftarrow \underline{a} \quad = \quad \underline{w} \longleftarrow \underline{h} \longleftarrow \underline{a}$$

Figure 66.1: Bnet interpretation of non-negative matrix factorization.

The TPMs, printed in blue, for bnet Fig.66.1, are as follows.

$$P(\underline{v} = w | \underline{a}) = \frac{V_{w,a}}{\sum_w V_{w,a}} \quad (66.2)$$

$$P(w|h) = \frac{W_{w,h}}{\sum_w W_{w,h}} \quad (66.3)$$

$$P(h|a) = \frac{\sum_w W_{w,h}}{\sum_w V_{w,a}} H_{h,a} \quad (66.4)$$

## 66.2 Simplest recursive algorithm

Initialize: Choose  $nh$ . Choose  $W^{(0)}$  and  $H^{(0)}$  that have non-negative entries.

Update: For  $n = 0, 1, \dots$ , do

$$H_{i,j}^{(n+1)} \leftarrow H_{i,j}^{(n)} \frac{[(W^{(n)})^T V]_{i,j}}{[(W^{(n)})^T \underbrace{W^{(n)} H^{(n)}}_{\approx V}]_{i,j}} \quad (66.5)$$

and

$$W_{i,j}^{(n+1)} \leftarrow W_{i,j}^{(n)} \frac{[V(H^{(n+1)})^T]_{i,j}}{\underbrace{[W^{(n)} H^{(n+1)} (H^{(n+1)})^T]_{i,j}}_{\approx V}}. \quad (66.6)$$

After each step, record error defined by

$$\mathcal{E}^{(n)} = \| V - W^{(n)} H^{(n)} \|_2. \quad (66.7)$$

Using 2-norm, a.k.a. Frobenius matrix norm. Continue until reach acceptable error.

Can also use Kullback-Leibler divergence for error:

$$\mathcal{E} = \sum_a P(a) D_{KL}(P(\underline{v} = w|a) \| \sum_h P(w|h)P(h|a)), \quad (66.8)$$

for some arbitrary choice of prior  $P(a)$ . For example, can choose  $P(a)$  uniform.

# Chapter 67

## Observationally Equivalent DAGs

This chapter is based on Chapter 1 of Ref.[52] and on a blog post by Bruno Gonçalves (Ref.[17]).

A probability distribution  $P$  is **compatible with a DAG**  $G$  if  $P$  and  $G$  have the same random variables, and they can be combined to form a bnet without contradictions; i.e., one can calculate all the TPMs from  $P$  and multiply them together to obtain  $P$  again. Let

$$\mathcal{P}(G) = \{P : P \text{ is compatible with } G\} . \quad (67.1)$$

**Two DAGs  $G$  and  $G'$  are observationally equivalent (OE)** if  $\mathcal{P}(G) = \mathcal{P}(G')$ . Hence, any total probability distribution that is compatible with one of them is compatible with the other. For example,  $a \rightarrow b$  and  $a \leftarrow b$  are OE because

$$P(a|b)P(b) = P(a, b) = P(b|a)P(a) . \quad (67.2)$$

We'll say two bnets are OE if their DAGs are OE.

Two DAGs  $G$  and  $G'$  are **d-separation equivalent** if  $DS(G) = DS(G')$ . See Chapter 23 for definition of  $DS(G)$ .

**Claim 96** *Two DAGs are OE iff their DAGs are d-separation equivalent.*

The **skeleton** of a DAG is its underlying undirected graph.

A **v-structure** in a DAG consists of two arrows converging to a node and such that their tails are not connected by a third arrow. Fig.67.1 shows in red all the v-structures of a particular DAG.

**Claim 97** *Observational Equivalence Theorem (by Verma and Pearl, 1990)*

*Two DAGs are OE iff they have the same skeletons and the same v-structures.*

### 67.1 Examples

The 3 DAGs in Fig.67.2 are OE. They form an equivalence class of OE DAGs that represent the same probability distribution. This equivalence class of DAGs can be

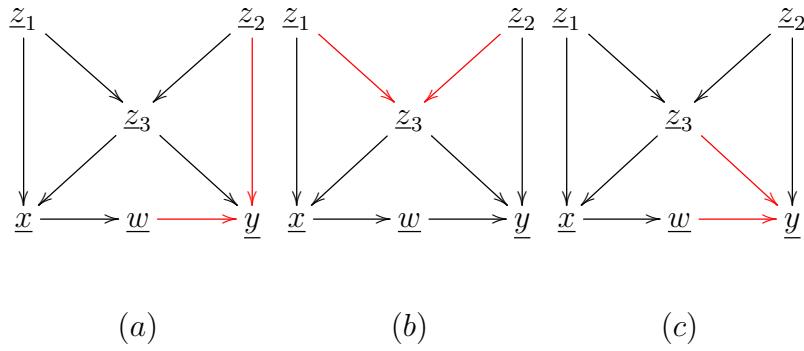


Figure 67.1: Example showing in red all v-structures of a particular DAG.

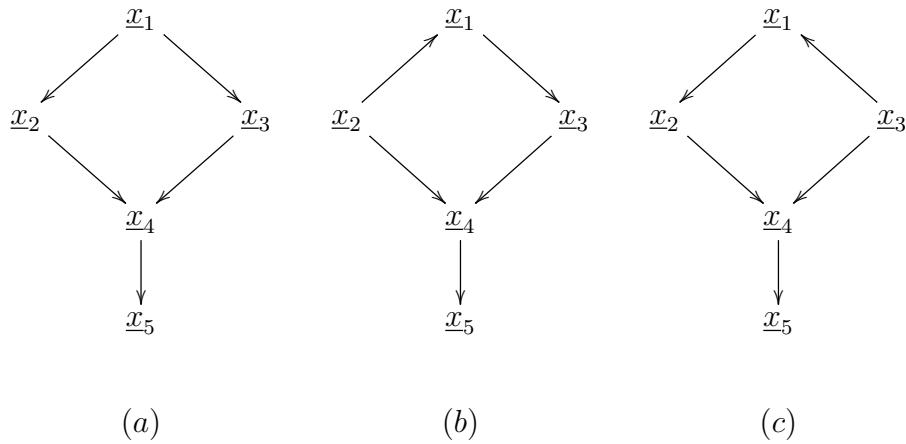


Figure 67.2: These 3 DAGs are observationally equivalent (OE).

represented by the partially directed graph Fig.67.3. These 3 DAGs can be proven to be OE in the following 3 ways:

1. Write the generic probability distributions represented by the 3 DAGs, and show that they are equal, as we did in Eq.(67.2). That is the low brow way of proving OE.
  2. Use d-separation (see Chapter 23). Consider DAG (a) first. Rename the nodes as  $\underline{\tau}_j$  with  $j = 1, 2, \dots$  so that the names are in topological order (i.e., so that the parents of  $\underline{\tau}_j$  have indices that are smaller than  $j$ ). The node names  $\underline{x}_j$  of DAG (a) are already in topological order, so we skip this step for DAG (a). Now write down its total probability distribution and notice which parents of a fully connected DAG were omitted.

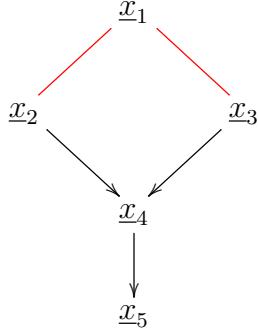


Figure 67.3: This partially directed graph represents the 3 DAGs in Fig.67.2.

$$P(x_1, x_2, x_3, x_4, x_5) = \underbrace{P(x_5|x_4)}_{x_3, x_2, x_1 \text{ omitted}} \underbrace{P(x_4|x_3, x_2)}_{x_1 \text{ omitted}} \underbrace{P(x_3|x_1)}_{x_2 \text{ omitted}} P(x_2|x_1) P(x_1) \quad (67.3)$$

The observations of which parents were omitted can be stated in d-separation lingo as the following 3 orthogonality relations:<sup>1</sup>

$$\underline{x}_3 \perp_P \underline{x}_2 \mid \underline{x}_1 \quad (67.4a)$$

$$\underline{x}_4 \perp_P \underline{x}_1 \mid \underline{x}_2, \underline{x}_3 \quad (67.4b)$$

$$\underline{x}_5 \perp_P (\underline{x}_1, \underline{x}_2, \underline{x}_3) \& \mid \underline{x}_4. \quad (67.4c)$$

Going through the same procedure for the other 2 DAGs yields, for each of them, an equivalent set of 3 orthogonality equations.<sup>2</sup>

This is enough to conclude that the 3 DAGs of Fig.67.2 are OE.

Note that Eqs.(67.4) encompass all that there is to say about the observability of DAG (a). These 3 equations can be checked empirically to assess how well the DAG fits the data. For example, one can do OLS (ordinary least squares) regression  $\underline{x}_5 \sim \underline{x}_1 + \underline{x}_2 + \underline{x}_3 + \underline{x}_4$  on the data, i.e., try to fit  $x_5 = \beta_0 + \sum_{i=1}^4 \beta_i x_i$  to the data, and find that, to a good approximation,  $\beta_1 = \beta_2 = \beta_3 = 0$ .

3. Use the OE Theorem. All three DAGs have the same skeleton, and the same single v-structure  $\underline{x}_2 \rightarrow \underline{x}_4 \leftarrow \underline{x}_3$ .

---

<sup>1</sup>Normally, if we had changed from the original node names to the  $\underline{\tau}_j$  node names, these orthogonality relations would first be stated in terms of the  $\underline{\tau}_j$  names, and we could translate them so that they were stated in terms of the original node names. But for DAG (a) there was no need to use the  $\underline{\tau}_j$  names.

<sup>2</sup>The  $\underline{x}_j$  node names are no longer in topological order for DAGs (b) and (c) so for them you should go through the intermediate step of renaming the nodes  $\underline{\tau}_j$ , and then, after obtaining the orthogonality relations in terms of the  $\underline{\tau}_j$  names, translating them back to the original  $\underline{x}_j$  names.

# Chapter 68

## Omitted Variable Bias

This paper is loosely based on Refs.[11] and [9].

This chapter assumes that the reader has read Section C.27 on Linear Regression (LR) and Section 72.12 which is an introduction to sensitivity analysis for the Potential Outcomes (PO) model.

We will use the terms “**PO Sensitivity Analysis**” and “**Omitted Variable Bias (OVB)**” to mean the same thing. In this chapter, we consider 2 types of OVB. LDEN bnets for these two cases are depicted in Fig.68.1. In Fig.68.1(a), the omitted variable is a confounder, and in Fig.68.1 (b), it’s a mediator.

Next we express OVB for these two cases as a product of gains along a path that goes through the unobserved node, and then we re-express the OVB in terms of correlations between the nodes.

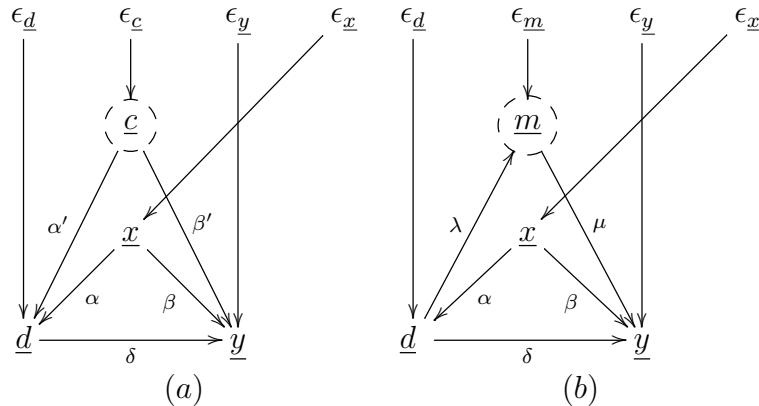


Figure 68.1: LDEN bnets used to do PO sensitivity analysis. Node  $\underline{c}$  in (a) is an unobserved confounder, and node  $\underline{m}$  in (b) is an unobserved mediator.

---

### CASE (a), confounder

Consider the LDEN bnet of Fig.68.1(a), whose structural equations, printed in blue, are as follows:

$$\begin{cases} \underline{c} = \epsilon_{\underline{c}} \\ \underline{x} = \epsilon_{\underline{x}} \\ \underline{d} = \alpha \underline{x} + \alpha' \underline{c} + \epsilon_{\underline{d}} \\ \underline{y} = \delta \underline{d} + \beta \underline{x} + \beta' \underline{c} + \epsilon_{\underline{y}} \end{cases} \quad (68.1)$$

In Section 72.12, we showed that for confounder case (a),

$$OV B_{con} = ATE - ATE|_{\beta'=0} = \frac{\beta'}{\alpha'} \quad (68.2)$$

This result is easy to understand.  $ATE|_{\beta'=0} = \delta$  due to the directed path  $\underline{d} \rightarrow \underline{y}$ , whereas  $ATE = \delta + \frac{\beta'}{\alpha'}$  due to the two directed paths  $\underline{d} \rightarrow \underline{y}$  and  $\underline{d} \rightarrow \underline{c} \rightarrow \underline{y}$ . Note that traveling from  $\underline{c}$  to  $\underline{d}$  has gain  $\alpha'$ , so traveling in the opposite direction has gain  $\frac{1}{\alpha'}$ .

Next we express  $OV B_{con}$  in terms of correlations between the nodes of the bnet.

### Claim 98

$$OV B_{con} = \frac{\beta'}{\alpha'} = \frac{[\rho_{y,c}\sigma_y]^{d,x}}{[\rho_{d,c}\sigma_d]^x} \quad (68.3)$$

If  $\sigma_{\epsilon_m} = \sigma_{\epsilon_d} = 0$ , then  $\rho_{y,c} = \rho_{d,c} = 1$  and

$$OV B_{con} = \frac{\sigma_y^{d,x}}{\sigma_d^x} \quad (68.4)$$

**proof:**<sup>1</sup>

Note that

$$\langle \underline{c}, \epsilon_{\underline{d}} \rangle = 0 \quad |x \quad (68.5)$$

because the paths from  $\underline{c}$  to  $\epsilon_{\underline{d}}$  are blocked by colliders. Hence,

$$\langle \underline{d}, \epsilon_{\underline{d}} \rangle = \langle \alpha' \underline{c} + \epsilon_{\underline{d}}, \epsilon_{\underline{d}} \rangle = \langle \epsilon_{\underline{d}}, \epsilon_{\underline{d}} \rangle \quad |x \quad (68.6)$$

$$\langle \underline{d}, \underline{d} \rangle = \langle \alpha' \underline{c} + \epsilon_{\underline{d}}, \alpha' \underline{c} + \epsilon_{\underline{d}} \rangle = (\alpha')^2 \langle \underline{c}, \underline{c} \rangle + \langle \epsilon_{\underline{d}}, \epsilon_{\underline{d}} \rangle \quad |x \quad (68.7)$$

$$\sigma_{\underline{d}} = |\alpha'| \sigma_{\underline{c}} \sqrt{1 + \left( \frac{\sigma_{\epsilon_{\underline{d}}}}{\alpha' \sigma_{\underline{c}}} \right)^2} \quad |x \quad (68.8)$$

---

<sup>1</sup>We use “|x” at the end of a line to mean all averages in that line are taken at fixed  $x = x$ .

$$\rho_{\underline{d}, \underline{c}} = \frac{\langle \underline{d}, \underline{c} \rangle}{\sqrt{\langle \underline{d}, \underline{d} \rangle \langle \underline{c}, \underline{c} \rangle}} |x| \quad (68.9)$$

$$= \frac{\langle \alpha' \underline{c} + \underline{\epsilon}_{\underline{d}}, \underline{c} \rangle}{\sqrt{\langle \alpha' \underline{c} + \underline{\epsilon}_{\underline{d}}, \alpha' \underline{c} + \underline{\epsilon}_{\underline{d}} \rangle \langle \underline{c}, \underline{c} \rangle}} |x| \quad (68.10)$$

$$= \frac{\alpha' \langle \underline{c}, \underline{c} \rangle}{\sqrt{((\alpha')^2 \langle \underline{c}, \underline{c} \rangle + \langle \underline{\epsilon}_{\underline{d}}, \underline{\epsilon}_{\underline{d}} \rangle) \langle \underline{c}, \underline{c} \rangle}} |x| \quad (68.11)$$

$$= \frac{\alpha' \sigma_{\underline{c}}}{\sqrt{(\alpha' \sigma_{\underline{c}})^2 + \sigma_{\underline{\epsilon}_{\underline{d}}}^2}} |x| \quad (68.12)$$

$$= \frac{\text{sign}(\alpha')}{\sqrt{1 + \left(\frac{\sigma_{\underline{\epsilon}_{\underline{d}}}}{\alpha' \sigma_{\underline{c}}}\right)^2}} |x| \quad (68.13)$$

$$\langle \underline{c}, \underline{d} \rangle = \alpha' \langle \underline{c}, \underline{c} \rangle |x| \quad (68.14)$$

$$\alpha' = \frac{\langle \underline{c}, \underline{d} \rangle}{\langle \underline{c}, \underline{c} \rangle} = \partial_{\underline{c}} \underline{d} = \rho_{\underline{c}, \underline{d}} \frac{\sigma_{\underline{d}}}{\sigma_{\underline{c}}} |x| \quad (68.15)$$

All equations between Eq.(68.5) and this point, remain valid if we make the following replacements:

$$\begin{aligned} \underline{d} &\rightarrow \underline{y} \\ \underline{\epsilon}_{\underline{d}} &\rightarrow \underline{\epsilon}_{\underline{y}} \\ \underline{c} &\rightarrow \underline{c} \\ \alpha' &\rightarrow \beta' \\ |x &\rightarrow |d, x \end{aligned} \quad (68.16)$$

In particular, the following are true

$$\sigma_{\underline{y}} = |\beta'| \sigma_{\underline{c}} \sqrt{1 + \left(\frac{\sigma_{\underline{\epsilon}_{\underline{y}}}}{\beta' \sigma_{\underline{c}}}\right)} |d, x| \quad (68.17)$$

$$\rho_{\underline{y}, \underline{c}} = \frac{\text{sign}(\beta')}{\sqrt{1 + \left(\frac{\sigma_{\underline{\epsilon}_{\underline{y}}}}{\beta' \sigma_{\underline{c}}}\right)^2}} |d, x| \quad (68.18)$$

$$\beta' = \partial_{\underline{c}} \underline{y} = \rho_{\underline{y}, \underline{c}} \frac{\sigma_{\underline{y}}}{\sigma_{\underline{c}}} |d, x| \quad (68.19)$$

Combining our newly found expressions for for  $\alpha'$  and  $\beta'$ , we get

$$\frac{\beta'}{\alpha'} = \left[ \frac{\rho_{\underline{y}, \underline{c}} \sigma_{\underline{y}}}{\sigma_{\underline{c}}} \right]^{|d, x|} \left[ \frac{\sigma_{\underline{c}}}{\rho_{\underline{d}, \underline{c}} \sigma_{\underline{d}}} \right]^{|x|} \quad (68.20)$$

Now note that

$$\sigma_{\underline{c}}^2 = \langle \underline{\epsilon}_{\underline{c}}, \underline{\epsilon}_{\underline{c}} \rangle \quad (68.21)$$

which is independent of  $\underline{d}$  and  $\underline{x}$ , so

$$\sigma_{\underline{c}}^{|\underline{x}} = \sigma_{\underline{c}}^{|\underline{d}, \underline{x}} \quad (68.22)$$

Therefore,

$$\frac{\beta'}{\alpha'} = \frac{[\rho_{y,\underline{c}} \sigma_y]^{|\underline{d}, \underline{x}}}{[\rho_{d,\underline{c}} \sigma_d]^{|\underline{x}}} \quad (68.23)$$

---

**QED**  
**CASE (b), mediator**

Consider the LDEN bnet of Fig.68.1(b), whose structural equations, printed in blue, are as follows:

$$\begin{cases} \underline{m} = \lambda \underline{d} + \underline{\epsilon}_m \\ \underline{x} = \underline{\epsilon}_x \\ \underline{d} = \alpha \underline{x} + \underline{\epsilon}_d \\ \underline{y} = \delta \underline{d} + \beta \underline{x} + \mu \underline{m} + \underline{\epsilon}_y \end{cases} \quad (68.24)$$

By an argument analogous to the one used previously in this chapter to prove that  $OVB_{con} = \frac{\beta'}{\alpha'}$ , we get

$$OVB_{med} = ATE - ATE|_{\mu=0} = \lambda \mu \quad (68.25)$$

Next we express  $OVB_{med}$  in terms of correlations between the nodes of the bnet.

**Claim 99** <sup>2</sup>

$$OVB_{med} = \lambda \mu = \frac{[\rho_{y,m} \sigma_y]^{|\underline{d}, \underline{x}}}{\sigma_d} \underbrace{\left[ \frac{\rho_{d,m}}{\sqrt{1 - \rho_{d,m}^2}} \right]}_{\tan \theta} \quad (68.26)$$

If  $|\tan \theta| \leq \eta$ , then<sup>3</sup>

$$|OVB_{med}| \leq \left| \frac{\sigma_y^{|\underline{d}, \underline{x}}}{\sigma_d} \right| \eta \quad (68.27)$$

---

<sup>2</sup>Eq.(68.26) appears in Ref.[11], but that paper claims it gives the bias for unobserved confounders instead of unobserved mediators. But the formula for the bias for unobserved confounders is given by Eq.(68.3).

<sup>3</sup>Recall that, by the Schwarz Inequality,  $|\rho_{a,b}| \leq 1$  for any correlation coefficient  $\rho_{a,b} = \frac{\langle a, b \rangle}{\sigma_a \sigma_b}$ .

**proof:**

Note that

$$\langle \underline{d}, \epsilon_{\underline{m}} \rangle = 0 \quad (68.28)$$

because paths from  $\underline{d}$  to  $\epsilon_{\underline{m}}$  are blocked by a collider. Hence,

$$\langle \underline{d}, \underline{m} \rangle = \lambda \langle \underline{d}, \underline{d} \rangle \quad (68.29)$$

$$\lambda = \frac{\langle \underline{d}, \underline{m} \rangle}{\langle \underline{d}, \underline{d} \rangle} = \frac{\partial \underline{m}}{\partial \underline{d}} = \rho_{\underline{d}, \underline{m}} \frac{\sigma_{\underline{m}}}{\sigma_{\underline{d}}} \quad (68.30)$$

Note that also

$$\langle \underline{m}, \epsilon_{\underline{y}} \rangle = 0 \quad |d, x \quad (68.31)$$

because the paths from  $\underline{m}$  to  $\epsilon_{\underline{y}}$  are blocked by a collider. Hence,

$$\langle \underline{m}, \underline{y} \rangle = \mu \langle \underline{m}, \underline{m} \rangle \quad |d, x \quad (68.32)$$

$$\mu = \frac{\langle \underline{m}, \underline{y} \rangle}{\langle \underline{m}, \underline{m} \rangle} = \frac{\partial \underline{y}}{\partial \underline{m}} = \rho_{\underline{y}, \underline{m}} \frac{\sigma_{\underline{y}}}{\sigma_{\underline{m}}} \quad |d, x \quad (68.33)$$

Combining our newly found expressions for  $\lambda$  and  $\mu$ , we get

$$\lambda \mu = \rho_{\underline{d}, \underline{m}} \frac{\sigma_{\underline{m}}}{\sigma_{\underline{d}}} \left[ \rho_{\underline{y}, \underline{m}} \frac{\sigma_{\underline{y}}}{\sigma_{\underline{m}}} \right]^{|\underline{d}, x} \quad (68.34)$$

Let

$$e_\lambda = \frac{\sigma_{\epsilon_{\underline{m}}}}{\lambda \sigma_{\underline{d}}} \quad (68.35)$$

Then

$$\sigma_{\underline{m}}^2 = \langle \underline{m}, \underline{m} \rangle \quad (68.36)$$

$$= \langle \lambda \underline{d} + \epsilon_{\underline{m}}, \lambda \underline{d} + \epsilon_{\underline{m}} \rangle \quad (68.37)$$

$$= \lambda^2 \langle \underline{d}, \underline{d} \rangle + \langle \epsilon_{\underline{m}}, \epsilon_{\underline{m}} \rangle \quad (68.38)$$

$$= \lambda^2 \sigma_{\underline{d}}^2 (1 + e_\lambda^2) , \quad (68.39)$$

and, since  $[\sigma_{\underline{d}}^2]^{|\underline{d}, x} = 0$ , we have

$$[\sigma_{\underline{m}}^{|\underline{d}, x}]^2 = \sigma_{\epsilon_{\underline{m}}}^2 \quad (68.40)$$

Hence,

$$\frac{\sigma_{\underline{m}}}{\sigma_{\underline{m}}^{|\underline{d}, x}} = \frac{1}{e_\lambda} \sqrt{1 + e_\lambda^2} \quad (68.41)$$

Furthermore,

$$\langle \underline{d}, \underline{m} \rangle = \langle \underline{d}, \lambda \underline{d} + \epsilon_{\underline{m}} \rangle \quad (68.42)$$

$$= \lambda \sigma_{\underline{d}}^2 \quad (68.43)$$

so

$$\rho_{\underline{d}, \underline{m}} = \frac{\langle \underline{d}, \underline{m} \rangle}{\sigma_{\underline{d}} \sigma_{\underline{m}}} \quad (68.44)$$

$$= \frac{\lambda \sigma_{\underline{d}}}{\sigma_{\underline{m}}} \quad (68.45)$$

$$= \frac{1}{\sqrt{1 + e_{\lambda}^2}} \quad (68.46)$$

Hence,

$$\sqrt{1 - \rho_{\underline{d}, \underline{m}}^2} = \frac{e_{\lambda}}{\sqrt{1 + e_{\lambda}^2}} = \left( \frac{\sigma_{\underline{m}}}{\sigma_{\underline{m}}^{|\underline{d}, \underline{x}|}} \right)^{-1} \quad (68.47)$$

$$\lambda \mu = \frac{[\rho_{\underline{y}, \underline{m}} \sigma_{\underline{y}}]^{|\underline{d}, \underline{x}|}}{\sigma_{\underline{d}}} \frac{\rho_{\underline{d}, \underline{m}}}{\sqrt{1 - \rho_{\underline{d}, \underline{m}}^2}} \quad (68.48)$$

### QED

Note that both  $OVB_{con}$  and  $OVB_{med}$  are equal to a product  $\mathcal{F}_{\underline{d}} \mathcal{F}_{\underline{y}}$  of two factors  $\mathcal{F}_{\underline{d}}$  and  $\mathcal{F}_{\underline{y}}$ . For  $OVB_{con}$

$$\mathcal{F}_{\underline{y}} = [\rho_{\underline{y}, \underline{c}} \sigma_{\underline{y}}]^{|\underline{d}, \underline{x}|}, \quad \mathcal{F}_{\underline{d}} = \frac{1}{[\rho_{\underline{d}, \underline{c}} \sigma_{\underline{d}}]^{|\underline{x}|}} \quad (68.49)$$

For  $OVB_{med}$ ,

$$\mathcal{F}_{\underline{y}} = [\rho_{\underline{y}, \underline{m}} \sigma_{\underline{y}}]^{|\underline{d}, \underline{x}|}, \quad \mathcal{F}_{\underline{d}} = \frac{\rho_{\underline{d}, \underline{m}}}{\sigma_{\underline{d}} \sqrt{1 - \rho_{\underline{d}, \underline{m}}^2}} \quad (68.50)$$

$\mathcal{F}_{\underline{y}}$  is the same for the confounder and mediator cases, except that the node  $\underline{c}$  in  $\mathcal{F}_{\underline{y}}$  for the confounder case is changed to  $\underline{m}$  in the mediator case. This is to be expected, because in both cases the arrow from the unobserved node points into  $\underline{y}$ . On the other hand,  $\mathcal{F}_{\underline{d}}$  is different for the confounder and mediator cases, because in the confounder case, the unobserved node  $\underline{c}$  points into  $\underline{d}$ , whereas in the mediator case,  $\underline{d}$  points into the unobserved node  $\underline{m}$ .

# Chapter 69

## Personalized Expected Utility

This chapter is based on Ref.[34].

This chapter assumes that the reader has already read Chapter 70 on Personalized Treatment Effects. Whereas Chapter 70 is concerned with finding bounds for  $PNS_z$ , this chapter will find bounds for  $EU_z$ , which is called the Personalized Expected Utility (PEU).

For  $y_0, y_1 \in \{0, 1\}$ , let us denote the **conditional joint experimental (causal, counterfactual) distribution** by:

$$P_{y_0, y_1 | z} = P(\underline{y}_0 = y_0, \underline{y}_1 = y_1 | z). \quad (69.1)$$

Suppose we are given a **Utility function**<sup>1</sup>

$$\alpha_{y_0, y_1} : \{0, 1\}^2 \rightarrow \mathbb{R} \quad (69.2)$$

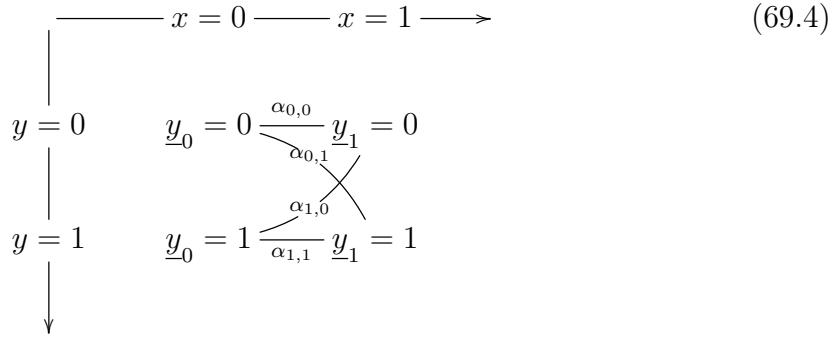
Let<sup>2</sup>

$$\begin{aligned} \beta &= \alpha_{0,1} & (y_0 = 0, y_1 = 1) & \text{compliers} \\ \gamma &= \alpha_{1,1} & (y_0 = 1, y_1 = 1) & \text{always takers} \\ \theta &= \alpha_{0,0} & (y_0 = 0, y_1 = 0) & \text{never takers} \\ \delta &= \alpha_{1,0} & (y_0 = 1, y_1 = 0) & \text{defiers} \end{aligned} \quad (69.3)$$

---

<sup>1</sup>Ref.[34] refers to the utility function as the benefit function.

<sup>2</sup>The notation  $\beta, \gamma, \theta, \delta$  won't be used again in this chapter. We mention it here so the reader can translate to and from our equations and the equations in Ref.[34] where this  $\beta, \gamma, \theta, \delta$  notation is used.



Define the **personalized expected utility (PEU)** by

$$EU = E[\alpha_{\underline{y}_0, \underline{y}_1}] = \alpha_{i,j} P_{i,j} \quad (69.5)$$

and the **conditional PEU** by

$$EU_z = E_{|z}[\alpha_{\underline{y}_0, \underline{y}_1}] = \alpha_{i,j} P_{i,j|z} \quad (69.6)$$

Note that

$$EU = \sum_z P(z) EU_z. \quad (69.7)$$

Above, we are using the Einstein summation convention (repeated indices are to be summed over) for the indices  $i, j \in \{0, 1\}$ .

Compare the definition of  $EU_z$  with that of two other causal effects used in his book:

$$PNS_z = P_{0,1||z} = P(\text{compliers}|z) \quad (69.8)$$

$$Uplift = ATE_z = E_{1|1,z} - E_{1|0,z} \quad (69.9)$$

As we shall see,  $EU_z$  contains the information in  $PNS_z$  and  $ATE_z$ , plus much more.

One can find the stratum  $z^*$  such that  $z^* = \operatorname{argmax}_z ATE_z$  (as is done A/B=RCT testing) or  $z^* = \operatorname{argmax}_z EU_z$  or  $z^* = \operatorname{argmax}_z PNS_z$ . This is called the **unit selection problem**. It's called "unit selection" rather than "stratum selection" because once the stratum  $z^*$  is found, one can find a unit (i.e., individual) within that stratum.

## 69.1 Goal of PEU Theory

Everything that we said in Chapter 70 in the section entitled "Goal of PTE Theory" applies to PEU theory too, if we just replace  $PNS_z$  by  $EU_z$ . As in Chapter 70, we

will consider two types of bounds (for  $EU_z$  instead of  $PNS_z$ ): (1) Bounds for an unspecified bnet, (2) Bounds for specific bnet families.

Here is an explanation of why  $EU_z$  varies within a bounded region, something that might not be obvious to the beginner. In Fig.69.1, we represent the utility function  $\alpha_{y_0,y_1}$  by a unit vector  $\hat{\alpha}$ , the probability distribution  $P_{y_0,y_1|z}$  by a vector  $\vec{P}$ , and  $EU_z$  by the dot product  $\vec{P} \cdot \hat{\alpha}$ . When the probability vector  $\vec{P}$  varies within a bounded region (shown in green), this causes the dot product  $EU_z = \vec{P} \cdot \hat{\alpha}$  to vary within a bounded interval (also shown in green).

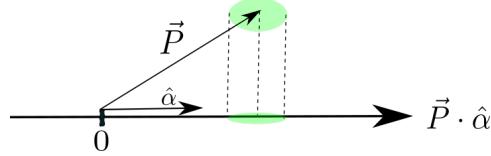


Figure 69.1: Bounds (shown in green) on the probability vector  $\vec{P}$  induce bounds (shown in green) on the dot product  $EU_z = \vec{P} \cdot \hat{\alpha}$ . Here  $\hat{\alpha}$  is a unit vector that stands for a normalized utility function.  $\hat{\alpha}$  does not vary but  $\vec{P}$  does.

## 69.2 Bnets for PEU Theory

Everything that we said in Chapter 70 in the section entitled “Bnets for PTE Theory” applies to PEU theory too, if we just replace  $PNS_z$  by  $EU_z$ .

## 69.3 Bounds on $EU$ for unspecified bnet

Define the **balanced utility** by

$$\alpha_B = \alpha_{0,0} + \alpha_{1,1} , \quad (69.10)$$

the **unbalanced utility** by

$$\alpha_U = \alpha_{1,0} + \alpha_{0,1} , \quad (69.11)$$

and their difference by:

$$\sigma = \alpha_U - \alpha_B . \quad (69.12)$$

We will also use the abbreviations:

$$\alpha_{1-0,j} = \alpha_{1,j} - \alpha_{0,j} \quad (69.13)$$

and

$$\alpha_{j,1-0} = \alpha_{j,1} - \alpha_{j,0} . \quad (69.14)$$

**Claim 100** *In general,*

$$\begin{cases} \max p_{[1\dots 4]} \leq EU_z \leq \min p_{[5\dots 8]} & \text{if } \sigma < 0 \\ \max p_{[5\dots 8]} \leq EU_z \leq \min p_{[1\dots 4]} & \text{if } \sigma > 0 \end{cases} \quad (69.15)$$

where<sup>3</sup>

$$\begin{cases} p_1 = \alpha_{0,1-0} E_{1|1,z} + \alpha_{j,0} E_{j|0,z} \\ p_2 = \alpha_{0-1,1} E_{0|0,z} + \alpha_{1,j} E_{j|1,z} \\ p_3 = p_5 + \sigma O_{*,*|z} \\ p_4 = p_1 - \sigma E_{1|0,z} + \sigma(1 - O_{*,*|z}) \end{cases} \quad (69.16)$$

$$\begin{cases} p_5 = \alpha_{1,1-0} E_{1|1,z} + \alpha_{j,0} E_{j|0,z} \\ p_6 = p_1 - \sigma E_{1|0,z} \\ p_7 = p_5 - \sigma E_{1|0,z} + \sigma P(\underline{y} = 1|z) \\ p_8 = p_1 - \sigma P(\underline{y} = 1|z) \end{cases} \quad (69.17)$$

**proof:** See Ref[34] or use the MRP (Matrix Representation of Probabilities) defined in Chapter 70.

**QED**

Later on, we will see that under monotonicity, these bounds collapse to a point estimate of  $EU_z$ . But what if monotonicity doesn't hold? In such cases, one can use the midpoint of the bounds as a non-rigorous point estimate of  $EU_z$ .

**Claim 101** *In general,*

$$P_{0,0|z} = E_{0|1,z} - P_{1,0|z} \quad (69.18)$$

$$P_{1,1|z} = E_{1|0,z} - P_{1,0|z} \quad (69.19)$$

$$P_{0,1|z} = 1 - P_{0,0|z} - P_{1,1|z} - P_{1,0|z} \quad (69.20)$$

$$= 1 - E_{0|1,z} - E_{1|0,z} + P_{1,0|z} \quad (69.21)$$

**proof:**

$$P_{0,0|z} + P_{1,0|z} = P(\underline{y}_1 = 0|z) = E_{0|1,z} \quad (69.22)$$

---

<sup>3</sup> $p_{[a\dots b]} = (p_a, p_{a+1}, \dots, p_b)$  for integers  $a, b$  such that  $a < b$ .

$$P_{1,1|z} + P_{1,0|z} = P(\underline{y}_0 = 1|z) = E_{1|0,z} \quad (69.23)$$

**QED**

Recall the definition of monotonicity. Monotonicity holds iff

$$P(\underline{y}_0 = 1, \underline{y}_1 = 0) = 0. \quad (69.24)$$

**Claim 102** *In general,*

$$EU_z = \alpha_{0,0}P_{0,0|z} + \alpha_{1,1}P_{1,1|z} + \alpha_{0,1}P_{0,1|z} + \alpha_{1,0}P_{1,0|z} \quad (69.25)$$

Hence, if monotonicity holds, or  $\alpha_{1,0} = 0$ , then

$$EU_z = \alpha_{0,0}P_{0,0|z} + \alpha_{1,1}P_{1,1|z} + \alpha_{0,1}P_{0,1|z} \quad (69.26)$$

**proof:** Trivial

**QED**

Claim 102 is trivial, but it provides a good motivation and inspiration for the following less trivial claim.

**Claim 103** *In general,*

$$EU_z = \alpha_{0,0} \underbrace{E_{0|1,z}}_{=1-E_{1|1,z}} + \alpha_{1,1}E_{1|0,z} + \alpha_{0,1} \underbrace{(1 - E_{0|1,z} - E_{1|0,z})}_{=E_{1|1,z}-E_{1|0,z}=ATE_z} + \sigma P_{1,0|z} \quad (69.27)$$

Hence, if monotonicity holds, or  $\sigma = 0$ , then

$$(EU_z)_{\sigma=0} = \alpha_{0,0}E_{0|1,z} + \alpha_{1,1}E_{1|0,z} + \alpha_{0,1}ATE_z \quad (69.28)$$

**proof:** In general,

$$EU_z = \begin{cases} \alpha_{0,0}P_{0,0|z} \\ + \alpha_{1,1}P_{1,1|z} \\ + \alpha_{0,1}P_{0,1|z} \\ + \alpha_{1,0}P_{1,0|z} \end{cases} = \begin{cases} \alpha_{0,0}(E_{0|1,z} - P_{1,0|z}) \\ + \alpha_{1,1}(E_{1|0,z} - P_{1,0|z}) \\ + \alpha_{0,1}(1 - E_{0|1,z} - E_{1|0,z} + P_{1,0|z}) \\ + \alpha_{1,0}P_{1,0|z} \end{cases} \quad (69.29)$$

Hence,

$$EU_z = (EU_z)_{\sigma=0} + \sigma P_{1,0|z} \quad (69.30)$$

**QED**

Perhaps this will make Claim 103 less mysterious to you. Note that Claims 102 and 103 imply the following:

$$\left[ \frac{\partial EU_z}{\partial \alpha_{1,0}} \right]_{\alpha_{0,0}, \alpha_{1,1}, \alpha_{0,1}} = \left[ \frac{\partial EU_z}{\partial \sigma} \right]_{\alpha_{0,0}, \alpha_{1,1}, \alpha_{0,1}} = P_{1,0|z} \quad (69.31)$$

## 69.4 Bounds on $EU$ for specific bnet families

# Chapter 70

## Personalized Treatment Effects

This chapter is based on the work of Pearl et al, as reported in Refs. [69] and [40].

Recall from Chapter 72 on Potential Outcomes (PO) and Beyond, that the **Average Treatment Effect (ATE)** is defined as

$$ATE = E[\underline{y}_1 - \underline{y}_0] \quad (70.1)$$

$$= P(\underline{y}_1 = 1) - P(\underline{y}_0 = 1) \quad (70.2)$$

The **Conditional ATE (CATE)** is defined as the conditional expected value

$$ATE_z = E_{|z}[\underline{y}_1 - \underline{y}_0] \quad (70.3)$$

$$= P(\underline{y}_1 = 1|z) - P(\underline{y}_0 = 1|z) . \quad (70.4)$$

Note that

$$ATE = \sum_z P(z)ATE_z \quad (70.5)$$

**Personalized Treatment Effect (PTE)** theory as envisioned by Pearl is the study of bounds for "personalized" treatment effects such as

$$PNS = P(\underline{y}_1 - \underline{y}_0 = 1) \quad (70.6)$$

and

$$PNS_z = P(\underline{y}_1 - \underline{y}_0 = 1|z) . \quad (70.7)$$

They are said to be **personalized** because they are averages over a *single* ensemble (i.e., population) of individuals  $\sigma$  with probability  $P(y_0^\sigma, y_1^\sigma)$ . *ATE*, on the other hand, is not personalized, because it equals the difference of two of those averages. Personalized effects equal the probability of a single event/person, whereas *ATE* equals the difference of the probabilities of 2 events/persons.

If the conditioning  $z$  is fine grained enough to pick out a single individual  $\sigma$  (i.e., if  $z = \sigma$ ), then we get

$$PNS_\sigma = \mathbb{1}(y_1^\sigma - y_0^\sigma = 1) \quad (70.8)$$

whereas

$$ATE_\sigma = \mathbb{1}(y_1^\sigma = 1) - \mathbb{1}(y_0^\sigma = 1) \quad (70.9)$$

$ATE$  and  $PNS$  measure different things.  $PNS$  measures the probability that a *single person* will switch outcomes from 0 to 1 when he/she switches treatments from 0 to 1.  $ATE$  measures the difference in populations between those who survive taking the drug and those who survive without it.

One very promising field in which PTE theory can be applied is in **Personalized Causal Medicine**. For example, suppose we want to use  $PNS_z$ , where the conditioning is on the sex of the patient (i.e.,  $z = male, female$ ), to advice a female patient whether to take a cancer drug or not.

## 70.1 Goal, Strategy and Rationale of PTE theory

In this section, we described briefly the goal, strategy and rationale behind PTE theory.

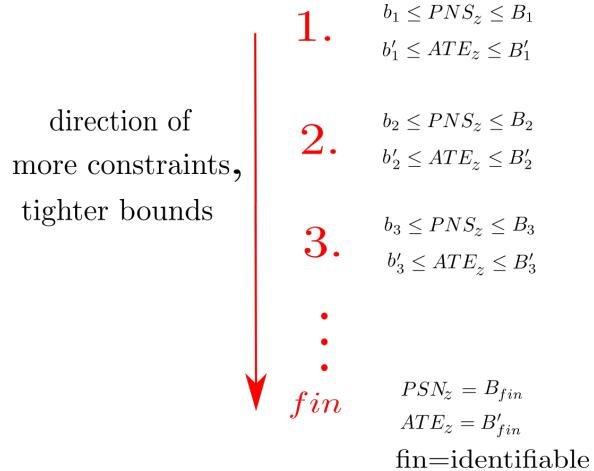


Figure 70.1: We use patient data to calculate at each step, increasingly tighter bounds  $b_j, b'_j, B_j, B'_j$  for  $PNS_z$  and  $ATE_z$ , ending in point bounds for both quantities.

The goal of PTE theory, as described by Fig. 70.1, is to find increasingly tighter bounds for PTEs such as  $PNS$ ,  $PNS_z$ ,  $ATE$ ,  $ATE_z$ , etc..

We say bounds, because it is not always possible to give a point estimate for  $PNS$  and other PTEs. If a point estimate for a PTE named  $Q$  is achievable, we say  $Q$  is **identifiable**. The same definition of identifiability has been used before in this

book for *ATE*. It's possible that *ATE* is identifiable, but *PNS* isn't, or vice versa, for certain kinds of data; i.e., both quantities need not become identifiable simultaneous at the same step above.

The bounds given by PTE theory are as tight as possible, depending on the available data, and on what bnet model assumptions the user is willing to make. We will consider two types of bounds: (1) Bounds for an unspecified bnet, (2) bounds for specific bnet families. Bounds for (2) will be tighter than bounds for (1).

The bounds are calculated from two types of data: **Observational Data (OD)** and **Experimental Data (ED)**.

For OD, one allows the patient to choose whether to take a drug or not ( $x = 0, 1$ ), and then we conduct a **survey** to record his/her value for  $x$  and whether the treatment worked or not ( $y = 0, 1$ ).

For ED, one conducts a **RCT** (Randomized Controlled Trial) instead of a survey. In the case of ED, we record, as in OD, the  $(x, y)$  for each patient, but the value of  $x$  for each patient is selected by the experimenter, at random, and, once selected, it is compulsory for the patient.

Unlike ED, OD is likely to be confounded, but it can still shed additional information that serves to tighten the bounds on  $PNS_z$  or other PTEs.

OD is usually collected first because it is easier and cheaper to collect than ED. Sometimes ED is too expensive or difficult or even impossible to collect, so only OD is available. Sometimes several ED (resp., several OD) need to be merged, before merging the merged ED with the merged OD. Pearl's PTE theory allows us to fuse together all the available data in all these types of situations.

Some purists such as the advocates of **EBM (Evidence Based Medicine)** advocate the use of only ED (i.e., only RCTs), no OD. This is reasonable in certain administrative professions to keep partisanship and chicanery out of the decision making process, but in other professions, throwing away OD would be foolish. A case in the history of medicine where OD was essential, was the case of John Snow (see Chapter 18). John Snow didn't have an RCT, but he was able to use OD to determine the driver of the cholera epidemic in London. He saved countless lives by doing so. An EBM purist would have thrown out his OD because it wasn't an RCT.

In the usual case, OD is collected first to aid in the design of an RCT, and then an RCT is conducted to collect ED. In this case, an EBM purist would throw away the OD, and only calculate an estimate of ATE. What PTE theory suggests is to calculate *both*, an estimate of ATE and bounds for PNS. Why? Because ATE and PNS measure different things. ATE utilizes only ED whereas PNS utilizes both OD and ED. Also, PNS is more personalized than ATE.

An RCT is called that because one chooses "at random", a subset  $\Sigma$  of a huge population  $\Sigma_\infty$ , and then one splits  $\Sigma$ , again at random, into 2 subsets,  $\Sigma_{control}$  and  $\Sigma_{treated}$ . All patients in  $\Sigma_{control}$  (resp.,  $\Sigma_{treated}$ ) are not treated (resp., treated). **Randomization** (i.e. choosing  $\Sigma$ ,  $\Sigma_{control}$ ,  $\Sigma_{treated}$ ), if perfect, averages out (i.e., cancels out) the effect of all confounders. The problem is that in practice, ideal random-

ization is hard to achieve. Hence, ideal RCTs are hard to achieve (and costly), plus they don't shed light on the confounders and mechanism involved. By mechanism, I mean a DAG.<sup>1</sup> A DAG is a hypothesis, and RCTs don't test it, whereas observational studies do. So it's a good idea to do a series of well designed observational studies (much cheaper than an RCT), with a hypothesis DAG, before doing the RCT. This elucidates the DAG, and helps design an RCT that achieves a good approximation to randomization.

Some people object to CI (Causal Inference) in general on the grounds that the causal DAGs are adhoc, arbitrary, a sort of unscientific voodoo. I think it's because they fail to grasp the true meaning and purpose of DAGs. I discuss this further in Section E.6.

## 70.2 Bnets for PTE theory

Let  $\bar{0} = 1$  and  $\bar{1} = 0$ .

Whenever we write  $P(\underline{a} = x, b)$ , we mean  $P(\underline{a} = x, \underline{b} = b)$ .

In this chapter, we will not use the notation  $P(y)$  and  $P(y')$  used by Pearl to discuss PTE theory. Instead, we will use  $P(\underline{y} = 1)$  and  $P(\underline{y} = 0)$  to denote his  $P(y)$  and  $P(y')$ , respectively.

On the other hand, in this chapter we will change the names of variables  $\underline{d}, \underline{y}, \underline{z}, \underline{y}(d)$  used in Chapter 72 on Potential Outcomes (PO) to the names favored by Pearl. Hence, we will replace  $\underline{d}, \underline{y}, \underline{x}, \underline{y}(d)$  by  $\underline{x}, \underline{y}, \underline{z}, \underline{y}_x$ , respectively.

PTE theory considers bnets of the form Fig.70.2. The bnet considered in Rubin's PO theory is a very simple special case of this where the box labeled "multiple nodes" is absent and there is an arrow pointing from  $\underline{z}$  to  $\underline{x}$ .

The TPM, printed in blue, for node  $\underline{y}$  of bnet Fig.70.2 is as follows:

$$P(\underline{y}|y_0, y_1, x) = \delta(\underline{y}, \underline{y}_x) \quad (70.10)$$

This TPM is used frequently in PTE theory. If  $x, y_0, y_1$  are arguments of  $P()$ , this TPM implies that one can swap  $\underline{y}_x = y_x$  and  $\underline{y} = y_x$  inside  $P()$ . For example,

$$P(y_0, y_1, x) = P(\underline{y}_x = y_x, y_{\bar{x}}, x) \quad (70.11)$$

$$= P(\underline{y} = y_x, y_{\bar{x}}, x) \quad (70.12)$$

According to Pearl, the defining property of  $y_x$  is that

$$P(\underline{y}_x = y) = P(\underline{y} = y | \mathcal{D}\underline{x} = x) \quad (70.13)$$

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<sup>1</sup>Note that DAGs are not unique. Some are a better causal fit than others for the physical situation being considered. See Chapter 34 for a discussion of Goodness of Causal Fit.

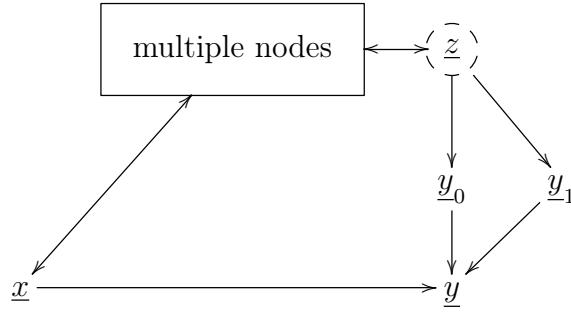


Figure 70.2: Type of Bnet considered in PTE theory. The box labeled “multiple nodes” contains various observed and hidden nodes with arrows to or from node  $\underline{x}$  and to or from node  $\underline{z}$ .  $\underline{z}$  can be a multinode.  $\underline{z}$  is shown as hidden but could be observed instead.

Pearl likes to call Eq.(70.13) the 1st Law. The 1st Law is also a consequence of bnet Fig.70.2 and the TPM Eq.(70.10). Indeed,  $\mathcal{D}\underline{x} = \underline{x}$  means one should amputate all arrows entering node  $\underline{x}$ , and one should set the TPM of  $\underline{x}$  to a delta function centered at  $\underline{x}$ . If that is done, then the values of  $\underline{y}$  and  $\underline{y}_x$  must be equal, because the TPM at node  $\underline{y}$  is a delta function that enforces this equality.

### 70.3 $ATE = PB - PH$

Define the **probability of benefit (PB)** (a.k.a. **Probability of Necessity and Sufficiency (PNS)**) by

$$PB = PNS = P(\underline{y}_0 = 0, \underline{y}_1 = 1) \quad (70.14)$$

and the **probability of harm (PH)** by

$$PH = P(\underline{y}_0 = 1, \underline{y}_1 = 0) \quad (70.15)$$

**Claim 104**

$$PB = P(\underline{y}_1 - \underline{y}_0 = 1) \quad (70.16)$$

$$PH = P(\underline{y}_1 - \underline{y}_0 = -1) \quad (70.17)$$

**proof:**

$$\underline{y}_1 - \underline{y}_0 = 1 \text{ iff } (\underline{y}_1 = 1 \text{ and } \underline{y}_0 = 0).$$

$$\underline{y}_1 - \underline{y}_0 = -1 \text{ iff } (\underline{y}_1 = 0 \text{ and } \underline{y}_0 = 1).$$

**QED**

**Claim 105**

$$ATE = PB - PH \quad (70.18)$$

**proof:**

$$ATE = E_\sigma[y_1^\sigma - y_0^\sigma] \quad (70.19)$$

$$= E[\underline{y}_1 - \underline{y}_0] \quad (70.20)$$

$$= \sum_y y [P(\underline{y}_1 = y) - P(\underline{y}_0 = y)] \quad (70.21)$$

$$= P(\underline{y}_1 = 1) - P(\underline{y}_0 = 1) \quad (70.22)$$

$$= \sum_{y_0} P(y_0, \underline{y}_1 = 1) - \sum_{y_1} P(\underline{y}_0 = 1, y_1) \quad (70.23)$$

$$= \underbrace{P(\underline{y}_0 = 0, \underline{y}_1 = 1)}_{PB} - \underbrace{P(\underline{y}_0 = 1, \underline{y}_1 = 0)}_{PH} \quad (70.24)$$

**QED**

See Fig.70.3 for an illustration of the constant  $ATE$  contours in the  $(PB, PH)$  plane.

See also Fig.70.4 for a vector representation of the identity  $ATE = PB - PH$ .

See also Fig.70.5 for an illustration of the region of possible points in the  $(ATE, PB)$  plane.

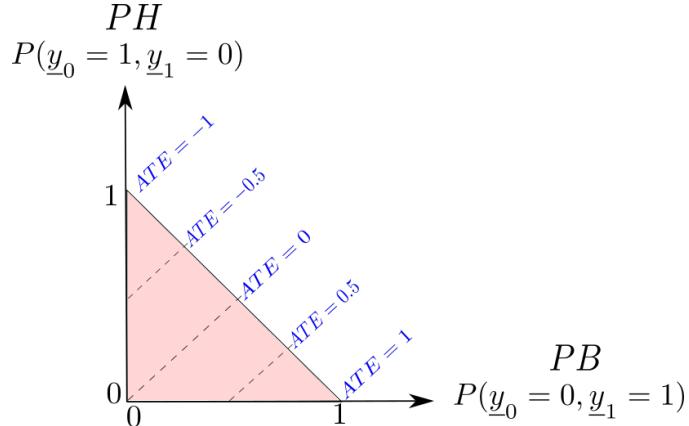


Figure 70.3: Shown in pink, the probability simplex  $\{(x, y) : x \geq 0, y \geq 0, x + y \leq 1\}$  with  $x = PB$  and  $y = PH$ . All points of that simplex are possible. Also shown are the constant  $ATE$  contours in the  $(PB, PH)$  plane.

## 70.4 Probabilities Relevant to PTE theory

Note<sup>2</sup>

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<sup>2</sup>To translate this section from our notation to the notation used by Tian and Pearl in Ref.[69], replace  $P(\underline{y}_1 = i, \underline{y}_0 = j, \underline{x} = k) \rightarrow p_{i,j,k} O_{1,0} \rightarrow P(x, y')$ ,  $O_{0|1} \rightarrow P(y'|x)$ ,  $E_{0|1} \rightarrow P(y'_x)$ , etc.

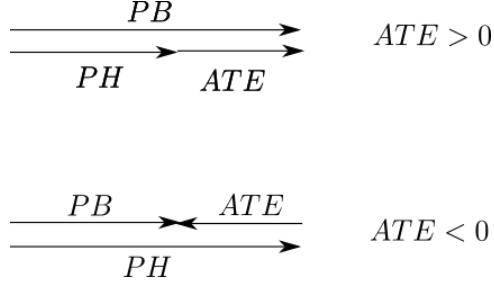


Figure 70.4: The identity  $ATE = PB - PH$  can be visualized as a vector sum in one dimension, where  $PB, PH \in [0, 1]$  and  $ATE \in [-1, 1]$ .

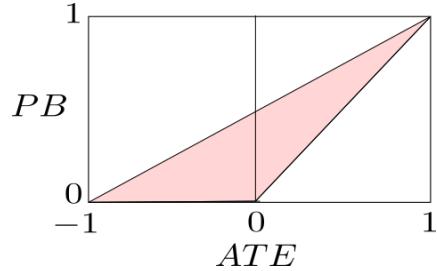


Figure 70.5: Shown in pink, the region of possible points in the  $(ATE, PB)$  plane.  $\max(0, ATE) \leq PB \leq (ATE + 1)/2$ .

Let  $x, y \in \{0, 1\}$  and  $z \in S_{\underline{z}}$  for some finite, not necessarily binary set  $S_{\underline{z}}$ . Define

$$\mathcal{P}_{x',y'|x,y} = P(\underline{y}_{x'} = y' | x, y) \quad (70.25)$$

**observational (non-causal) probabilities**

$$O_{x,y} = P(\underline{x} = x, \underline{y} = y) \quad (70.26)$$

$$O_{y|x} = P(\underline{y} = y | \underline{x} = x) \quad (70.27)$$

$$\pi_x = P(\underline{x} = x) \quad (70.28)$$

**experimental (causal) probabilities**

$$E_{y|x} = P(\underline{y}_x = y) \quad (70.29)$$

**Average Treatment Effect (ATE)**

$$ATE = P(\underline{y}_1 = 1) - P(\underline{y}_0 = 1) \quad (70.30)$$

$$= E_{1|1} - E_{1|0} \quad (70.31)$$

$$= E_{1|1} + E_{0|0} - 1 \quad (70.32)$$

## Conditional ATE (CATE)

$$ATE_z = P(\underline{y}_1 = 1|z) - P(\underline{y}_0 = 1|z) \quad (70.33)$$

$$= E_{1|1,z} + E_{0|0,z} - 1 \quad (70.34)$$

## Average Causal Effect

$$ACE = P(\underline{y} = 1|\mathcal{D}\underline{x} = 1) - P(\underline{y} = 1|\mathcal{D}\underline{x} = 0) \quad (70.35)$$

Note that

$$ACE = \underbrace{P(\underline{y} = 1|\mathcal{D}\underline{x} = 1)}_{P(\underline{y}_1=1)} - \underbrace{P(\underline{y} = 1|\mathcal{D}\underline{x} = 0)}_{P(\underline{y}_0=1)} = ATE \quad (70.36)$$

## Conditional ACE (CACE)

This is what is called  $ACE_z$  in Chapter 72. Note that  $ACE_z = ATE_z$ .

**Effect of Treatment on the Treated (ETT)** (i.e.,  $ATE$  for the treated)

$$ETT = \underbrace{P(\underline{y}_1 = 1|\underline{x} = 1)}_{\mathcal{E}_1} - \underbrace{P(\underline{y}_0 = 1|\underline{x} = 1)}_{\mathcal{E}_0} \quad (70.37)$$

Note that

$$\mathcal{E}_1\pi_1 = P(\underline{y}_1 = 1, \underline{x} = 1) \quad (70.38)$$

$$= O_{1,1} \quad (70.39)$$

and

$$\mathcal{E}_0\pi_1 = P(\underline{y}_0 = 1, \underline{x} = 1) \quad (70.40)$$

$$= P(\underline{y}_0 = 1) - \underbrace{P(\underline{x} = 0, \underline{y}_0 = 1)}_{P(\underline{x}=0, \underline{y}=1)} \quad (70.41)$$

$$= E_{1|0} - O_{0,1} \quad (70.42)$$

so

$$ETT\pi_1 = \sum_x O_{x,1} - E_{1|0} \quad (70.43)$$

## Probability of Necessity ( $PN$ )<sup>3</sup>

$$PN = \mathcal{P}_{0,0|1,1} \quad (70.44)$$

---

<sup>3</sup>I like to call  $PN$  the Probability of Nullifying, because it goes from 11 to 00

### Probability of Sufficiency ( $PS$ )<sup>4</sup>

$$PS = \mathcal{P}_{1,1|0,0} \quad (70.45)$$

### Probability of Necessity and Sufficiency (PNS) (a.k.a. Probability of Benefit (PB))

$$PNS = PB = P(\underline{y}_0 = 0, \underline{y}_1 = 1) \quad (70.46)$$

Henceforth, we will use  $PNS3$  to denote the trio

$$PNS3 = (PNS, PN, PS) . \quad (70.47)$$

### Probability of Harm (PH)

$$PH = P(\underline{y}_0 = 1, \underline{y}_1 = 0) \quad (70.48)$$

### Risk ratio or relative risk (RR)

$$RR = \frac{O_{1|1}}{O_{1|0}} \quad (70.49)$$

### Excess Risk Ratio (ERR)

$$ERR = \frac{O_{1|1} - O_{1|0}}{O_{1|1}} = 1 - \frac{1}{RR} \quad (70.50)$$

### Corrected ERR (CERR)

$$CERR = ERR + \frac{O_{1|0} - E_{1|0}}{O_{1,1}} \quad (70.51)$$

You might be wondering how  $P(\underline{y}_x = y|\underline{x} = 0)$  and  $P(\underline{y}_x = y|\underline{x} = 1)$  for  $x, y \in \{0, 1\}^2$  are related to  $O_{y|x}$  and  $E_{y|x}$ . The following claim shows how.

### Claim 106

$$P(\underline{y}_x = y|\underline{x} = x) = O_{y|x} \quad (70.52a)$$

$$P(\underline{y}_x = y|\underline{x} = \bar{x}) = \frac{E_{y|x} - O_{y|x}\pi_x}{\pi_{\bar{x}}} \quad (70.52b)$$

**proof:** Before we begin the proof, note that summing both sides of Eqs.(70.52) gives  $1 = 1$ , so these 2 equations pass that test.

$$P(\underline{y}_x = y|\underline{x} = x) = P(y = y|\underline{x} = x) = O_{y|x} \quad (70.53)$$

---

<sup>4</sup>I like to call  $PS$  the Probability of Surging, because it goes from 00 to 11

$$P(\underline{y}_x = y | \underline{x} = \bar{x}) = \frac{P(\underline{y}_x = y, \underline{x} = \bar{x})}{\pi_{\bar{x}}} \quad (70.54)$$

$$= \frac{P(\underline{y}_x = y) - P(\underline{y}_x = y, \underline{x} = x)}{\pi_{\bar{x}}} \quad (70.55)$$

$$= \frac{P(\underline{y}_x = y) - P(\underline{y}_x = y | \underline{x} = x)\pi_x}{\pi_{\bar{x}}} \quad (70.56)$$

$$= \frac{E_{y|x} - O_{y|x}\pi_x}{\pi_{\bar{x}}} \quad (70.57)$$

**QED**

**Claim 107**

$$P(y_0, y_1 | x) = P(y_{\bar{x}} | x, \underline{y} = y_x)P(\underline{y} = y_x | x) \quad (70.58)$$

$$= \begin{array}{c} y_{\bar{x}} \\ \nearrow \\ x \longrightarrow \underline{y} = y_x \end{array} \quad (70.59)$$

**proof:**

$$P(y_0, y_1 | x) = \frac{P(y_0, y_1, x)}{P(x)} \quad (70.60)$$

$$= \frac{P(y_{\bar{x}}, x, \underline{y} = y_x)}{P(x)} \quad (70.61)$$

$$= \frac{P(y_{\bar{x}} | x, \underline{y} = y_x)P(x, \underline{y} = y_x)}{P(x)} \quad (70.62)$$

$$= P(y_{\bar{x}} | x, \underline{y} = y_x)P(\underline{y} = y_x | x) \quad (70.63)$$

**QED**

**Claim 108**

$$\underbrace{PNS}_{P(\underline{y}_0=0, \underline{y}_1=1)} = PN * O_{1,1} + PS * O_{0,0} \quad (70.64)$$

Hence, if we know any two of  $(PN, PS, PNS)$ , we can calculate the third.

**proof:**

$$P(y_0, y_1) = \sum_x P(y_0, y_1|x)P(x) \quad (70.65)$$

$$= \sum_x P(y_{\bar{x}}|x, \underline{y} = y_x)P(x, \underline{y} = y_x) \quad (\text{see Claim 107.}) \quad (70.66)$$

$$= \begin{cases} P(y_1|\underline{x} = 0, \underline{y} = y_0)P(\underline{x} = 0, \underline{y} = y_0) \\ + P(y_0|\underline{x} = 1, \underline{y} = y_1)P(\underline{x} = 1, \underline{y} = y_1) \end{cases} \quad (70.67)$$

Thus,

$$P(\underline{y}_0 = 0, \underline{y}_1 = 1) = \begin{cases} P(\underline{y}_1 = 1|\underline{x} = 0, \underline{y} = 0)P(\underline{x} = 0, \underline{y} = 0) \\ + P(\underline{y}_0 = 0|\underline{x} = 1, \underline{y} = 1)P(\underline{x} = 1, \underline{y} = 1) \end{cases} \quad (70.68)$$

$$= PS * O_{0,0} + PN * O_{1,1} \quad (70.69)$$

**QED**

Note that  $PNS$  refers to both  $\underline{y}_0$  and  $\underline{y}_1$ ,  $PN$  refers only to  $\underline{y}_0$  and  $PS$  refers only to  $\underline{y}_1$ . Thus,  $PN$  and  $PS$  serve to separate the pair of variables  $(\underline{y}_0, \underline{y}_1)$  and to isolate them individually. Claim 108 is a quantitative expression of that separation.

Pearl likes to say that  $PNS$  belongs to Rung 3 because it's a probability that involves both  $\underline{y}_0$  and  $\underline{y}_1$ , and one of those two must be a counterfactual (an event that never occurred). On the other hand,  $PN, PS, ATE$ , etc., are defined in terms of probabilities that involve either  $\underline{y}_0$  or  $\underline{y}_1$  but not both. Probabilities that involve only one of them, can be expressed with the do operator, so they belong to Rung 2. Conditional probabilities like  $P(y|x)$  that involve neither  $\underline{y}_0$  nor  $\underline{y}_1$  belong to Rung 1.<sup>5</sup>

## 70.5 Symmetry

Define  $\sim$  to be an operator that swaps zeros and ones in  $P(\underline{y}_0 = y, \underline{y}_1 = y', x)$ . Hence

$$[P(\underline{y}_0 = y, \underline{y}_1 = y', \underline{x} = x)]^\sim = P(\underline{y}_1 = \bar{y}, \underline{y}_0 = \bar{y}', \underline{x} = \bar{x}) \quad (70.70)$$

$$(\mathcal{P}_{x', y'|x, y})^\sim = \mathcal{P}_{\bar{x}', \bar{y}'|\bar{x}, \bar{y}} \quad (70.71)$$

$$(O_{x,y})^\sim = O_{\bar{x}, \bar{y}} \quad (70.72)$$

$$(O_{y|x})^\sim = O_{\bar{y}|\bar{x}} \quad (70.73)$$

---

<sup>5</sup>Probabilities such as  $P(\underline{y}_0 = 1, \underline{y} = 0, \underline{x} = 1) = P(\underline{y}_0 = 1, \underline{y}_1 = 0, \underline{x} = 1)$  are considered Rung 3.

$$(\pi_x)^\sim = \pi_{\bar{x}} \quad (70.74)$$

$$(E_{y|x})^\sim = E_{\bar{y}|\bar{x}} \quad (70.75)$$

$$(PN)^\sim = PS, \quad (PS)^\sim = PN \quad (70.76)$$

$$(PNS)^\sim = PNS \quad (70.77)$$

$$(RR)^\sim = \frac{O_{0|0}}{O_{0|1}} \quad (70.78)$$

Recall

$$ERR = \frac{O_{1|1} - O_{1|0}}{O_{1|1}} = 1 - \frac{1}{RR} \quad (70.79)$$

Therefore, define

$$(ERR)^\sim = \frac{O_{0|0} - O_{0|1}}{O_{0|0}} = 1 - \frac{1}{(RR)^\sim} \quad (70.80)$$

Note that

$$O_{1|1} - O_{1|0} = O_{1|1} + O_{0|0} - 1 \quad (70.81)$$

$$= O_{0|0} - O_{0|1} \quad (70.82)$$

$$= (O_{1|1} - O_{1|0})^\sim \quad (70.83)$$

## 70.6 Linear Programming Problem

### Probability Simplex

$$\mathcal{S} = \left\{ P(y_0, y_1, x) : \begin{array}{l} P(y_0, y_1, x) \geq 0 \\ y_0, y_1, x \in \{0, 1\} \\ \sum_{y_0=0}^1 \sum_{y_1=0}^1 \sum_{x=0}^1 P(y_0, y_1, x) = 1 \end{array} \right\} \quad (70.84)$$

Note that  $\mathcal{S}$  has 7 degrees of freedom (dofs).

1. observational (non-causal) constraints on  $\mathcal{S}$  (3 constraints)

$$O_{x,y} = P(x, y) = \sum_{y'} P(\underline{y}_x = y, \underline{y}_{\bar{x}} = y', x) \quad \text{for } (x, y) \in \{(0, 1), (1, 0), (1, 1)\} \quad (70.85)$$

## 2. experimental (causal) constraints on $\mathcal{S}$ (2 constraints)<sup>6</sup>

$$E_{1|x} = P(\underline{y}_x = 1) = \sum_{x'} \sum_{y'} P(\underline{y}_x = 1, \underline{y}_{\bar{x}} = y', x = x') \quad \text{for } x \in \{0, 1\} \quad (70.86)$$

$\mathcal{S}$  has 7 dofs but the 3 observational constraints reduce the number of dofs to 4. The 5 observational and experimental constraints reduce the number of dofs to 2.  $\mathcal{S}$  is embedded in  $\mathbb{R}^8$  and then the 6 constraints (unit probability, 2 observational and 3 experimental) reduce it to the interior of a 6 or less sided figure in  $\mathbb{R}^2$ .

Henceforth, we will refer to the observational and experimental constraints together as the **minimal constraints**.

This is half of a linear programming problem. Recall that a **linear programming problem** can be stated as finding the column vector  $\xi$  that minimizes a cost  $\mathcal{C} = c^T \xi$  subject to  $A\xi = b$  and  $\xi \geq 0$ . Here we have no cost function or minimization, but we have  $A\xi = b$  and  $\xi \geq 0$  where  $\xi = [P(y_0, y_1, x)]_{\forall y_0, y_1, x}$ . Also  $b = [1, O_{0,1}, O_{1,0}, O_{1,1}, E_{1|0}, E_{1|1}]^T$ , and  $A$  = a matrix of zeros and ones.

Note that

$$PNS = P(\underline{y}_0 = 0, \underline{y}_1 = 1) \quad (70.87)$$

$$= \sum_x P(\underline{y}_0 = 0, \underline{y}_1 = 1, x) \quad (70.88)$$

$$PN = P(\underline{y}_0 = 0 | \underline{x} = 1, \underline{y} = 1) \quad (70.89)$$

$$= \frac{P(\underline{y}_0 = 0, \underline{y}_1 = 1, \underline{x} = 1)}{O_{1,1}} \quad (70.90)$$

$$PS = P(\underline{y}_1 = 1 | \underline{x} = 0, \underline{y} = 0) \quad (70.91)$$

$$= \frac{P(\underline{y}_0 = 0, \underline{y}_1 = 1, \underline{x} = 0)}{O_{0,0}} \quad (70.92)$$

## 70.7 Special constraints

- **Exogeneity (a.k.a. no-confounding)** holds for simplex  $\mathcal{S}$  if  $\underline{y}_x \perp \underline{x}$  for  $x \in \{0, 1\}$ . Hence

$$\underbrace{P(\underline{y}_x = 1)}_{E_{1|x}} = P(\underline{y}_x = 1 | x) = \underbrace{P(\underline{y} = 1 | x)}_{O_{1|x}} \quad \text{for } x \in \{0, 1\} \quad (70.93)$$

---

<sup>6</sup> $E_{0|x}$  follows from  $E_{0|x} = 1 - E_{1|x}$ .

Exogeneity gives **2 constraints**.

Note that exogeneity is the same thing as identifiability of  $P(\underline{y}_x = \underline{y}) = P(\underline{y} = \underline{y} | \mathcal{D}\underline{x} = \underline{x})$ . But identifiability (i.e., do-identifiability) is a more general concept. One can speak of the identifiability of  $P(y_x | z)$  or of  $P(y_0, y_1, a)$ , etc. In general, any expression with do operators is do-identifiable if it can be expressed as an expression without do-operators.

- **Strong Exogeneity** holds for simplex  $\mathcal{S}$  if  $(\underline{y}_0, \underline{y}_1)_{joint} \perp \underline{x}$ . Hence

$$P(y_0, y_1 | x) = P(y_0, y_1) \quad (70.94)$$

Strong exogeneity gives **3 constraints**. Strong exogeneity implies exogeneity but not the converse.<sup>7</sup>

- **Monotonicity**<sup>8</sup> holds for simplex  $\mathcal{S}$  if

$$PH = P(\underline{y}_0 = 1, \underline{y}_1 = 0) = 0 \quad (70.95)$$

. Equivalently,

$$\sum_x P(\underline{y}_0 = 1, \underline{y}_1 = 0, x) = 0 \quad (70.96)$$

which is true iff

$$P(\underline{y}_0 = 1, \underline{y}_1 = 0, x) = 0 \quad \text{for } x \in \{0, 1\} \quad (70.97)$$

Monotonicity gives **2 constraints**.

Note that when  $PH = 0$ ,  $PNS = ATE$ .

**Claim 109** *Monotonicity and exogeneity together imply strong exogeneity.*

**proof:**

This proof is presented here for completeness. Later on, we will give a much simpler proof of this result. I advise the reader to skip this proof on first reading of this chapter.

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<sup>7</sup>In this book, we use both  $(\underline{a}, \underline{b})_\& \perp \underline{x}$  and  $(\underline{a}, \underline{b})_{joint} \perp \underline{x}$ . When we write  $(\underline{a}, \underline{b})_\& \perp \underline{x}$ , we mean that  $\underline{a} \perp \underline{x}$  and  $\underline{b} \perp \underline{x}$ , or, equivalently,  $P(a|x) = P(a)$  and  $P(b|x) = P(b)$ . When we write  $(\underline{a}, \underline{b})_{joint} \perp \underline{x}$  or simply  $(\underline{a}, \underline{b}) \perp \underline{x}$ , we mean  $P(a, b|x) = P(a, b)$ . Summing  $P(a, b|x) = P(a, b)$  over  $a$  gives  $P(b|x) = P(b)$ , and summing it over  $b$  gives  $P(a|x) = P(a)$ . Hence we see that  $(\underline{a}, \underline{b})_{joint} \perp \underline{x}$  implies  $(\underline{a}, \underline{b})_\& \perp \underline{x}$  but not the converse. If  $\underline{a}$  and  $\underline{b}$  are independent at fixed  $\underline{x}$  so that  $P(a, b|x) = P(a|x)P(b|x)$  then  $(\underline{a}, \underline{b})_{joint} \perp \underline{x}$  iff  $(\underline{a}, \underline{b})_\& \perp \underline{x}$

<sup>8</sup>This property is called monotonicity because it's equivalent to the statement that  $y_0^\sigma \leq y_1^\sigma$  for all individuals  $\sigma$  in the population. Indeed,  $y_0^\sigma \leq y_1^\sigma$  includes the 3 cases  $(y_0^\sigma, y_1^\sigma) = (0, 0), (1, 1), (0, 1)$ , but excludes the only other case, namely  $(1, 0)$ .

Let  $a \in \{0, 1\}$ .

$$P(\underline{y}_a = \bar{a}, x) = \sum_{a'} P(\underline{y}_a = \bar{a}, \underline{y}_{\bar{a}} = a', x) \quad (70.98)$$

$$= P(\underline{y}_a = \bar{a}, \underline{y}_{\bar{a}} = \bar{a}, x) \quad (\text{by monotonicity}) \quad (70.99)$$

Thus,

$$P(\underline{y}_a = \bar{a} | \underline{x} = a) = P(\underline{y}_a = \bar{a}, \underline{y}_{\bar{a}} = \bar{a} | \underline{x} = a) \quad (70.100)$$

and

$$P(\underline{y}_a = \bar{a}) = P(\underline{y}_a = \bar{a}, \underline{y}_{\bar{a}} = \bar{a}) \quad (70.101)$$

By exogeneity, the left hand side of Eq.(70.100) and the left hand side of Eq.(70.101) are equal, so the right hand sides of those equations must be equal too.

$$P(\underline{y}_a = \bar{a}, \underline{y}_{\bar{a}} = \bar{a} | \underline{x} = a) = P(\underline{y}_a = \bar{a}, \underline{y}_{\bar{a}} = \bar{a}) \quad (70.102)$$

This immediately implies<sup>9</sup>

$$P(\underline{y}_a = \bar{a}, \underline{y}_{\bar{a}} = \bar{a} | x) = P(\underline{y}_a = \bar{a}, \underline{y}_{\bar{a}} = \bar{a}) \quad (70.103)$$

for  $x \in \{0, 1\}$ . This gives for  $a = 0$

$$P(\underline{y}_0 = 1, \underline{y}_1 = 1 | x) = P(\underline{y}_0 = 1, \underline{y}_1 = 1) \quad (70.104)$$

and for  $a = 1$

$$\underbrace{P(\underline{y}_1 = 0, \underline{y}_0 = 0 | x)}_{P(\underline{y}_0 = 0, \underline{y}_1 = 0 | x)} = \underbrace{P(\underline{y}_1 = 0, \underline{y}_0 = 0)}_{P(\underline{y}_0 = 0, \underline{y}_1 = 0)} \quad (70.105)$$

Monotonicity itself gives

$$P(\underline{y}_0 = 1, \underline{y}_1 = 0 | x) = 0 = P(\underline{y}_0 = 1, \underline{y}_1 = 0) \quad (70.106)$$

The remaining strong exogeneity constraint, given by

$$P(\underline{y}_0 = 0, \underline{y}_1 = 1 | x) = P(\underline{y}_0 = 0, \underline{y}_1 = 1), \quad (70.107)$$

follows because

$$\sum_{y_0, y_1} P(y_0, y_1 | x) = \sum_{y_0, y_1} P(y_0, y_1) = 1 \quad (70.108)$$

**QED**

---

<sup>9</sup>If  $x \in \{0, 1\}$  and  $P(a | \underline{x} = 0) = P(a)$ , then  $P(a) - P(a, \underline{x} = 0) = P(a)[1 - P(\underline{x} = 0)]$ , so  $P(a, \underline{x} = 1) = P(a)P(\underline{x} = 1)$ . Hence,  $P(a | \underline{x} = 1) = P(a)$ .

## 70.8 Matrix representation of probabilities

Suppose  $\epsilon_x(y_0, y_1)$  for  $x, y_0, y_1 \in \{0, 1\}$  are eight vectors in a vector space  $V$ .  $\epsilon_x(y_0, y_1)$  will only be used at position  $(y_0, y_1)$  of a  $2 \times 2$  matrix, where the positions are defined as follows:

$$\begin{array}{ccc} & y_1 & \\ \uparrow & & \\ 1 & (0, 1) & (1, 1) \\ | & & \\ 0 & (0, 0) & (1, 0) \\ | & & \\ 0 & \longrightarrow & 1 \longrightarrow y_0 \end{array} \quad (70.109)$$

When  $\epsilon_x(y_0, y_1)$  is used inside a  $2 \times 2$  matrix, we will not write the argument  $(y_0, y_1)$ , leaving it implicit, unless confusion may arise. Thus, for example, we will represent

$$\mathcal{P} \begin{bmatrix} \epsilon_0(0, 1) & 0 \\ 0 & 0 \end{bmatrix} \text{ by } \mathcal{P} \begin{bmatrix} \epsilon_0 & 0 \\ 0 & 0 \end{bmatrix}.$$

For  $x \in \{0, 1\}$ , let

$$P_{\underline{y}_0, \underline{y}_1, \underline{x}}(0, 0, x) = \mathcal{P} \begin{bmatrix} 0 & 0 \\ \epsilon_x & 0 \end{bmatrix} \quad (70.110a)$$

$$P_{\underline{y}_0, \underline{y}_1, \underline{x}}(0, 1, x) = \mathcal{P} \begin{bmatrix} \epsilon_x & 0 \\ 0 & 0 \end{bmatrix} \quad (70.110b)$$

$$P_{\underline{y}_0, \underline{y}_1, \underline{x}}(1, 0, x) = \mathcal{P} \begin{bmatrix} 0 & 0 \\ 0 & \epsilon_x \end{bmatrix} \quad (70.110c)$$

$$P_{\underline{y}_0, \underline{y}_1, \underline{x}}(1, 1, x) = \mathcal{P} \begin{bmatrix} 0 & \epsilon_x \\ 0 & 0 \end{bmatrix} \quad (70.110d)$$

Define a map  $\mathcal{P}[\quad] : V \rightarrow \mathbb{R}$  that we will call the **matrix representation of probabilities (MRP)** (mnemonic, Mr. P). We will assume that the map  $\mathcal{P}[\quad]$  is linear. Hence, for instance,

$$\mathcal{P} \begin{bmatrix} 4\epsilon_0 + 3\epsilon_1 & -5\epsilon_0 \\ 0 & 0 \end{bmatrix} = 4\mathcal{P} \begin{bmatrix} \epsilon_0 & 0 \\ 0 & 0 \end{bmatrix} + 3\mathcal{P} \begin{bmatrix} \epsilon_1 & 0 \\ 0 & 0 \end{bmatrix} - 5\mathcal{P} \begin{bmatrix} 0 & \epsilon_0 \\ 0 & 0 \end{bmatrix} \quad (70.111)$$

Henceforth, we will use the abbreviation

$$\epsilon_+ = \epsilon_0 + \epsilon_1 \quad (70.112)$$

Note that

$$\mathcal{P} \begin{bmatrix} \epsilon_+ & \epsilon_+ \\ \epsilon_+ & \epsilon_+ \end{bmatrix} = 1 \quad (70.113)$$

$$\pi_x = \mathcal{P} \begin{bmatrix} \epsilon_x & \epsilon_x \\ \epsilon_x & \epsilon_x \end{bmatrix} \quad (70.114)$$

$$E_{0|0} = \mathcal{P} \begin{bmatrix} \epsilon_+ & 0 \\ \epsilon_+ & 0 \end{bmatrix}, \quad O_{0,0} = \mathcal{P} \begin{bmatrix} \epsilon_0 & 0 \\ \epsilon_0 & 0 \end{bmatrix} \quad (70.115)$$

$$E_{0|1} = \mathcal{P} \begin{bmatrix} 0 & 0 \\ \epsilon_+ & \epsilon_+ \end{bmatrix}, \quad O_{1,0} = \mathcal{P} \begin{bmatrix} 0 & 0 \\ \epsilon_1 & \epsilon_1 \end{bmatrix} \quad (70.116)$$

$$E_{1|0} = \mathcal{P} \begin{bmatrix} 0 & \epsilon_+ \\ 0 & \epsilon_+ \end{bmatrix}, \quad O_{0,1} = \mathcal{P} \begin{bmatrix} 0 & \epsilon_0 \\ 0 & \epsilon_0 \end{bmatrix} \quad (70.117)$$

$$E_{1|1} = \mathcal{P} \begin{bmatrix} \epsilon_+ & \epsilon_+ \\ 0 & 0 \end{bmatrix}, \quad O_{1,1} = \mathcal{P} \begin{bmatrix} \epsilon_1 & \epsilon_1 \\ 0 & 0 \end{bmatrix} \quad (70.118)$$

$$P(\underline{y} = 0) = O_{0,0} + O_{1,0} = \mathcal{P} \begin{bmatrix} \epsilon_0 & 0 \\ \epsilon_+ & \epsilon_1 \end{bmatrix} \quad (70.119)$$

$$P(\underline{y} = 1) = O_{0,1} + O_{1,1} = \mathcal{P} \begin{bmatrix} \epsilon_1 & \epsilon_+ \\ 0 & \epsilon_0 \end{bmatrix} \quad (70.120)$$

$$PN * O_{1,1} = \mathcal{P} \begin{bmatrix} \epsilon_0 & 0 \\ 0 & 0 \end{bmatrix} \quad (70.121)$$

$$PS * O_{0,0} = \mathcal{P} \begin{bmatrix} \epsilon_1 & 0 \\ 0 & 0 \end{bmatrix} \quad (70.122)$$

$$PNS = \mathcal{P} \begin{bmatrix} \epsilon_+ & 0 \\ 0 & 0 \end{bmatrix} \quad (70.123)$$

$$PH = \mathcal{P} \begin{bmatrix} 0 & 0 \\ 0 & \epsilon_+ \end{bmatrix} \quad (70.124)$$

$$ATE = PNS - PH = \mathcal{P} \begin{bmatrix} \epsilon_+ & 0 \\ 0 & -\epsilon_+ \end{bmatrix} \quad (70.125)$$

When  $PH = 0$ ,

$$P(\underline{y} = 1)|_{PH=0} = \mathcal{P} \begin{bmatrix} \epsilon_1 & \epsilon_+ \\ 0 & 0 \end{bmatrix} \quad (70.126)$$

The special constraints of exogeneity, strong exogeneity and monotonicity have a very simple in the MRP.

Suppose that  $\pi_0, \pi_1 \geq 1$  and  $\pi_0 + \pi_1 = 1$ . Note that

$$\left. \begin{array}{l} \epsilon_+ = \frac{\epsilon_0}{\pi_0} \\ \text{or} \\ \epsilon_+ = \frac{\epsilon_1}{\pi_1} \end{array} \right\} \implies \epsilon_+ = \frac{\epsilon_0}{\pi_0} = \frac{\epsilon_1}{\pi_1} \quad (70.127)$$

Below, we will abbreviate

$$\hat{\epsilon}_x = \frac{\epsilon_x}{\pi_x} \quad (70.128)$$

for  $x \in \{0, 1\}$ .

### Claim 110

(a) *Exogeneity holds iff (“4 sides can change color”)*

$$\mathcal{P} \begin{bmatrix} \hat{\epsilon}_0 & 0 \\ \hat{\epsilon}_0 & 0 \end{bmatrix} = \mathcal{P} \begin{bmatrix} \hat{\epsilon}_1 & 0 \\ \hat{\epsilon}_1 & 0 \end{bmatrix} = \mathcal{P} \begin{bmatrix} \epsilon_+ & 0 \\ \epsilon_+ & 0 \end{bmatrix} \quad (70.129a)$$

$$\mathcal{P} \begin{bmatrix} \hat{\epsilon}_0 & \hat{\epsilon}_0 \\ 0 & 0 \end{bmatrix} = \mathcal{P} \begin{bmatrix} \hat{\epsilon}_1 & \hat{\epsilon}_1 \\ 0 & 0 \end{bmatrix} = \mathcal{P} \begin{bmatrix} \epsilon_+ & \epsilon_+ \\ 0 & 0 \end{bmatrix} \quad (70.129b)$$

$$\mathcal{P} \begin{bmatrix} 0 & \hat{\epsilon}_0 \\ 0 & \hat{\epsilon}_0 \end{bmatrix} = \mathcal{P} \begin{bmatrix} 0 & \hat{\epsilon}_1 \\ 0 & \hat{\epsilon}_1 \end{bmatrix} = \mathcal{P} \begin{bmatrix} 0 & \epsilon_+ \\ 0 & \epsilon_+ \end{bmatrix} \quad (70.129c)$$

$$\mathcal{P} \begin{bmatrix} 0 & 0 \\ \hat{\epsilon}_0 & \hat{\epsilon}_0 \end{bmatrix} = \mathcal{P} \begin{bmatrix} 0 & 0 \\ \hat{\epsilon}_1 & \hat{\epsilon}_1 \end{bmatrix} \mathcal{P} \begin{bmatrix} 0 & 0 \\ \epsilon_+ & \epsilon_+ \end{bmatrix} \quad (70.129d)$$

(b) *Monotonicity holds iff*

$$\mathcal{P} \begin{bmatrix} 0 & 0 \\ 0 & \epsilon_x \end{bmatrix} = 0 \quad (70.130)$$

for  $x \in \{0, 1\}$ .

(c) *Strong exogeneity holds iff (“4 corners can change color”)*

$$\mathcal{P} \begin{bmatrix} \hat{\epsilon}_0 & 0 \\ 0 & 0 \end{bmatrix} = \mathcal{P} \begin{bmatrix} \hat{\epsilon}_1 & 0 \\ 0 & 0 \end{bmatrix} = \mathcal{P} \begin{bmatrix} \epsilon_+ & 0 \\ 0 & 0 \end{bmatrix} \quad (70.131a)$$

$$\mathcal{P} \begin{bmatrix} 0 & \hat{\epsilon}_0 \\ 0 & 0 \end{bmatrix} = \mathcal{P} \begin{bmatrix} 0 & \hat{\epsilon}_1 \\ 0 & 0 \end{bmatrix} = \mathcal{P} \begin{bmatrix} 0 & \epsilon_+ \\ 0 & 0 \end{bmatrix} \quad (70.131b)$$

$$\mathcal{P} \begin{bmatrix} 0 & 0 \\ 0 & \hat{\epsilon}_0 \end{bmatrix} = \mathcal{P} \begin{bmatrix} 0 & 0 \\ 0 & \hat{\epsilon}_1 \end{bmatrix} = \mathcal{P} \begin{bmatrix} 0 & 0 \\ 0 & \epsilon_+ \end{bmatrix} \quad (70.131c)$$

$$\mathcal{P} \begin{bmatrix} 0 & 0 \\ \hat{\epsilon}_0 & 0 \end{bmatrix} = \mathcal{P} \begin{bmatrix} 0 & 0 \\ \hat{\epsilon}_1 & 0 \end{bmatrix} = \mathcal{P} \begin{bmatrix} 0 & 0 \\ \epsilon_+ & 0 \end{bmatrix} \quad (70.131d)$$

**proof:**

(a) This follows from the definitions of  $E_{y|x}$  and  $O_{x,y}$  for  $x, y \in \{0, 1\}$ , as stated above in the MRP.

(b) This follows from the identity

$$P_{\underline{y}_0, \underline{y}_1, \underline{x}}(1, 0|x) = \mathcal{P} \begin{bmatrix} 0 & 0 \\ 0 & \frac{\epsilon_x}{\pi_x} \end{bmatrix} \quad (70.132)$$

for  $x \in \{0, 1\}$ .

(c) This follows from definitions of  $P_{\underline{y}_0, \underline{y}_1, \underline{x}}(y_0, y_1, x)$  for  $y_0, y_1, x \in \{0, 1\}$ , as stated above in the MRP.

**QED**

Note that it is obvious from Claim 110 that strong exogeneity implies exogeneity.

Claim 110 also makes it easy peasy to prove that exogeneity and monotonicity imply strong exogeneity. Indeed, here is a much simpler proof than the one we presented earlier.

**Claim 111** *Exogeneity and monotonicity imply strong exogeneity.*

**proof:** Let's call  $E(a), E(b), E(c), E(d)$  the four Eqs.(70.129) that define Exogeneity, and  $SE(a), SE(b), SE(c), SE(d)$  the four Eqs.(70.131) that define Strong Exogeneity.

- Monotonicity implies the lower right entry is zero, so  $SE(c)$  is true.
- Setting to zero the lower right entry in  $E(c)$  and  $E(d)$  implies  $SE(b)$  and  $SE(d)$ .
- Subtracting  $SE(d)$  from  $E(a)$  gives  $SE(a)$ .

**QED**

## 70.9 Bounds on Exp. Probs. imposed by Obs. Probs.

**Claim 112** *In general,*

$$O_{x,1} \leq E_{1|x} \leq 1 - O_{x,0} \quad \text{for } x \in \{0, 1\}. \quad (70.133)$$

*In other words,*

$$O_{1,1} \leq E_{1|1} \leq 1 - O_{1,0} \quad (70.134)$$

$$O_{0,1} \leq E_{1|0} \leq 1 - O_{0,0} \quad (70.135)$$

*With monotonicity, we get the tighter bounds*

$$\overbrace{O_{1,1} + O_{0,1}}^{P(\underline{y}=1)} \leq E_{1|1} \leq 1 - O_{1,0} \quad (70.136)$$

$$O_{0,1} \leq E_{1|0} \leq \overbrace{1 - O_{0,0} - O_{1,0}}^{P(\underline{y}=1)} \quad (70.137)$$

**proof:**

$$O_{1,1} \leq E_{1|1} \leq \underbrace{1 - O_{1,0}}_{O_{1,1} + O_{0,0} + O_{0,1}} \quad (70.138)$$

has the MRP

$$\mathcal{P} \begin{bmatrix} \epsilon_1 & \epsilon_1 \\ 0 & 0 \end{bmatrix} \leq \mathcal{P} \begin{bmatrix} \epsilon_+ & \epsilon_+ \\ 0 & 0 \end{bmatrix} \leq \mathcal{P} \begin{bmatrix} \epsilon_1 & \epsilon_1 \\ 0 & 0 \end{bmatrix} + \mathcal{P} \begin{bmatrix} \epsilon_0 & 0 \\ \epsilon_0 & 0 \end{bmatrix} + \mathcal{P} \begin{bmatrix} 0 & \epsilon_0 \\ 0 & \epsilon_0 \end{bmatrix} \quad (70.139)$$

which is obviously true.

$$O_{0,1} \leq E_{1|0} \leq \underbrace{1 - O_{0,0}}_{O_{1,1} + O_{0,1} + O_{1,0}} \quad (70.140)$$

has the MRP

$$\mathcal{P} \begin{bmatrix} 0 & \epsilon_0 \\ 0 & \epsilon_0 \end{bmatrix} \leq \mathcal{P} \begin{bmatrix} 0 & \epsilon_+ \\ 0 & \epsilon_+ \end{bmatrix} \leq \mathcal{P} \begin{bmatrix} \epsilon_1 & \epsilon_1 \\ 0 & 0 \end{bmatrix} + \mathcal{P} \begin{bmatrix} 0 & \epsilon_0 \\ 0 & \epsilon_0 \end{bmatrix} + \mathcal{P} \begin{bmatrix} 0 & 0 \\ \epsilon_1 & \epsilon_1 \end{bmatrix} \quad (70.141)$$

which is obviously true.

$$P(\underline{y} = 1)|_{PH=0} \leq E_{1|1} \quad (70.142)$$

has the MRP

$$\mathcal{P} \begin{bmatrix} \epsilon_1 & \epsilon_+ \\ 0 & 0 \end{bmatrix} \leq \mathcal{P} \begin{bmatrix} \epsilon_+ & \epsilon_+ \\ 0 & 0 \end{bmatrix} \quad (70.143)$$

which is obviously true.

$$E_{1|0}|_{PH=0} \leq P(\underline{y} = 1)|_{PH=0} \quad (70.144)$$

has the MRP

$$\mathcal{P} \begin{bmatrix} 0 & \epsilon_+ \\ 0 & 0 \end{bmatrix} \leq \mathcal{P} \begin{bmatrix} \epsilon_1 & \epsilon_+ \\ 0 & 0 \end{bmatrix} \quad (70.145)$$

which is obviously true.

**QED**

## 70.10 Bounds on $PNS_3$ for unspecified bnet

**Claim 113** *If  $P(a, b)$  is a probability distribution, then*

$$\max\{0, P(a) + P(b) - 1\} \leq P(a, b) \leq \min\{P(a), P(b)\} \quad (70.146)$$

**proof:**  $P(a|b) \leq 1$  and  $P(b|a) \leq 1$  implies  $P(a, b) \leq P(b)$  and  $P(a, b) \leq P(a)$ . Hence,  $P(a, b) \leq \min\{P(a), P(b)\}$ .

$$P(a) + P(b) - 1 = \sum_{a', b'} P(a', b') \underbrace{[\delta(a, a') + \delta(b, b') - 1]}_T \quad (70.147)$$

$$\leq P(a, b) \quad (T \text{ biggest when } a = a' \text{ and } b = b') \quad (70.148)$$

QED

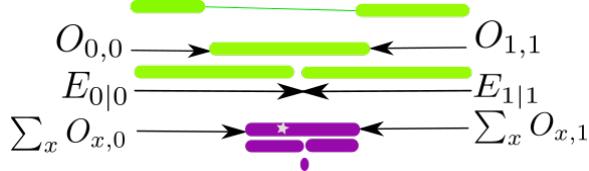


Figure 70.6: Minimal bounds for  $PNS$ .  $PNS$  is larger than maximum of the purple segments and smaller than the minimum of the green ones. The purple segment of almost zero length represents zero. The green segment interrupted by a thin green line represents  $O_{0,0} + O_{1,1}$ . Note that  $\sum_x O_{x,0} + \sum_x O_{x,1} = 1$ . When monotonicity holds,  $PNS$  equals  $E_{1|1} + E_{0|0} - 1$  which is the purple segment marked with a star.

**Claim 114** *Minimal bounds (see Fig. 70.6)*

*If the minimal constraints hold for simplex  $\mathcal{S}$ , then*

$$\max \left\{ \begin{array}{l} 0 \\ E_{1|1} + E_{0|0} - 1 \\ E_{0|0} - \sum_x O_{x,0} \\ E_{1|1} - \sum_x O_{x,1} \end{array} \right\} \leq PNS \leq \min \left\{ \begin{array}{l} E_{1|1} \\ E_{0|0} \\ O_{1,1} + O_{0,0} \\ E_{1|1} + E_{0|0} - O_{1,1} - O_{0,0} \end{array} \right\} \quad (70.149)$$

$$\max \left\{ \frac{0}{E_{0|0} - \sum_x O_{x,0}} \right\} \leq PN \leq \min \left\{ \frac{1}{E_{0|0} - O_{0,0}} \right\} \quad (70.150)$$

$$\max \left\{ \frac{0}{E_{1|1} - \sum_x O_{x,1}} \right\} \leq PS \leq \min \left\{ \frac{1}{E_{1|1} - O_{1,1}} \right\} \quad (70.151)$$

**proof:** These bounds were copied directly from Ref.[69], except the notation was changed. In certain cases, we have slightly rewritten the bounds from Ref.[69] to exhibit more explicitly their symmetry under swaps of zeros and ones. For example, instead of using  $(E_{1|0}, E_{1|1})$  as parameters, we use  $(E_{1|1}, E_{0|0})$ .

These bounds are obviously true in the MRP. Indeed, in the MRP, the following holds. For  $PNS$ , we have

$$\begin{bmatrix} 0 \\ E_{1|1} + E_{0|0} - 1 \\ E_{0|0} - \sum_x O_{x,0} \\ E_{1|1} - \sum_x O_{x,1} \end{bmatrix} = \begin{bmatrix} 0 \\ \mathcal{P} \begin{bmatrix} \epsilon_+ & 0 \\ 0 & -\epsilon_+ \end{bmatrix} \\ \mathcal{P} \begin{bmatrix} \epsilon_1 & 0 \\ 0 & -\epsilon_1 \end{bmatrix} \\ \mathcal{P} \begin{bmatrix} \epsilon_0 & 0 \\ 0 & -\epsilon_0 \end{bmatrix} \end{bmatrix} \quad (70.152)$$

$$PNS = \mathcal{P} \begin{bmatrix} \epsilon_+ & 0 \\ 0 & 0 \end{bmatrix} \quad (70.153)$$

$$\begin{bmatrix} E_{1|1} \\ E_{0|0} \\ O_{1,1} + O_{0,0} \\ E_{1|1} + E_{0|0} - O_{1,1} - O_{0,0} \end{bmatrix} = \begin{bmatrix} \mathcal{P} \begin{bmatrix} \epsilon_+ & 0 \\ \epsilon_+ & 0 \end{bmatrix} \\ \mathcal{P} \begin{bmatrix} \epsilon_+ & \epsilon_+ \\ 0 & 0 \end{bmatrix} \\ \mathcal{P} \begin{bmatrix} \epsilon_+ & \epsilon_1 \\ \epsilon_0 & 0 \end{bmatrix} \\ \mathcal{P} \begin{bmatrix} \epsilon_+ & \epsilon_0 \\ \epsilon_1 & 0 \end{bmatrix} \end{bmatrix} \quad (70.154)$$

For  $PN$ , we have

$$\begin{bmatrix} 0 \\ E_{1|1} - \sum_x O_{x,1} \end{bmatrix} = \begin{bmatrix} 0 \\ \mathcal{P} \begin{bmatrix} \epsilon_0 & 0 \\ 0 & -\epsilon_0 \end{bmatrix} \end{bmatrix} \quad (70.155)$$

$$PN * O_{1,1} = \mathcal{P} \begin{bmatrix} \epsilon_0 & 0 \\ 0 & 0 \end{bmatrix} \quad (70.156)$$

$$\begin{bmatrix} 1 \\ E_{1|1} - O_{1,1} \end{bmatrix} = \begin{bmatrix} 1 \\ \mathcal{P} \begin{bmatrix} \epsilon_0 & \epsilon_0 \\ 0 & 0 \end{bmatrix} \end{bmatrix} \quad (70.157)$$

For  $PS$ , we have

$$\begin{bmatrix} 0 \\ E_{0|0} - \sum_x O_{x,0} \end{bmatrix} = \begin{bmatrix} 0 \\ \mathcal{P} \begin{bmatrix} \epsilon_1 & 0 \\ 0 & -\epsilon_1 \end{bmatrix} \end{bmatrix} \quad (70.158)$$

$$PS * O_{0,0} = \mathcal{P} \begin{bmatrix} \epsilon_1 & 0 \\ 0 & 0 \end{bmatrix} \quad (70.159)$$

$$\begin{bmatrix} 1 \\ E_{0|0} - O_{0,0} \end{bmatrix} = \begin{bmatrix} 1 \\ \mathcal{P} \begin{bmatrix} \epsilon_1 & \epsilon_1 \\ 0 & 0 \end{bmatrix} \end{bmatrix} \quad (70.160)$$

The first two lines of the bound for  $PNS$  are a simple consequence of Claim 113. Indeed, Claim 113 implies

$$\max \left\{ \frac{0}{P(y_0) + P(y_1) - 1} \right\} \leq P(y_0, y_1) \leq \min \left\{ \frac{P(y_0)}{P(y_1)} \right\} \quad (70.161)$$

When  $y_0 = 0, y_1 = 1$ , we get

$$\max \left\{ \frac{0}{E_{0|0} + E_{1|1} - 1} \right\} \leq PNS \leq \min \left\{ \frac{E_{0|0}}{E_{1|1}} \right\} \quad (70.162)$$

**QED**

In Claim 114, note that

- $\sum_x O_{x,y} = P(\underline{y} = y)$  for  $y = 0, 1$ .
- Let

$$E'_{0|0} = E_{0|0} - \sum_x O_{x,0} = \mathcal{P} \begin{bmatrix} \epsilon_1 & 0 \\ 0 & -\epsilon_1 \end{bmatrix} \quad (70.163)$$

$$E'_{1|1} = E_{1|1} - \sum_x O_{x,1} = \mathcal{P} \begin{bmatrix} \epsilon_0 & 0 \\ 0 & -\epsilon_0 \end{bmatrix} \quad (70.164)$$

$$ATE = E_{1|1} + E_{0|0} - 1 = E'_{1|1} + E'_{0|0} = \mathcal{P} \begin{bmatrix} \epsilon_+ & 0 \\ 0 & -\epsilon_+ \end{bmatrix} \quad (70.165)$$

- Claim 114 applies if we have both observational data (OD) and experimental data (ED). If we only have OD (resp., ED), ignore all bounds that involve an  $E$  (resp., involve an  $O$ ) probability.

Hence, with only OD<sup>10</sup>

$$0 \leq PNS \leq O_{1,1} + O_{0,0} \quad (70.166)$$

---

<sup>10</sup>The bounds Eq.(70.166) assume exogeneity does not hold. For the case when exogeneity does hold, stronger bounds will be given later on in the chapter.

and  $PN, PS \in [0, 1]$ , whereas with only ED,

$$\max \left\{ \frac{0}{E_{1|1} + E_{0|0} - 1} \right\} \leq PNS \leq \min \left\{ \frac{E_{1|1}}{E_{0|0}} \right\} \quad (70.167)$$

and  $PN, PS \in [0, 1]$ .

- At first blush, there seem to be 3 possible cases to consider: (1) Only OD. (2) Both OD and ED. (3) Only ED. Actually, Case (1) plus the assumption of exogeneity is the same as Case (3). Indeed, recall that exogeneity means no confounding, and ED (i.e., an RCT) also has no confounding. So we don't have to consider Case (3) if we consider Case (1) without and with exogeneity. Exogeneity is built into case (2), so case (2) without exogeneity is meaningless.

**Claim 115** *If minimal and exogeneity constraints hold for simplex  $\mathcal{S}$ , then*

$$\max \left\{ \frac{0}{O_{1|1} + O_{0|0} - 1}, \frac{O_{0|0} - \sum_x O_{x,0}}{O_{1|1} - \sum_x O_{x,1}} \right\} \leq PNS \leq \min \left\{ \frac{O_{1|1}}{O_{0|0}}, \frac{O_{1,1} + O_{0,0}}{O_{1|1} + O_{0|0} - O_{1,1} - O_{0,0}} \right\} \quad (70.168)$$

$$\max \left\{ \frac{0}{ERR} \right\} \leq PN \leq \min \left\{ \frac{1}{\frac{O_{0|0}}{O_{1|1}}} \right\} \quad (70.169)$$

$$\max \left\{ \frac{0}{(ERR)^\sim} \right\} \leq PS \leq \min \left\{ \frac{1}{\frac{O_{1|1}}{O_{0|0}}} \right\} \quad (70.170)$$

**proof:** Just replace  $E_{y|x}$  by  $O_{y|x}$  in the minimal bounds given in Claim 114.

The canceled terms do not improve the bounds and can be dropped. We show this next using MRP.

In the MRP, the minimal bounds for  $PNS$  are

$$\begin{bmatrix} 0 \\ E_{1|1} + E_{0|0} - 1 \\ E_{0|0} - \sum_x O_{x,0} \\ E_{1|1} - \sum_x O_{x,1} \end{bmatrix} = \begin{bmatrix} 0 \\ \mathcal{P} \begin{bmatrix} \epsilon_+ & 0 \\ 0 & -\epsilon_+ \end{bmatrix} \\ \mathcal{P} \begin{bmatrix} \epsilon_1 & 0 \\ 0 & -\epsilon_1 \end{bmatrix} \\ \mathcal{P} \begin{bmatrix} \epsilon_0 & 0 \\ 0 & -\epsilon_0 \end{bmatrix} \end{bmatrix} \quad (70.171)$$

$$PNS = \mathcal{P} \begin{bmatrix} \epsilon_+ & 0 \\ 0 & 0 \end{bmatrix} \quad (70.172)$$

$$\begin{bmatrix} E_{1|1} \\ E_{0|0} \\ O_{1,1} + O_{0,0} \\ E_{1|1} + E_{0|0} - O_{1,1} - O_{0,0} \end{bmatrix} = \begin{bmatrix} \mathcal{P} \begin{bmatrix} \epsilon_+ & 0 \\ \epsilon_+ & 0 \end{bmatrix} \\ \mathcal{P} \begin{bmatrix} \epsilon_+ & \epsilon_+ \\ 0 & 0 \end{bmatrix} \\ \mathcal{P} \begin{bmatrix} \epsilon_+ & \epsilon_1 \\ \epsilon_0 & 0 \end{bmatrix} \\ \mathcal{P} \begin{bmatrix} \epsilon_+ & \epsilon_0 \\ \epsilon_1 & 0 \end{bmatrix} \end{bmatrix} \quad (70.173)$$

If exogeneity holds, we can replace all  $E$ 's by  $O$ 's on the left hand sides. We can also use  $\epsilon_+ = \hat{\epsilon}_0 = \hat{\epsilon}_1$  on the right hand sides to conclude that

$$O_{1|1} + O_{0|0} - 1 = \mathcal{P} \begin{bmatrix} \epsilon_+ & \epsilon_+ - \epsilon_+ \\ 0 & -\epsilon_+ \end{bmatrix} = \mathcal{P} \begin{bmatrix} \hat{\epsilon}_x & \hat{\epsilon}_x - \hat{\epsilon}_x \\ 0 & -\hat{\epsilon}_x \end{bmatrix} = \frac{1}{\pi_x} \mathcal{P} \begin{bmatrix} \epsilon_x & 0 \\ 0 & -\epsilon_x \end{bmatrix} \quad (70.174)$$

for both  $x \in \{0, 1\}$ . Note that  $\frac{1}{\pi_x} \mathcal{P} \begin{bmatrix} \epsilon_x & 0 \\ 0 & -\epsilon_x \end{bmatrix}$  will always be greater or equal to  $\mathcal{P} \begin{bmatrix} \epsilon_x & 0 \\ 0 & -\epsilon_x \end{bmatrix}$  when  $\mathcal{P} \begin{bmatrix} \epsilon_x & 0 \\ 0 & -\epsilon_x \end{bmatrix} \geq 0$  (if it's negative, the 0 bound takes precedence). Hence, the two canceled lower bound terms can be dropped. A similar argument shows that the two canceled upper bound terms can be dropped too.

**QED**

**Claim 116** *If the minimal and strong exogeneity constraints hold for simplex  $\mathcal{S}$ , then the inequalities for exogeneity Claim 115 hold. In addition,*

$$PN = \frac{PNS}{O_{1|1}} \quad (70.175)$$

and

$$PS = \frac{PNS}{O_{0|0}} \quad (70.176)$$

**proof:**

$$PN * O_{1|1} = P(\underline{y}_0 = 0, \underline{y} = 1 | \underline{x} = 1) \quad (70.177)$$

$$= P(\underline{y}_0 = 0, \underline{y}_1 = 1) \quad (70.178)$$

$$= PNS \quad (70.179)$$

$$PS * O_{0|0} = P(\underline{y}_1 = 1, \underline{y} = 0 | \underline{x} = 0) \quad (70.180)$$

$$= P(\underline{y}_0 = 0, \underline{y}_1 = 1) \quad (70.181)$$

$$= PNS \quad (70.182)$$

**QED**

**Claim 117** *If the minimal and monotonicity constraints hold for simplex  $\mathcal{S}$ , then*

$$PNS = E_{1|1} + E_{0|0} - 1 \quad (70.183)$$

$$PN = \frac{E_{0|0} - \sum_x O_{x,0}}{O_{1,1}} = \frac{\sum_x O_{x,1} - E_{1|0}}{O_{1,1}} = CERR \quad (70.184)$$

$$PS = \frac{E_{1|1} - \sum_x O_{x,1}}{O_{0,0}} = \frac{\sum_x O_{x,0} - E_{0|1}}{O_{0,0}} = (CERR)^\sim \quad (70.185)$$

**proof:** These results can be easily proven using the MRP.

Note that

$$\frac{\sum_x O_{x,1} - E_{1|0}}{O_{1,1}} = \frac{O_{1|1}\pi_1 + O_{1|0}(1 - \pi_1) - E_{1|0}}{O_{1|1}\pi_1} \quad (70.186)$$

$$= 1 - \frac{O_{1|0}}{O_{1|1}} + \frac{O_{1|0} - E_{1|0}}{O_{1,1}} \quad (70.187)$$

$$= CERR \quad (70.188)$$

**QED**

**Claim 118** *If the minimal, exogeneity and monotonicity constraints hold for simplex  $\mathcal{S}$ , then  $PNS, PN, PS$  are identifiable, and*

$$PNS = O_{1|1} + O_{0|0} - 1 \quad (70.189)$$

$$PN = \frac{O_{0|0} - \sum_x O_{x,0}}{O_{1,1}} = \frac{\sum_x O_{x,1} - O_{1|0}}{O_{1,1}} = ERR \quad (70.190)$$

$$PS = \frac{O_{1|1} - \sum_x O_{x,1}}{O_{0,0}} = \frac{\sum_x O_{x,0} - O_{0|1}}{O_{0,0}} = (ERR)^\sim \quad (70.191)$$

**proof:** Set  $E_{y|x} = O_{y|x}$  in Claim 117.

**QED**

## 70.11 Bounds on $PNS3$ for specific bnet families

### 70.12 Bounds on $ATE$ imposed by Obs. Probs.

**Claim 119**

$$O_{0,0} + O_{1,1} - 1 \leq ATE \leq O_{0,0} + O_{1,1} \quad (70.192)$$

**proof:**

$$O_{0,0} + O_{1,1} - 1 = \mathcal{P} \begin{bmatrix} 0 & -\epsilon_0 \\ -\epsilon_1 & -\epsilon_+ \end{bmatrix} \quad (70.193)$$

$$ATE = \mathcal{P} \begin{bmatrix} \epsilon_+ & 0 \\ 0 & -\epsilon_+ \end{bmatrix} \quad (70.194)$$

$$O_{0,0} + O_{1,1} = \mathcal{P} \begin{bmatrix} \epsilon_+ & \epsilon_1 \\ \epsilon_0 & 0 \end{bmatrix} \quad (70.195)$$

QED

### 70.13 Bounds on $PNS$ in terms of $ATE$ and Obs. Probs.

**Claim 120**

$$\max \left\{ \frac{0}{ATE} \right\} \leq PNS \leq \min \left\{ \frac{O_{0,0} + O_{1,1}}{O_{0,1} + O_{1,0} + ATE} \right\} \quad (70.196)$$

Hence,

$$\max \left\{ \frac{0}{ATE} \right\} \leq PNS \leq \min \left\{ \frac{1}{1 + ATE} \right\} \quad (70.197)$$

**proof:**

Note that

$$ATE = \mathcal{P} \begin{bmatrix} \epsilon_+ & 0 \\ 0 & -\epsilon_+ \end{bmatrix} \quad (70.198)$$

and

$$PNS = \mathcal{P} \begin{bmatrix} \epsilon_+ & 0 \\ 0 & 0 \end{bmatrix} \quad (70.199)$$

so

$$\max \left\{ \begin{array}{c} 0 \\ ATE \end{array} \right\} = \max \left\{ \begin{array}{c} 0 \\ \mathcal{P} \begin{bmatrix} \epsilon_+ & 0 \\ 0 & -\epsilon_+ \end{bmatrix} \end{array} \right\} \leq \mathcal{P} \begin{bmatrix} \epsilon_+ & 0 \\ 0 & 0 \end{bmatrix} = PNS \quad (70.200)$$

Next note that

$$O_{0,0} + O_{1,1} = \mathcal{P} \begin{bmatrix} \epsilon_+ & \epsilon_1 \\ \epsilon_0 & 0 \end{bmatrix} \quad (70.201)$$

$$O_{1,0} + O_{0,1} = \mathcal{P} \begin{bmatrix} 0 & \epsilon_0 \\ \epsilon_1 & \epsilon_+ \end{bmatrix} \quad (70.202)$$

$$O_{1,0} + O_{0,1} + ATE = \mathcal{P} \begin{bmatrix} \epsilon_+ & \epsilon_0 \\ \epsilon_1 & 0 \end{bmatrix} \quad (70.203)$$

so

$$PNS = \mathcal{P} \begin{bmatrix} \epsilon_+ & 0 \\ 0 & 0 \end{bmatrix} \leq \min \left\{ \begin{array}{c} \mathcal{P} \begin{bmatrix} \epsilon_+ & \epsilon_1 \\ \epsilon_0 & 0 \end{bmatrix} \\ \mathcal{P} \begin{bmatrix} \epsilon_+ & \epsilon_0 \\ \epsilon_1 & 0 \end{bmatrix} \end{array} \right\} = \min \left\{ \begin{array}{c} O_{0,0} + O_{1,1} \\ O_{1,0} + O_{0,1} + ATE \end{array} \right\} \quad (70.204)$$

**QED**

## 70.14 Numerical Examples

I've written an open source Python program (See Ref[73]) that calculates the bounds given in this chapter. The program is called "JudeasRx", in honor of Judea Pearl. Fig.70.7 is an example of its interface with data entered by Boris Sobolev from a real life case. JudeasRx considers  $z = g = gender \in \{m, f\}$ .

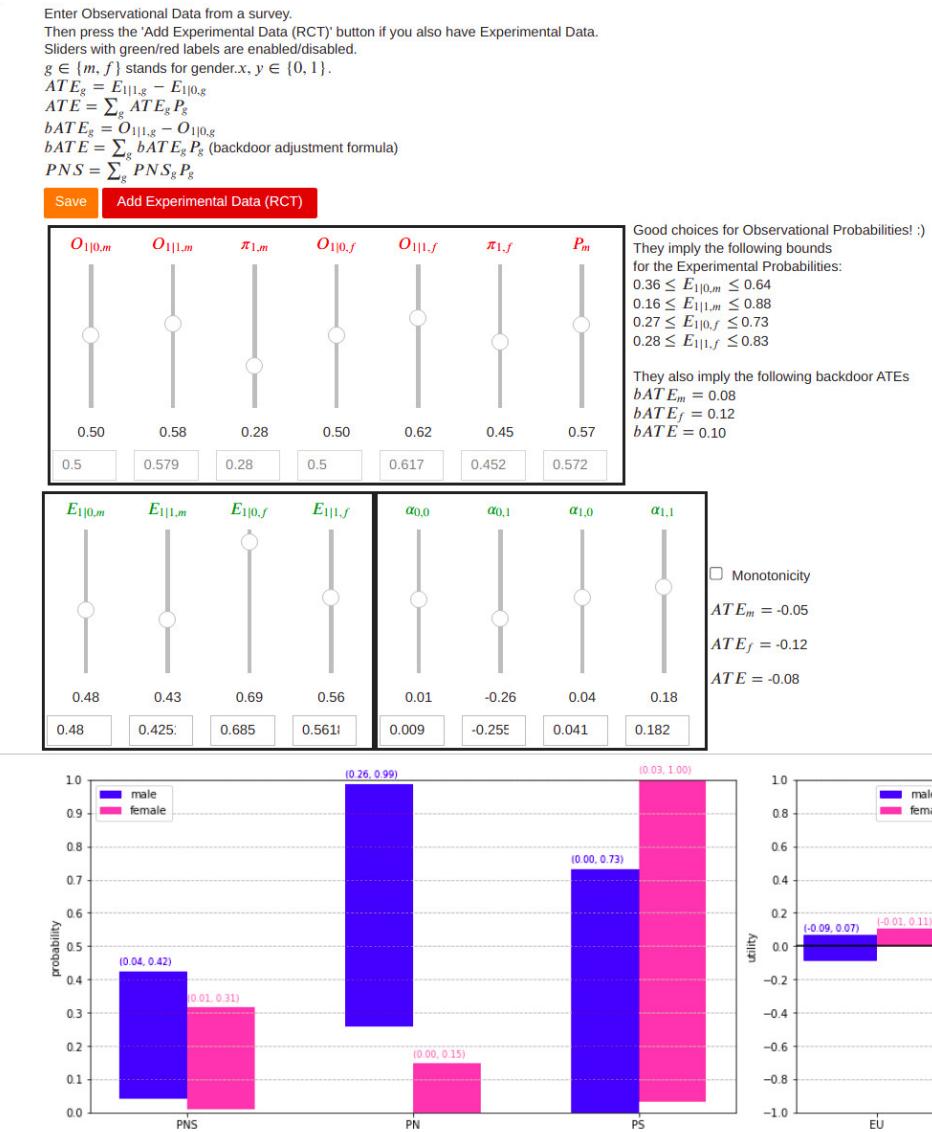


Figure 70.7: Interface for the Python program JudeasRx, with data entered by Boris Sobolev.

# Chapter 71

## Plate Notation

In this chapter, we will use the Numpy-like tensor notation discussed in Section C.48. In particular, note that  $[n] = [0 : n] = \{0, 1, \dots, n - 1\}$  and that  $T^{[n], [m]}$  is an  $n \times m$  matrix.

**Plate notation** is used to simplify equal parts of a bnet that occur in parallel. Suppose you have a bnet containing as a subset,  $\Lambda$  node sets  $S_\lambda$ , where  $\lambda \in [\Lambda]$ . Suppose any two  $S_\lambda$  have the same number of equivalent nodes, and two equivalent nodes have the same TPM. Rather than drawing all  $\Lambda$  sets, we think of them as **layers** of a **plate** (or stack) that come out of the page like a stack of pancakes with the pancakes lying flat on the page. That way we only have to draw one pancake, instead of  $\Lambda$ . We only draw once instead of  $\Lambda$  times, each node and the arrows entering and exiting that node. Quite a saving in labor and bnet complexity! And a bnet can have more than one plate, and a node can belong to more than one plate!

Plates are often used in Machine Learning (see, for example, Chapter 95 on Transformers Networks).

Fig.71.1 gives an example of a bnet with 2 nested plates<sup>1</sup>. The TPMs for this bnet are of the following form (we print them in blue).

$$P(A^{[20]} | Q^{[20], [10]}, K^{[20], [10]}, V^{[20], [10]}) = \quad (71.1a)$$

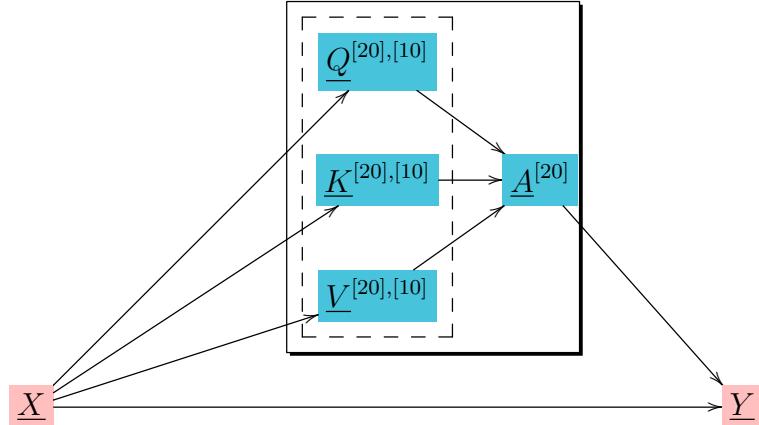
$$P(K^{[20], [10]} | X) = \quad (71.1b)$$

$$P(Q^{[20], [10]} | X) = \quad (71.1c)$$

$$P(V^{[20], [10]} | X) = \quad (71.1d)$$

---

<sup>1</sup>Fig.71.1 and the blue TPMs were rendered with my free, open source software `texnn` (see Ref.[80]) `texnn` can keep track of the tensor shapes of each node, for bnets with one or more plates.



□ □ 10 layers

■ 20 layers

Figure 71.1: Example of a bnet with 2 nested plates. In general, multiple plates need not be nested.

$$P(X) = \quad (71.1e)$$

$$P(Y|X, A^{[20]}) = \quad (71.1f)$$

# Chapter 72

## Potential Outcomes and Beyond

This chapter is based on Ref.[12], a book by Stephen Cunningham entitled “Causal inference: the mixtape”.

The theory of potential outcomes (PO) was for the most part invented in a seminal 1974 paper by Donald B. Rubin. Rubin has also made important extensions to PO theory since 1974. However, he does not use Pearl’s causal DAGs to discuss PO theory. Pearl has shown that PO theory can be substantially clarified and extended by using the language of causal DAGs. The d-separation theorem and do operator that we discuss in Chapters 23 and 72 are especially useful in this regard. In this chapter, we stress the connection of PO theory to Pearl’s causal DAGs and bnets.

$\sigma$	$d^\sigma$	$y^\sigma$	$y^\sigma(0)$	$y^\sigma(1)$
Edith	0	5	5	.
Frank	0	7	7	.
George	0	8	8	.
Hank	0	10	10	.
Andy	1	10	.	10
Ben	1	5	.	5
Chad	1	16	.	16
Daniel	1	3	.	3

Table 72.1: PO dataset describing whether individual  $\sigma$  took a treatment drug ( $d^\sigma = 1$ ) or didn’t ( $d^\sigma = 0$ ). The treatment outcome is measured by the real number  $y^\sigma$ .

Suppose a **population of individuals**  $\sigma = 0, 1, 2, \dots, nsam - 1$  is given ( $d^\sigma = 1$ ) or is not given ( $d^\sigma = 0$ ) a **treatment decision**  $d^\sigma$ , and that the **treatment outcome (i.e., response)** is measured by a real number  $y^\sigma$ . Table 72.1 gives a possible **PO dataset** for this scenario. As you can see from that table, each individual either takes a drug or doesn’t, but not both. PO theory can be viewed as a **missing data (MD) problem**. MD problems are discussed in Chapter 59. However, the PO MD problem is much more specialized than the generic MD problems discussed in Chapter 59. In the PO MD problem, we can fill in the blank cells by matching each

individual that took the drug with another *similar* individual that didn't. We will have much more to say about this matching strategy later in this chapter.

One can define similar individuals as individuals that have the same value for  $nx$  features  $x^\sigma = (x_i^\sigma)_{i=0,1,\dots,nx-1}$ . One can add to Table 72.1  $nx$  extra columns giving the value of the feature vector  $x^\sigma$  for each individual. Members of a population with the same  $x^\sigma$  are referred to as a **subpopulation or stratum (i.e., layer)**.

In a **randomized controlled trial (RCT)**<sup>1</sup>, the effect of the variable  $x^\sigma$  on the value of  $d^\sigma$  is eliminated by randomizing the population and therefore making the effect of  $x^\sigma$  on  $d^\sigma$  average out to zero. However, there are many situations in which carrying out an RCT is not possible or desirable. PO theory is a way of predicting the result of an RCT in situations where doing a real RCT is not possible or desirable.

In this chapter,  $x^\sigma$  will be called the confounders. Implicit throughout this chapter is the assumption that there are **no unmeasured confounders**. Because if there are some unmeasured confounders, those can send secret messages that influence the value that  $d^\sigma$  takes. This would ruin the predictions of someone trying to predict the results of an RCT without being privy to those secret messages. When there are **some unmeasured confounders**, it might still be possible to predict the effect of an RCT. This might be possible using instrumental variables. See Chapter 41 for a discussion of **instrumental variables**.

## 72.1 $G$ and $G_{den}$ bnets, the starting point bnets

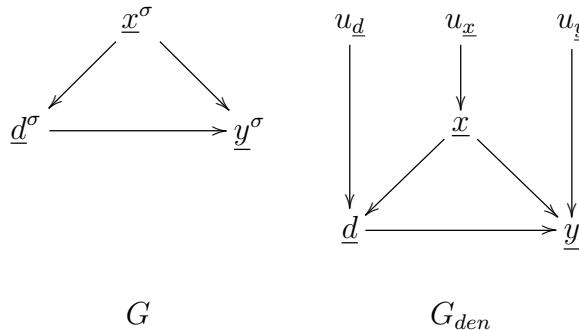


Figure 72.1: Bnets  $G$  and  $G_{den}$  are our starting point in discussing PO theory.  $G$  is for a single individual  $\sigma$  of the population. Bnet  $G_{den}$  is the DEN counterpart to  $G$ . DEN (Deterministic with External Noise) bnets are discussed in Chapter 48.

---

<sup>1</sup>The term **A/B test** is often used to mean an RCT where A and B are the treated and control groups. However, sometimes the term is used to refer to an experiment that conditions on confounders, which violates the definition of an RCT, and is the same as a PO test.

In this chapter, we will abbreviate  $\underline{X}[\sigma] = \underline{X}^\sigma$  for  $X \in \{d, x, y\}$ , where  $\sigma \in \{0, 1, 2, \dots, nsam - 1\}$ .

For each individual (a.k.a. unit, sample)  $\sigma = 0, 1, 2, \dots, nsam - 1$ , let:

$\underline{d}^\sigma \in \{0, 1\}$  be the treatment decision or drug dose. It equals 1 if treated and 0 if untreated.

$\underline{y}^\sigma \in \mathbb{R}$  be the treatment potential outcome

$\underline{x}^\sigma$  be the column vector of treatment confounders (a.k.a. covariates because they are often used as covariates (i.e., independent variables) in linear regression.)

Consider bnets  $G$  and  $G_{den}$  in Fig.72.1.  $G$  reflects the language used in Ref.[12] to discuss PO theory. And  $G_{den}$  reflects the language that Judea Pearl prefers to use to discuss PO theory. Both languages are equivalent. To go from one language to the other, one need only perform the following swaps, where  $\underline{u}$  is the external noise of the DEN bnet.

$$\underline{X}^\sigma \leftrightarrow \underline{X}(\underline{u}) \text{ for } X \in \{d, x, y\}.$$

$$P(\sigma) = \frac{1}{nsam} \leftrightarrow P(u)$$

$$\sum_\sigma P(\sigma)(\cdot) \leftrightarrow \sum_u P(u)(\cdot)$$

The TPMs, printed in blue, for the bnet  $G$  in Fig.72.1, are as follows:

$$P(x^\sigma) = P_{\underline{x}}(x^\sigma) \quad (72.1)$$

$$P(d^\sigma|x^\sigma) = P_{\underline{d}|x}(d^\sigma|x^\sigma) \quad (72.2)$$

$$P(y^\sigma|d^\sigma, x^\sigma) = P_{\underline{y}|d,x}(y^\sigma|d^\sigma, x^\sigma) \quad (72.3)$$

Now let:

$\underline{d} \in \{0, 1\}$  be the treatment decision. It equals 1 if treated and 0 if untreated

$\underline{y} \in \mathbb{R}$  be the treatment potential outcome

$\underline{x}$  be the column vector of treatment confounders (a.k.a. covariates)

$\underline{u} = (\underline{u}_d, \underline{u}_x, \underline{u}_y)$  be the external noise

The TPMs, printed in blue, for the bnet  $G_{den}$  in Fig.72.1, are as follows:

$$P(x|u_{\underline{x}}) = \mathbb{1}(x = u_{\underline{x}}) \quad (72.4)$$

$$P(d|x, u_{\underline{d}}) = \mathbb{1}(d = f_d(x, u_{\underline{d}})) \quad (72.5)$$

$$P(y|d, x, u_{\underline{y}}) = \mathbb{1}(y = f_y(d, x, u_{\underline{y}})) \quad (72.6)$$

If we linearize  $f_{\underline{y}}$  in Eq.(72.6), we get

$$\underline{y} = \delta \underline{d} + \beta \underline{x} + \underline{u}_y , \quad (72.7)$$

where  $\delta, \beta \in \mathbb{R}$ . Assuming that  $\underline{x}, \underline{y} \in \mathbb{R}$  and  $\underline{d} \in \{0, 1\}$ , Eq.(72.7) can be plotted. The resulting plot is given in Fig.72.2. This plot is a very special case of the PO problem, but it gives a crude idea of the “effects”  $\delta = y(1) - y(0)$  that PO theory gives estimates for. Any individual participating in the experiment experiences either  $y(1)$  or  $y(0)$ , but not both.

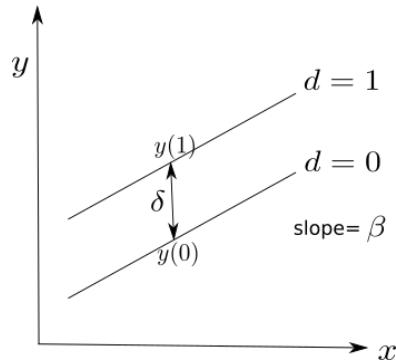


Figure 72.2: Plot of Eq.(72.7)

## 72.2 $G$ bnet with nodes $y^\sigma(0), y^\sigma(1)$ added to it.

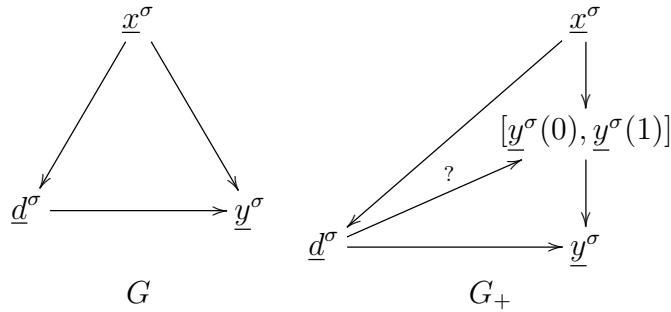


Figure 72.3: Bnet  $G_+$  is bnet  $G$  with two new nodes  $y^\sigma(0)$  and  $y^\sigma(1)$  added to it. The tuple node  $[y^\sigma(0), y^\sigma(1)]$  can also be represented by two nodes  $\underline{c} \rightarrow \underline{y}(\underline{c})$ , where  $\underline{c} \in \{0, 1\}$ .

Consider Fig.72.3. Bnet  $G_+$  was obtained by adding two new nodes  $y^\sigma(0)$  and  $y^\sigma(1)$  to bnet  $G$ . The TPMs, printed in blue, for bnet  $G_+$ , are as follows. Note that we define them in terms of the TPMs for bnet  $G$ .

$$P(x^\sigma) = P_{\underline{x}}(x^\sigma) \quad (72.8)$$

$$P(d^\sigma|x^\sigma) = P_{d|\underline{x}}(d^\sigma|x^\sigma) \quad (72.9)$$

For  $c \in \{0, 1\}$ ,

$$P(y^\sigma(c)|d^\sigma, x^\sigma) = \begin{cases} P_{y(c)|\underline{d}, \underline{x}}(y^\sigma(c)|d^\sigma, x^\sigma) & \text{if INCLUDE arrow with question mark} \\ P_{\underline{y}(c)|\underline{x}}(y^\sigma(c)|x^\sigma) & \text{if EXCLUDE arrow with question mark} \end{cases} \quad (72.10)$$

$$P(y^\sigma|y^\sigma(0), y^\sigma(1), d^\sigma) = \mathbb{1}(y^\sigma = d^\sigma y^\sigma(1) + (1 - d^\sigma)y^\sigma(0)) \quad (72.11a)$$

$$= \mathbb{1}(y^\sigma = y^\sigma(d^\sigma)) \quad (72.11b)$$

Eq.(72.11) is often referred to as the **SUTVA or Consistency assumption**.

If we sum over the nodes  $\underline{y}(0)$  and  $\underline{y}(1)$  of this bnet, we should get the bnet  $G$ . This is easy to check. Indeed,

$$P(y^\sigma|d^\sigma, x^\sigma) = \sum_{y^\sigma(0)} \sum_{y^\sigma(1)} \mathbb{1}(y^\sigma = y^\sigma(d^\sigma)) P(y^\sigma(0)|d^\sigma, x^\sigma) P(y^\sigma(1)|d^\sigma, x^\sigma) \quad (72.12)$$

$$= \begin{cases} P_{\underline{y}(0)|\underline{d}, \underline{x}}(y^\sigma|d^\sigma, x^\sigma) & \text{if } d^\sigma = 0 \\ P_{\underline{y}(1)|\underline{d}, \underline{x}}(y^\sigma|d^\sigma, x^\sigma) & \text{if } d^\sigma = 1 \end{cases}. \quad (72.13)$$

Henceforth, we will refer to the case where the question mark arrow is included as the general case, and to the case when it's excluded as the **weak-d limit**. Henceforth, we will first present results for the general case, and then describe how those results change for the weak-d limit. Rubinologists always assume the weak-d limit, but we find that with little effort, we can derive many results for general case, and then compare those results to their weak-d limit. I find such comparisons instructive.

Note that in the general case,  $P(\underline{y}(c) = y|\underline{d} = d, x)$  for  $c, d \in \{0, 1\}$  are four different probability distributions, and that  $P(\underline{y} = y|d = d, x)$  is defined in terms of two of them, the so called **factual distributions** with  $c = d$ . By measuring  $\underline{y}$ , we can't access the other 2 probability distributions, the so called **counter-factual distributions** with  $c \neq d$ .

In the weak-d limit,  $P(\underline{y}(c) = y|\underline{d} = d, x) = P(\underline{y}(c) = y|x)$  are two probability distributions, and they both can be accessed by measuring  $\underline{y}$ .

## 72.3 Expected Values of treatment outcome $y^\sigma$

It is convenient to define the following expected values of  $\underline{y}^\sigma$  in terms of the TPMs of bnet  $G_+$ :

$$\mathcal{Y}_{c|d,x} = E_{\sigma|d,x}[\underline{y}^\sigma(c)] \rightarrow E_{\underline{y}(c)|d,x}[\underline{y}(c)] = \sum_y y P(\underline{y}(c) = y | \underline{d} = d, x) \quad (72.14)$$

$$\mathcal{Y}_{c|d} = E_{\sigma|d}[\underline{y}^\sigma(c)] \rightarrow E_{\underline{y}(c)|d}[\underline{y}(c)] = \sum_x \mathcal{Y}_{c|d,x} P(x|d) \quad (72.15)$$

$$\mathcal{Y}_{c|x} = E_{\sigma|x}[\underline{y}^\sigma(c)] \rightarrow E_{\underline{y}(c)|x}[\underline{y}(c)] = \sum_d \mathcal{Y}_{c|d,x} P(d|x) \quad (72.16)$$

$$\mathcal{Y}_c = E_\sigma[\underline{y}^\sigma(c)] \rightarrow E_{\underline{y}(c)}[\underline{y}(c)] = \sum_{x,d} \mathcal{Y}_{c|d,x} P(x, d) \quad (72.17)$$

Note that in the weak-d limit,

$$\mathcal{Y}_c = \sum_x \mathcal{Y}_{c|d,x} P(x) . \quad (72.18)$$

Note also that in the weak-d limit,  $\mathcal{Y}_{c|d,x}$  is independent of  $d$ , but  $\mathcal{Y}_{c|d}$  can depend on  $d$  if  $P(x|d)$  depends on  $d$ .

$\mathcal{Y}_{0|0}, \mathcal{Y}_{1|1}$  are said to be **factual** (indicating compliant patients) whereas  $\mathcal{Y}_{0|1}, \mathcal{Y}_{1|0}$  are said to be **counterfactual** (indicating non-compliant patients).

Also let

$$\mathcal{Y}_{|d,x} = E_{\sigma|d,x}[\underline{y}^\sigma] \rightarrow E_{\underline{y}|d,x}[\underline{y}] = \sum_y y P(\underline{y} = y | \underline{d} = d, x) \quad (72.19)$$

$$\mathcal{Y}_{|d} = E_{\sigma|d}[\underline{y}^\sigma] \rightarrow E_{\underline{y}|d}[\underline{y}] = \sum_x \mathcal{Y}_{|d,x} P(x|d) \quad (72.20)$$

$$\mathcal{Y}_{|x} = E_{\sigma|x}[\underline{y}^\sigma] \rightarrow E_{\underline{y}|x}[\underline{y}] = \sum_d \mathcal{Y}_{|d,x} P(d|x) \quad (72.21)$$

$$\mathcal{Y} = E_\sigma[\underline{y}^\sigma] \rightarrow E_{\underline{y}}[\underline{y}] = \sum_d \mathcal{Y}_{|d,x} P(d, x) \quad (72.22)$$

In the weak-d limit,  $\mathcal{Y}_{|d,x}$  is independent of  $d$ , but  $\mathcal{Y}_{|d}$  can still depend if  $P(x|d)$  depends on  $d$ , then  $\mathcal{Y}_{|d}$  depends on  $d$  too.

## 72.4 Translation Dictionary

Table 72.2 gives a dictionary for translating from the standard PO notation of Ref.[12] to our notation.

In standard PO notation	In our notation
$i$ , individual (i.e., unit, sample) index	$\sigma$
$D_i = d_i$ , treatment decision	$\underline{d}^\sigma = d^\sigma$
$Y_i = y_i$ , treatment outcome	$\underline{y}^\sigma = y^\sigma$
$X_i = x_i$ , treatment confounders	$\underline{x}^\sigma = x^\sigma$
$E[Y_i(c)]$	$E_\sigma[\underline{y}^\sigma(c)] = \mathcal{Y}_c$
$E[Y_i(c) D_i = d]$	$E_{\sigma d}[\underline{y}^\sigma(c)] = \mathcal{Y}_{c d}$
$E[Y_i(c) D_i = d, X_i = x]$	$E_{\sigma d,x}[\underline{y}^\sigma(c)] = \mathcal{Y}_{c d,x}$
$E[Y_i]$	$E_\sigma[\underline{y}^\sigma] = \mathcal{Y}$
$E[Y_i D_i = d]$	$E_{\sigma d}[\underline{y}^\sigma] = \mathcal{Y}_{ d}$
$E[Y_i D_i = d, X_i = x]$	$E_{\sigma d,x}[\underline{y}^\sigma] = \mathcal{Y}_{ d,x}$

Table 72.2: Dictionary for translating from standard PO notation of Ref.[12] to our notation.  $c, d \in \{0, 1\}$ .

## 72.5 $\mathcal{Y}_{|d,x} = \mathcal{Y}_{d|d,x}$ (SUTVA)

**Claim 121** <sup>2</sup>

$$\mathcal{Y}_{|d,x} = \mathcal{Y}_{d|d,x} \quad (72.23)$$

$$\mathcal{Y}_{|d} = \mathcal{Y}_{d|d} \quad (72.24)$$

**proof:**

$$\mathcal{Y}_{|d,x} = \sum_y y P(\underbrace{y}_{=y(d) \text{ by Eq.(72.11)}} = y | d, x) \quad (72.25)$$

$$= \mathcal{Y}_{d|d,x}. \quad (72.26)$$

Applying  $\sum_x P(x|d)$  to both sides of Eq.(72.23) gives Eq.(72.24).

**QED**

---

<sup>2</sup>In the standard PO notation, this is the frequently used identity

$$E[Y|D = d, x] = E[Y(d)|D = d, x]$$

.

## 72.6 Conditional Independence Assumption (CIA)

The **Conditional Independence Assumption** (CIA) is said to hold if

$$(\underline{y}^\sigma(0), \underline{y}^\sigma(1), \underline{y}^\sigma) \& \perp_P \underline{d}^\sigma | \underline{x}^\sigma . \quad (72.27)$$

This is satisfied by  $G_+$  in the weak-d limit. To prove this, check that

$$(\underline{y}^\sigma(0), \underline{y}^\sigma(1), \underline{y}^\sigma) \perp_{G_+} \underline{d}^\sigma | \underline{x}^\sigma \quad (72.28)$$

and then invoke the d-separation theorem (see Chapter 23).

I think CIA only makes sense if the individuals are treatment blind (i.e., have no knowledge of whether they are in the treated or control groups.) Otherwise, that extra knowledge becomes a confounder not being included in  $x$ .

A **Randomized Controlled Trial (RCT)** is defined to satisfy Eq.(72.27) without the  $\underline{x}^\sigma$  conditioning; i.e., it satisfies

$$(\underline{y}^\sigma(0), \underline{y}^\sigma(1), \underline{y}^\sigma) \& \perp_P \underline{d}^\sigma . \quad (72.29)$$

This means that in an RCT, the arrow from  $\underline{x}^\sigma$  to  $\underline{d}^\sigma$  in  $G_+$  is omitted.

Note that if we assume both CIA (i.e., weak-d limit) and SUTVA, we get

$$\mathcal{Y}_{|d,x} = E_{\sigma|d,x}[\underline{y}^\sigma] \quad (72.30a)$$

$$= E_\sigma[\underline{y}^\sigma | \underline{d}^\sigma = d, \underline{x}^\sigma = x] \quad (72.30b)$$

$$= E_\sigma[\underline{y}^\sigma(d) | \underline{d}^\sigma = d, \underline{x}^\sigma = x] \text{ (by SUTVA)} \quad (72.30c)$$

$$= E_\sigma[\underline{y}^\sigma(d) | \underline{x}^\sigma = x] \text{ (by CIA)} \quad (72.30d)$$

$$= E_{\sigma|x}[\underline{y}^\sigma(d)] \quad (72.30e)$$

$$= \mathcal{Y}_{d|x} . \quad (72.30f)$$

In an RCT, Eq.(72.30f) is valid without the  $x$  conditioning.

## 72.7 Treatment Effects

A **treatment effect** is a difference of two  $\mathcal{Y}_{c|d}$ . It is convenient to define the following treatment effects. See Figs.72.4 and 72.5.

- average treatment effect (ATE).

$$\textcolor{red}{ATE} = \mathcal{Y}_1 - \mathcal{Y}_0 = \delta \quad (72.31)$$

- average treatment effect of the treated (ATT)

$$\textcolor{red}{ATT} = \mathcal{Y}_{1|1} - \mathcal{Y}_{0|1} \quad (72.32)$$

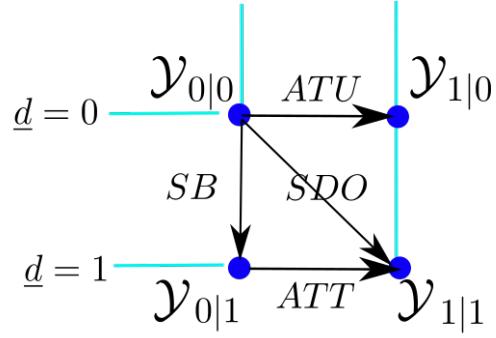


Figure 72.4: Different treatment effects. A treatment effect is a difference of two  $\mathcal{Y}_{c|d}$ .

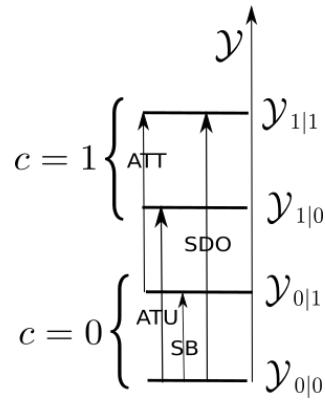


Figure 72.5: Alternative representation of the same information that is contained in Fig.72.4.

- average treatment effect of the untreated (ATU)

$$\textcolor{red}{ATU} = \mathcal{Y}_{1|0} - \mathcal{Y}_{0|0} \quad (72.33)$$

- selection bias (SB)

$$\textcolor{red}{SB} = \mathcal{Y}_{0|1} - \mathcal{Y}_{0|0} \quad (72.34)$$

- simple difference in outcomes (SDO)

$$\textcolor{red}{SDO} = \mathcal{Y}_{1|1} - \mathcal{Y}_{0|0} \quad (72.35)$$

Let

$$\pi_d = P(\underline{d} = d) \quad (72.36)$$

for  $d \in \{0, 1\}$ .

Note that there exist some linear constraints between these treatment effects.

$$\underbrace{\mathcal{Y}_1 - \mathcal{Y}_0}_{ATE} = \underbrace{\mathcal{Y}_{1|1}\pi_1 + \mathcal{Y}_{1|0}\pi_0}_{\mathcal{Y}_1} - \underbrace{(\mathcal{Y}_{0|1}\pi_1 + \mathcal{Y}_{0|0}\pi_0)}_{\mathcal{Y}_0} \quad (72.37)$$

$$= \underbrace{(\mathcal{Y}_{1|1} - \mathcal{Y}_{0|1})\pi_1}_{ATT} + \underbrace{(\mathcal{Y}_{1|0} - \mathcal{Y}_{0|0})\pi_0}_{ATU} \quad (72.38)$$

$$\underbrace{\mathcal{Y}_{1|1} - \mathcal{Y}_{0|0}}_{SDO} = \underbrace{(\mathcal{Y}_{1|1} - \mathcal{Y}_{0|1})}_{ATT} + \underbrace{\mathcal{Y}_{0|1} - \mathcal{Y}_{0|0}}_{SB} \quad (72.39)$$

$$\begin{aligned} \underbrace{\mathcal{Y}_{1|1} - \mathcal{Y}_{0|0}}_{SDO} &= \underbrace{(\mathcal{Y}_{1|1} - \mathcal{Y}_{0|1})\pi_1 + (\mathcal{Y}_{1|0} - \mathcal{Y}_{0|0})\pi_0}_{ATE} \\ &\quad + \underbrace{\mathcal{Y}_{0|1} - \mathcal{Y}_{0|0}}_{SB} \\ &\quad + \underbrace{(\mathcal{Y}_{1|1} - \mathcal{Y}_{0|1})}_{ATT}\pi_0 \\ &\quad - \underbrace{(\mathcal{Y}_{1|0} - \mathcal{Y}_{0|0})}_{ATU}\pi_0 \end{aligned} \quad (72.40)$$

By virtue of Eq.(72.38),

$$ATT = ATU \implies ATT = ATU = ATE \quad (72.41)$$

and

$$ATE = 0 \iff \frac{ATU}{ATT} = -\left(\frac{\pi_1}{\pi_0}\right). \quad (72.42)$$

Whenever  $ATT = ATU$ , we will say there is **T-U symmetry**.

In general,  $SDO = ATT + SB$ , but if there is T-U symmetry, then  $SDO = ATE + SB$ .

If there is T-U symmetry and zero bias  $SB = 0$ , then  $SDO = ATE = ATT = ATU$ .

If there is a null result for an RCT (i.e.,  $ATE = 0$ ), T-U symmetry and zero bias  $SB = 0$ , then  $SDO = ATE = ATT = ATU = 0$ .

Let

$$\mathcal{Y}_{c,d|x} = \mathcal{Y}_{c|d,x}P(d|x) \quad (72.43)$$

For each  $\mathcal{E} \in \{ATE, ATT, ATU, SB, SDO\}$ , we can define its restriction  $\mathcal{E}_x$  to a fixed stratum  $x$  by replacing each  $\mathcal{Y}_{c|d}$  with  $\mathcal{Y}_{c,d|x}$ . For example,

$$ATT = \mathcal{Y}_{1|1} - \mathcal{Y}_{0|1} \text{ so } ATT_x = \mathcal{Y}_{1,1|x} - \mathcal{Y}_{0,1|x}. \quad (72.44)$$

We can calculate  $\mathcal{E}$  from  $\mathcal{E}_x$  using

$$\mathcal{E} = E_x[\mathcal{E}_x] = \sum_x P(x)\mathcal{E}_x . \quad (72.45)$$

## 72.8 Insights into what makes treatment effects equal and $\mathcal{Y}_{1|0} = \mathcal{Y}_1$

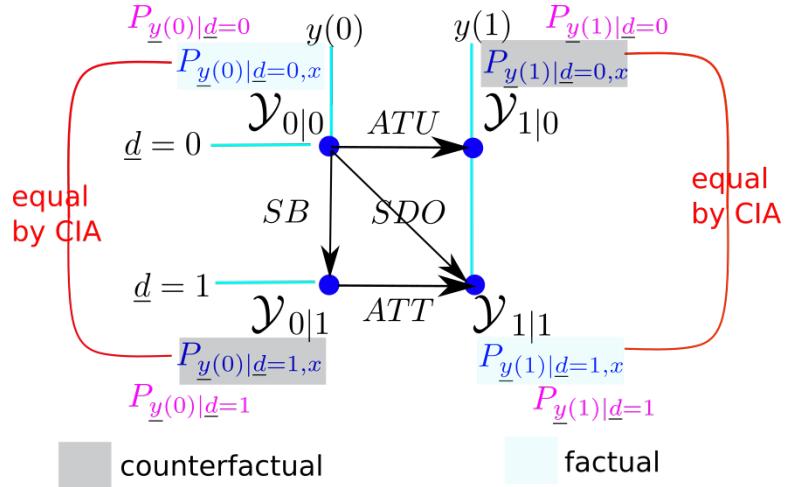


Figure 72.6: Figure 72.4 with added information about probability distributions used to obtain each expected value  $\mathcal{Y}_{c|d}$ .

1. Is it possible for  $SDO = 0$  but  $ATE \neq 0$  or vice versa, and what is going on when this is true?
2. What is going on when two treatment effects are equal; for instance, when  $ATT = ATU$ ?
3. When is  $\mathcal{Y}_{1|0} = \mathcal{Y}_1$ , and what is going on when this is true?

Fig.72.6 gives some intuition about what is going on when any of these things happen.

Recall that each expected value  $\mathcal{Y}_{c|d}$  is associated with a probability distribution  $P_{\underline{y}(c)|\underline{d},x}$ .

$$\mathcal{Y}_{c|d} = \sum_y y \underbrace{\sum_x P_{\underline{y}(c)|\underline{d},x}(y|d, x)P(x|d)}_{P_{\underline{y}(c)|\underline{d}}(y|d)} \quad (72.46)$$

for  $c, d \in \{0, 1\}$ . Fig.72.6 reminds us of which  $P$  is used to generate each  $\mathcal{Y}$ . From this figure, we see that

1. A sufficient condition for  $SDO = 0$  is that  $P_{\underline{y}(1)|\underline{d}=1} = P_{\underline{y}(0)|\underline{d}=0}$ . A sufficient condition for  $ATE = 0$  is that  $P_{\underline{y}(1)|x} = P_{\underline{y}(0)|x}$ .
2. A sufficient condition for  $ATT = ATU$  is that  $P_{\underline{y}(1)|\underline{d}=1,x} - P_{\underline{y}(0)|\underline{d}=1,x}$  equals  $P_{\underline{y}(1)|\underline{d}=0,x} - P_{\underline{y}(0)|\underline{d}=0,x}$ .
3. A sufficient condition for  $\mathcal{Y}_{1|0} = \mathcal{Y}_1$  is that  $P_{\underline{y}(1)|\underline{d}=0} = P_{\underline{y}(1)}$ . Note that the CIA implies that  $P_{\underline{y}(1)|\underline{d}=0,x} = P_{\underline{y}(1)|x}$  always, but this does not imply that  $P_{\underline{y}(1)|\underline{d}=0} = P_{\underline{y}(1)}$ .

## 72.9 $G_{do+}$ bnet

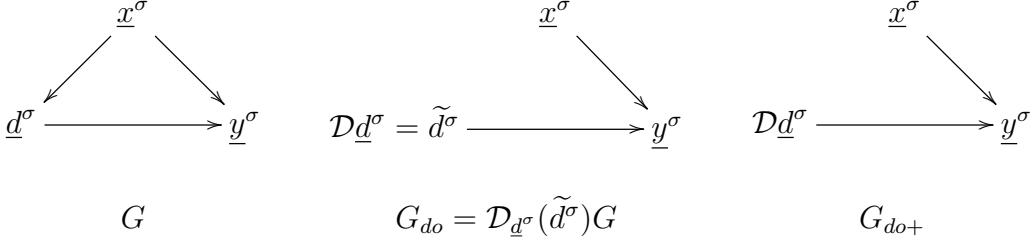


Figure 72.7: Bnet  $G_{do} = \mathcal{D}_{\underline{d}^{\sigma}}(\tilde{d}^{\sigma})G$  is obtained by applying the do operator to node  $\underline{d}^{\sigma}$  of bnet  $G$ . Bnet  $G_{do+}$  is obtained by adding a prior probability distribution  $P(\tilde{d}^{\sigma})$  to node  $\mathcal{D}\underline{d}^{\sigma}$  of bnet  $G_{do}$ .

Fig.72.7 shows how bnet  $G_{do}$  is obtained by applying the do operator to bnet  $G$ , and how bnet  $G_{do+}$  is obtained by adding a prior probability distribution to one of the nodes of  $G_{do}$ . In bnet  $G_{do}$ , node  $\underline{d}^{\sigma}$  has been stripped of all outside influences and fixed to a specific state  $\tilde{d}^{\sigma}$ . This is what an RCT does.

The TPMs, printed in blue, for the bnets  $G_{do}$  and  $G_{do+}$ , are as follows. Note that the TPMs for bnets  $G_{do}$  and  $G_{do+}$  are defined in terms of the TPMs of bnet  $G$ .

$$P(x^{\sigma}) = P_{\underline{x}}(x^{\sigma}) \quad (72.47)$$

$$P_{\mathcal{D}\underline{d}}(\tilde{d}) = \sum_x P_{\underline{d}|\underline{x}}(\tilde{d}|x)P_{\underline{x}}(x) \quad (72.48)$$

$$P(\tilde{d}^{\sigma}) = \begin{cases} \delta(\tilde{d}^{\sigma}, \tilde{d}^{\sigma}) & \text{for } G_{do} \\ P_{\mathcal{D}\underline{d}}(\tilde{d}^{\sigma}) & \text{for } G_{do+} \end{cases} \quad (72.49)$$

$$P(y^\sigma | \tilde{d}^\sigma, x^\sigma) = P_{\underline{y}|\underline{d}, \underline{x}}(y^\sigma | \tilde{d}^\sigma, x^\sigma) \quad (72.50)$$

Note that in  $G_{do}$ ,

$$P(\underline{y} = y | \mathcal{D}\underline{d} = d, \underline{x} = x) = P(y | \underline{d} = d, x) \quad (72.51)$$

because, by the d-separation theorem, when we condition on the confounder  $\underline{x}$ , we block information from being transmitted from  $\underline{d}$  to  $\underline{y}$  through  $\underline{x}$ , and this is equivalent to amputating the arrow  $\underline{x} \rightarrow \underline{d}$ .

Using Eq.(72.51), we get

$$P(\underline{y} = y | \mathcal{D}\underline{d} = d) = \sum_x P(\underline{y} = y | \mathcal{D}\underline{d} = d, x) P(x | \mathcal{D}\underline{d} = d) \quad (72.52)$$

$$= \sum_x P(y | d, x) P(x) \quad (72.53)$$

Eq.(72.53) is called the **backdoor adjustment formula**. It allows us to express a probability with a do operator in its definition in terms of probabilities without do operators.

## 72.10 $ACE = ATE$

Define the Average Causal Effect ( $ACE$ ) by

$$ACE = \sum_y y [P(y | \mathcal{D}\underline{d} = 1) - P(y | \mathcal{D}\underline{d} = 0)] \quad (72.54)$$

$$= \sum_x P(x) \sum_y y [P(y | \underline{d} = 1, x) - P(y | \underline{d} = 0, x)] . \text{ (by Eq.(72.53))} \quad (72.55)$$

**Claim 122** *If we assume both SUTVA and CIA (i.e., weak-d limit), then*

$$ACE = ATE \quad (72.56)$$

**proof:**

$$ACE = \sum_x P(x) \sum_y y [P(\underline{y} = y | \underline{d} = 1, x) - P(\underline{y} = y | \underline{d} = 0, x)] \quad (72.57)$$

$$= \sum_x P(x) [\mathcal{Y}_{1|x} - \mathcal{Y}_{0|x}] \text{ (by SUTVA)} \quad (72.58)$$

$$= \sum_x P(x) [\mathcal{Y}_{1|x} - \mathcal{Y}_{0|x}] \text{ (by CIA)} \quad (72.59)$$

$$= \mathcal{Y}_1 - \mathcal{Y}_0 \quad (72.60)$$

$$= ATE \quad (72.61)$$

**QED**

We will say there is a **null result in an RCT** when  $ACE = 0$ . By the previous claim, this is true iff  $ATE = 0$  (assuming weak-d limit).

## 72.11 Good, Bad Controls

The bnet  $G_+$  of Fig.72.3, —the cornerstone of Rubin’s PO theory— is limited in scope and is easily misapplied, leading to incorrect results. The problem is some features that are available and could be conditioned on shouldn’t because they would introduce spurious contributions to ATE. Such features are called “bad controls”<sup>3</sup>

Examples:

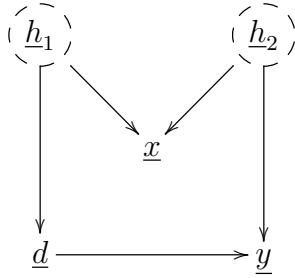


Figure 72.8: In this bnet,  $\underline{x}$  is a bad control (i.e., should not be conditioned on). Nodes  $\underline{h}_1$  and  $\underline{h}_2$  are hidden and therefore cannot be conditioned on.

1. Consider the bnet Fig.72.8, which Pearl calls M-bias, because it looks like an M. In that figure,  $\underline{x}$  is a “bad control” because calculating  $ATE$  by conditioning on

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<sup>3</sup>In this section, the word “controls” refers to the covariates (i.e., independent variables), other than  $\underline{d}$ , in a regression with  $\underline{y}$  as target (i.e., independent) variable. This should not be confused with the control (i.e., untreated) individuals of a RCT.

it, and using the formula  $ATE = \sum_x P(x)[\mathcal{Y}_{1|x} - \mathcal{Y}_{0|x}]$ , yields a value of  $ATE$  that is different from  $ACE$ . This value for  $ATE$  is unacceptable because it does not give the result of an RCT whereas  $ACE$  defined in terms of do operators always does. The reason<sup>4</sup>  $ATE \neq ACE$  for this figure is that in it,  $\underline{x}$  is a collider node, and conditioning on it allows rather than prevents information to flow from  $\underline{d}$  to  $\underline{y}$  via the path  $\underline{d} - \underline{h}_1 - \underline{x} - \underline{h}_2 - \underline{y}$ .

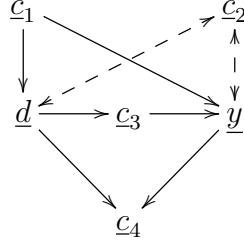


Figure 72.9: In this bnet, node  $\underline{c}_1$  is a good control and nodes  $\underline{c}_2, \underline{c}_3, \underline{c}_4$  are bad ones.

2. In Fig.72.9, node  $\underline{c}_1$  is a good control and nodes  $\underline{c}_2, \underline{c}_3, \underline{c}_4$  are bad ones.

Conditioning on  $\underline{c}_1$  blocks path  $\underline{d} - \underline{c}_1 - \underline{y}$ , good

Conditioning on  $\underline{c}_2$  opens path  $\underline{d} - \underline{c}_2 - \underline{y}$ , bad

Conditioning on  $\underline{c}_3$  blocks path  $\underline{d} - \underline{c}_3 - \underline{y}$ , bad

Conditioning on  $\underline{c}_4$  opens path  $\underline{d} - \underline{c}_4 - \underline{y}$ , bad

Pearl et al have a paper (Ref.[10]) that I highly recommend that gives 20 examples of good, neutral and bad controls in an  $ATE$  calculation. Those 20 examples are also analyzed by my software SCuMpy (see Ref.[77]).

## 72.12 PO Confounder Sensitivity Analysis

There are various “sensitivity analysis” strategies that are commonly used (for example, by the software PyWhy) as a sanity check for a PO analysis.

- **vary columns of dataset**

1. **randomize  $\underline{y}$  column** (random outcome) This should make  $ATE = 0$ .
2. **randomize  $\underline{x}$  column** (random common cause) This should make  $ATE = 0$ .

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<sup>4</sup>We are using here arguments based on the d-separation theorem which is discussed in Chapter 23.

- 3. **randomize  $d$  column** (placebo treatment dose) This should make  $ATE = 0$ .
  - 4. **add new column  $u$** , where  $u$  is an “unobserved common cause”. This should change  $ATE$  in a predictable manner. See below.
  - 5. **add new column  $u$** , where  $u$  is a “randomized common cause”. This should not change  $ATE$ .  
  - **vary rows of dataset**, either all of them or some of them. Replace them by a dataset that should obey same DAG. This should not change  $ATE$ .
  - **vary good controls**. If using a DAG that is more complicated than the naive triangular PO DAG, vary from one set of good controls to another. This should not change  $ATE$ .

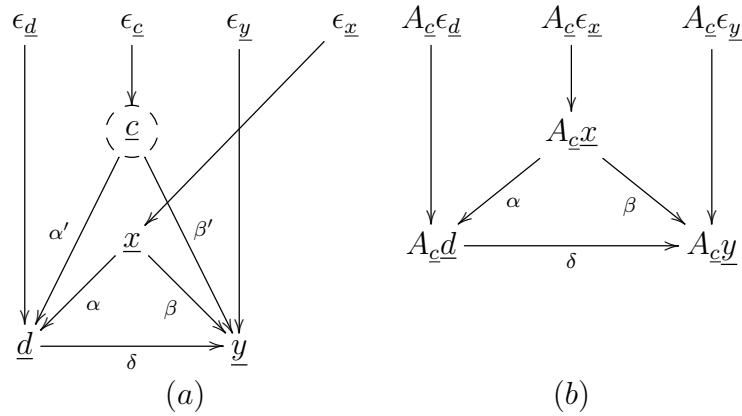


Figure 72.10: LDEN bnets used to do PO confounder sensitivity analysis. Node  $\underline{c}$  is an unobserved common cause confounder. The operator  $A_{\underline{c}}$  in bnet (b) annihilates  $\underline{c}$  (i.e.,  $A_{\underline{c}\underline{c}} = 0$ )

We end this section by deriving a formula for the change in *ATE* when an unobserved common cause  $c$  is added to the naive triangular PO DAG. (See Fig.72.10)

Consider the LDEN bnet of Fig.72.10 (a), whose structural equations, printed in blue, are as follows:

$$\underline{d} = \alpha \underline{x} + \alpha' \underline{c} + \epsilon_d \quad (72.62)$$

$$\underline{y} = \beta \underline{x} + \beta' \underline{c} + \delta \underline{d} + \epsilon_y \quad (72.63)$$

where  $\epsilon_d$  and  $\epsilon_y$  are root nodes with zero mean. Therefore,

$$\underline{c} = \frac{1}{\alpha'} (\underline{d} - \epsilon_{\underline{d}} - \alpha \underline{x}) \quad (72.64)$$

$$\underline{y} = \left( \beta - \frac{\alpha \beta'}{\alpha'} \right) \underline{x} + \left( \delta + \frac{\beta'}{\alpha'} \right) (\underline{d} - \epsilon_{\underline{d}}) + \epsilon_{\underline{y}} \quad (72.65)$$

$$\mathcal{Y}_{d|x,c} = E[\underline{y}(d)|x,c] = E[\underline{y}|d,x,c] = \beta x + \beta' c + \delta d \quad (72.66)$$

$$\mathcal{Y}_{d|x} = E[\underline{y}(d)|x] = E[\underline{y}|d,x] = \left( \beta - \frac{\alpha \beta'}{\alpha'} \right) x + \left( \delta + \frac{\beta'}{\alpha'} \right) d \quad (72.67)$$

$$ATE = E_x[ATE_x] = E_x[\mathcal{Y}_{1|x} - \mathcal{Y}_{0|x}] = \delta + \frac{\beta'}{\alpha'} \quad (72.68)$$

$$ATE|_{\beta'=0} = \delta \quad (72.69)$$

$$ATE - ATE|_{\beta'=0} = \frac{\beta'}{\alpha'} \quad (72.70)$$

Note that the right hand side of Eq.(72.70) is the product of the gains along the path  $\underline{d} \rightarrow \underline{c} \rightarrow \underline{y}$ . The gain  $1/\alpha'$  for  $\underline{d} \rightarrow \underline{c}$  equals the inverse of the gain  $\alpha'$  for  $\underline{c} \rightarrow \underline{d}$ .

Neither  $\alpha'$  nor  $\beta'$  are observed, but the right hand side of Eq.(72.70) can be bounded above by an observable quantity. This is done in Chapter 68.

## 72.13 $(SDO, ATE)$ space

If we substitute  $y^\sigma \rightarrow y^\sigma(d^\sigma)$  and  $y^{m(\sigma)} \rightarrow y^\sigma(1 - d^\sigma)$  into the estimate Eq.(72.83) for  $ATE$  and the estimate Eq.(72.89) for  $SDO$ , we get

$$\widehat{ATE}_x = \frac{1}{N_x} \sum_{\sigma \in A_x} (2d^\sigma - 1)[y^\sigma(d^\sigma) - y^\sigma(1 - d^\sigma)] \quad (72.71)$$

$$= \frac{1}{N_x} \sum_{\sigma \in A_x} [y^\sigma(1) - y^\sigma(0)] \quad (72.72)$$

and

$$\widehat{SDO}_x = \frac{1}{N_{1,x}} \sum_{\sigma \in A_x} d^\sigma y^\sigma(d^\sigma) - \frac{1}{N_{0,x}} \sum_{\sigma \in A_x} (1 - d^\sigma) y^\sigma(d^\sigma) \quad (72.73)$$

$$= \frac{1}{N_{1,x}} \sum_{\sigma \in A_{1,x}} y^\sigma(1) - \frac{1}{N_{0,x}} \sum_{\sigma \in A_{0,x}} y^\sigma(0). \quad (72.74)$$

Recall that  $\widehat{\mathcal{E}} = E_x[\widehat{\mathcal{E}}_x] = \sum_x \frac{N_x}{N} \widehat{\mathcal{E}}_x$  for  $\mathcal{E} \in \{ATE, SDO\}$ .

Recall also that  $ACE = ATE = 0$  is the null result in an RCT.

Suppose that the treatment outcome  $y^\sigma$  has only two possible values, 0 and 1. Then,  $-1 \leq ATE \leq 1$  and  $-1 \leq SDO \leq 1$ . But does  $ATE = 0$  imply  $SDO = 0$  or vice versa? Next, we answer that question and more by finding the region of accessibility in the  $(SDO, ATE)$  plane, assuming  $y^\sigma \in \{0, 1\}$ .

$\sigma$	$d^\sigma$	$y^\sigma(0)$	$y^\sigma(1)$
1	0	1	0
2	0	1	0
3	0	1	0
4	1	1	0
5	1	1	0
6	1	1	0

(a)  $ATE = -1$  ( $SDO = -1$ )  
point A

$\sigma$	$d^\sigma$	$y^\sigma(0)$	$y^\sigma(1)$
1	0	0	1
2	0	0	1
3	0	0	1
4	1	0	0
5	1	0	0
6	1	0	0

(b)  $ATE = \frac{1}{2}$  ( $SDO = 0$ )  
point B

$\sigma$	$d^\sigma$	$y^\sigma(0)$	$y^\sigma(1)$
1	0	0	1
2	0	0	1
3	0	0	1
4	1	0	1
5	1	0	1
6	1	0	1

(c)  $ATE = 1$  ( $SDO = 1$ )  
point C

Figure 72.11: Examples of PO datasets. Exploring  $ATE$  extremes.

$\sigma$	$d^\sigma$	$y^\sigma(0)$	$y^\sigma(1)$
1	0	1	1
2	0	1	1
3	0	1	1
4	1	0	0
5	1	0	0
6	1	0	0

(a)  $SDO = -1$  ( $ATE = 0$ )  
point D

$\sigma$	$d^\sigma$	$y^\sigma(0)$	$y^\sigma(1)$
1	0	1	0
2	0	1	0
3	0	1	0
4	1	1	1
5	1	1	1
6	1	1	1

(b)  $SDO = 0$  ( $ATE = -\frac{1}{2}$ )  
point E

$\sigma$	$d^\sigma$	$y^\sigma(0)$	$y^\sigma(1)$
1	0	0	0
2	0	0	0
3	0	0	0
4	1	1	1
5	1	1	1
6	1	1	1

(c)  $SDO = 1$  ( $ATE = 0$ )  
point F

Figure 72.12: Examples of PO datasets. Exploring  $SDO$  extremes.

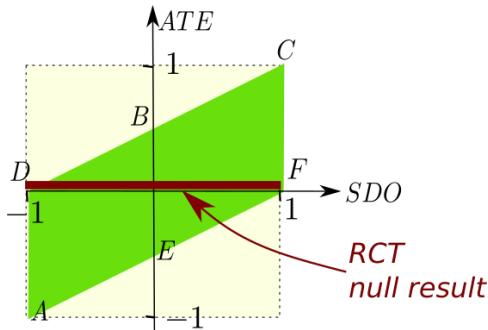


Figure 72.13: Green parallelogram is accessible region in  $(SDO, ATE)$  plane, assuming  $y^\sigma \in \{0, 1\}$ . Each of the six points A, B, ... F corresponds to one of the six tables in Figs. 72.11 and 72.12. Segment DF corresponds to the null result in an RCT.

## 72.14 Strata-Matching

For a situation described by the bnet  $G_+$  in the weak-d limit, we can match *similar* individuals to fill the blank cells of Table 72.1. By “similar”, we mean that they have the same or almost the same value of  $x^\sigma$ .

The reason the weak-d limit is required is because it implies that  $P(y(c)|d = 0, x) = P(y(c)|d = 1, x)$  for  $c \in \{0, 1\}$ . Hence, we can sample from a known factual ( $c = d$ ) distribution to fill the missing data in the unknown counterfactual ( $c \neq d$ ) distribution.

### 72.14.1 Exact strata-matching

#### Estimates of Treatment Effects

For  $d \in \{0, 1\}$  and all strata  $x$ , define the sets of individuals  $A_{d,x} = \{\sigma : d^\sigma = d, x^\sigma = x\}$ ,  $A_x = A_{0,x} \cup A_{1,x}$  and  $A = \cup_x A_x$ . Let  $N_{d,x} = |A_{d,x}|$ ,  $N_x = |A_x|$  and  $N = |A|$ .

In an exact strata-matching, we match each individual with  $d^\sigma = d, x^\sigma = x$  with exactly one individual with  $d^\sigma = 1 - d, x^\sigma = x$ . Define a map  $m : A \rightarrow A$  such that, for each  $x$ , and for  $d \in \{0, 1\}$ , if  $\sigma \in A_{d,x}$ , then  $m(\sigma) \in A_{1-d,x}$ . This assumes  $A_{0,x}$  and  $A_{1,x}$  are non-empty for all  $x$ . The purpose of map  $m()$  is to fill in the missing data in the PO dataset. See Fig.72.3 for a pictorial representation of this.

	$y^\sigma(0)$	$y^\sigma(1)$
$d^\sigma = 0$	$y^\sigma$	$y^{m(\sigma)}$
$d^\sigma = 1$	$y^{m(\sigma)}$	$y^\sigma$

Table 72.3: Illustration of the purpose of the map  $m()$ . Note that  $y^\sigma = y^\sigma(d^\sigma)$  and  $y^{m(\sigma)} = y^\sigma(1 - d^\sigma)$ .

Note that

$$\sum_{\sigma \in A_x} \frac{d^\sigma}{N_{1,x}} = \sum_{\sigma \in A_{1,x}} \frac{1}{N_{1,x}} = 1. \quad (72.75)$$

Thus

$$\sum_{\sigma \in A_x} \frac{d^\sigma}{N_{1,x}} y^\sigma = E_{\sigma|d=1,x}[y^\sigma] = \mathcal{Y}_{1|x} \quad (72.76)$$

Table 72.4 gives estimates of  $\mathcal{Y}_{c|d,x}$

Recall that

$$\mathcal{Y}_{c,d|x} = \mathcal{Y}_{c|d,x} P(d|x) \quad (72.77)$$

Hence,

	$y^\sigma(0)$	$y^\sigma(1)$
$d^\sigma = 0$	$\frac{1}{N_{0,x}} \sum_{\sigma \in A_x} (1 - d^\sigma) y^\sigma = \mathcal{Y}_{0 0,x}$	$\frac{1}{N_{0,x}} \sum_{\sigma \in A_x} (1 - d^\sigma) y^{m(\sigma)} = \mathcal{Y}_{1 0,x}$
$d^\sigma = 1$	$\frac{1}{N_{1,x}} \sum_{\sigma \in A_x} d^\sigma y^{m(\sigma)} = \mathcal{Y}_{0 1,x}$	$\frac{1}{N_{1,x}} \sum_{\sigma \in A_x} d^\sigma y^\sigma = \mathcal{Y}_{1 1,x}$

Table 72.4: Estimates of  $\mathcal{Y}_{c|d,x}$ .

	$y^\sigma(0)$	$y^\sigma(1)$
$d^\sigma = 0$	$\frac{1}{N_x} \sum_{\sigma \in A_x} (1 - d^\sigma) y^\sigma = \mathcal{Y}_{0,0 x}$	$\frac{1}{N_x} \sum_{\sigma \in A_x} (1 - d^\sigma) y^{m(\sigma)} = \mathcal{Y}_{1,0 x}$
$d^\sigma = 1$	$\frac{1}{N_x} \sum_{\sigma \in A_x} d^\sigma y^{m(\sigma)} = \mathcal{Y}_{0,1 x}$	$\frac{1}{N_x} \sum_{\sigma \in A_x} d^\sigma y^\sigma = \mathcal{Y}_{1,1 x}$

Table 72.5: Estimates of  $\mathcal{Y}_{c,d|x}$ .

$$\mathcal{Y}_{c,d|x} = (N_{d,x} \mathcal{Y}_{c|d,x}) \frac{P(d|x)}{N_{d,x}} \quad (72.78)$$

$$= (N_{d,x} \mathcal{Y}_{c|d,x}) \frac{1}{N_x} \quad (72.79)$$

Table 72.5 gives estimates of  $\mathcal{Y}_{c,d|x}$

The treatment effects  $\mathcal{E} \in \{ATE, ATT, ATU, SB, SDO\}$  can be estimated from the data via the following estimates.

$$\widehat{ATE}_x = \overbrace{\mathcal{Y}_{1|1,x} P(1|x) + \mathcal{Y}_{1|0,x} P(0|x)}^{\mathcal{Y}_{1|x}} - \overbrace{\mathcal{Y}_{0|1,x} P(1|x) + \mathcal{Y}_{0|0,x} P(0|x)}^{\mathcal{Y}_{0|x}} \quad (72.80)$$

$$= \frac{1}{N_x} [\widehat{ATT}_x N_{1,x} + \widehat{ATU}_x N_{0,x}] \quad (72.81)$$

$$= \frac{1}{N_x} \left[ \sum_{\sigma \in A_x} d^\sigma [y^\sigma - y^{m(\sigma)}] + \sum_{\sigma \in A_x} (1 - d^\sigma) [y^{m(\sigma)} - y^\sigma] \right] \quad (72.82)$$

$$= \frac{1}{N_x} \sum_{\sigma \in A_x} (2d^\sigma - 1) [y^\sigma - y^{m(\sigma)}] \quad (72.83)$$

$$\widehat{ATT}_x = \overbrace{\frac{1}{N_x} \sum_{\sigma \in A_x} d^\sigma y^\sigma}^{\mathcal{Y}_{1,1|x}} - \overbrace{\frac{1}{N_x} \sum_{\sigma \in A_x} d^\sigma y^{m(\sigma)}}^{\mathcal{Y}_{0,1|x}} \quad (72.84)$$

$$= \frac{1}{N_x} \sum_{\sigma \in A_x} d^\sigma [y^\sigma - y^{m(\sigma)}] \quad (72.85)$$

$$\widehat{ATU}_x = \overbrace{\frac{1}{N_x} \sum_{\sigma \in A_x} (1 - d^\sigma) y^{m(\sigma)}}^{\mathcal{Y}_{1,0|x}} - \overbrace{\frac{1}{N_x} \sum_{\sigma \in A_x} (1 - d^\sigma) y^\sigma}^{\mathcal{Y}_{0,0|x}} \quad (72.86)$$

$$= \frac{1}{N_x} \sum_{\sigma \in A_x} (1 - d^\sigma) [y^{m(\sigma)} - y^\sigma] \quad (72.87)$$

$$\widehat{SB}_x = \overbrace{\frac{1}{N_x} \sum_{\sigma \in A_x} d^\sigma y^{m(\sigma)}}^{\mathcal{Y}_{0,1|x}} - \overbrace{\frac{1}{N_x} \sum_{\sigma \in A_x} (1 - d^\sigma) y^\sigma}^{\mathcal{Y}_{0,0|x}} \quad (72.88)$$

$$\widehat{SDO}_x = \overbrace{\frac{1}{N_x} \sum_{\sigma \in A_x} d^\sigma y^\sigma}^{\mathcal{Y}_{0,1|x}} - \overbrace{\frac{1}{N_x} \sum_{\sigma \in A_x} (1 - d^\sigma) y^\sigma}^{\mathcal{Y}_{0,0|x}} \quad (72.89)$$

Suppose we do linear regression to fit a hyperplane  $y(x)$  to the dataset set  $\{(x^\sigma, y^\sigma) : \sigma\}$ , and then we calculate  $\frac{\partial y}{\partial d} = \delta$ . Out of all the treatment effects, this  $\delta$  is probably (?) closest to  $ACE = ATE$ . Note also that the linear regression method of estimating  $\delta$  does imputation (guesses missing values) by doing a linear fit. One can also use machine learning to do a non-linear fit. In contrast, the estimates of treatment effects presented in this section do imputation by non-linear strata-matching.

### Example, estimation of treatment effects

For  $\sigma \in \{1, 2, \dots, 10\}$ , define

$$m(\sigma) = \begin{cases} \sigma + 5 & \text{if } \sigma \leq 5 \\ \sigma - 5 & \text{if } \sigma > 5 \end{cases} \quad (72.90)$$

Let  $N(\mathcal{S})$  be the number of individuals  $\sigma$  that satisfy condition  $\mathcal{S}$ . For example,  $N(\underline{d^\sigma} = d)$  is the number of individuals such that  $\underline{d^\sigma} = d$ .

$$N_1 = N(d^\sigma = 1) = 5 \quad (72.91)$$

$$N_0 = N(d^\sigma = 0) = 5 \quad (72.92)$$

$$N = N_0 + N_1 = 10 \quad (72.93)$$

$$\mathcal{Y}_{1|1} = \frac{1}{N_1} \sum_{\sigma} d^\sigma y^\sigma = \frac{4}{5} \quad (72.94)$$

$\sigma$	$d^\sigma$	$y^\sigma$	$d^\sigma y^\sigma$	$(1 - d^\sigma)y^\sigma$	$d^\sigma y^{m(\sigma)}$	$(1 - d^\sigma)y^{m(\sigma)}$
1	0	0	0	0	0	0
2	0	0	0	0	0	1
3	0	1	0	1	0	1
4	0	1	0	1	0	1
5	0	1	0	1	0	1
6	1	0	0	0	0	0
7	1	1	1	0	0	0
8	1	1	1	0	1	0
9	1	1	1	0	1	0
10	1	1	1	0	1	0

Table 72.6: Estimates of treatment effects are calculated for this example.

$N(d, y)$	$y = 0$	$y = 1$
$d = 0$	2	3
$d = 1$	1	4

Table 72.7:  $N(\underline{d}^\sigma = d, \underline{y}^\sigma = y)$  for the data in Table 72.6.

$$\mathcal{Y}_{0|0} = \frac{1}{N_0} \sum_{\sigma} (1 - d^\sigma) y^\sigma = \frac{3}{5} \quad (72.95)$$

$$\mathcal{Y}_{0|1} = \frac{1}{N_1} \sum_{\sigma} d^\sigma y^{m(\sigma)} = \frac{3}{5} \quad (72.96)$$

$$\mathcal{Y}_{1|0} = \frac{1}{N_0} \sum_{\sigma} (1 - d^\sigma) y^{m(\sigma)} = \frac{4}{5} \quad (72.97)$$

$$ATT = \mathcal{Y}_{1|1} - \mathcal{Y}_{0|1} = \frac{1}{5} \quad (72.98)$$

$$ATE = ATT = ATU = SDO = \frac{1}{5}, \quad SB = 0 \quad (72.99)$$

This example is unusual in that it has a single stratum  $x$ , and for that stratum, the treated and untreated populations are **balanced** (of equal size). Also, the map  $m()$  is 1-1 onto. If, for instance,  $m(\sigma) = 6$  for all  $\sigma \in A_0$  and  $m(\sigma) = 5$  for  $\sigma \in A_1$ , then  $ATE, ATT, ATU, SDO$  would not all be same, and  $SB$  would not be zero.

In fact, whenever there is a single balanced stratum and the map  $m()$  is 1-1 onto, Eq.(72.99) can be proven to be true using the methods of section 72.8.

## 72.14.2 Approximate strata-matching

It is very often the case that one can't find for a given individual  $\sigma$  another individual that has opposite  $d^\sigma$  but exactly the same value of  $x^\sigma$ . In such cases, one can discard all matchless individuals. But that would entail a loss of precious information. Instead of discarding orphans, a better way is to relax our demands and match individual  $\sigma$  with another individual  $m(\sigma)$  such that  $x^\sigma$  and  $x^{m(\sigma)}$  are very close in some metric. Alternatively, the matching individual might not be real; it might be a composite of individuals.

More precisely, for some arbitrary parameter  $\epsilon > 0$ , and an individual  $\sigma$ , define the **strata-matching set**  $\mathcal{M}_\epsilon(\sigma)$  by<sup>5</sup>

$$\mathcal{M}_\epsilon(\sigma) = \{m : d^m = 1 - d^\sigma, \text{dist}(x^\sigma, x^m) \leq \epsilon\}, \quad (72.100)$$

where

$$\text{dist}(x^\sigma, x^m) = [x^\sigma]^T [\Sigma]^{-1} x^m, \quad (72.101)$$

where  $\Sigma = \langle x^\sigma, [x^m]^T \rangle$ . This metric  $\text{dist}(x^\sigma, x^m)$  is called the **Mahalanobis distance**. We will call the case  $\epsilon = 0$  an **exact strata-matching**, and the case  $\epsilon \neq 0$  an **approximate strata-matching**. To do an approximate strata-matching, replace  $y^{m(\sigma)}$  by  $\langle y \rangle^{\mathcal{M}_\epsilon(\sigma)}$  in the estimates given above for an exact strata-matching.  $\langle y \rangle^{\mathcal{M}_\epsilon(\sigma)}$  is defined by

$$\langle y \rangle^{\mathcal{M}_\epsilon(\sigma)} = \frac{1}{|\mathcal{M}_\epsilon(\sigma)|} \sum_{m \in \mathcal{M}_\epsilon(\sigma)} y^m. \quad (72.102)$$

## 72.14.3 Unbiased strata-matching estimates

The estimates we obtained via strata-matching are biased because strata-matching, due to its non-uniqueness, introduces noise into the estimate. However, one can define new bias-corrected estimates. Following Ref.[12], we will next find an unbiased estimate of  $ATT_x$  using the biased estimate of  $ATT_x$  that we obtained by strata-matching.

Let  $\hat{\mathcal{Y}}_{|d,x}$  be an estimate of  $\mathcal{Y}_{|d,x} = E_{|d,x}[y]$  that is obtained, for example, via Linear Regression.

**Claim 123** *The quantity*

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<sup>5</sup>One can use an  $\epsilon$  that depends on  $\sigma$ . For example, let  $\epsilon(\sigma, 5)$  satisfy  $|\mathcal{M}_{\epsilon(\sigma, 5)}(\sigma)| = 5$ .

$$\widehat{ATT}_x^{unbi} = \frac{1}{N_x} \sum_{\sigma \in A_x} d^\sigma \left[ (y^\sigma - y^{m(\sigma)}) - (\widehat{\mathcal{Y}}_{|0,x^\sigma} - \widehat{\mathcal{Y}}_{|0,x^{m(\sigma)}}) \right] \quad (72.103)$$

is an unbiased estimate of  $ATT_x$ .

**proof:**

We begin by assuming a special case of SUTVA. Let

$$\underline{y}^\sigma = \underline{y}(d^\sigma) = \widehat{\mathcal{Y}}_{|d^\sigma,x^\sigma} + \underline{\epsilon}^\sigma \quad (72.104)$$

where

$$\left\langle \widehat{\mathcal{Y}}_{|d^\sigma,x^\sigma}, \underline{\epsilon}^\sigma \right\rangle_\sigma = 0 \quad (72.105)$$

Recall that the biased estimate of  $ATT_x$  obtained by strata-matching is

$$\widehat{ATT}_x^{bi} = \frac{1}{N_x} \sum_{\sigma \in A_x} d^\sigma (y^\sigma - y^{m(\sigma)}) \quad (72.106)$$

where  $\sigma$  and  $m(\sigma)$  are matched (i.e.,  $x^\sigma \approx x^{m(\sigma)}$  and  $d^{m(\sigma)} = 1 - d^\sigma$ ).

$$\widehat{ATT}_x^{bi} = \frac{1}{N_x} \sum_{\sigma \in A_x} d^\sigma \left( \widehat{\mathcal{Y}}_{|1,x^\sigma} - \widehat{\mathcal{Y}}_{|0,x^{m(\sigma)}} \right) \quad (72.107)$$

$$+ \frac{1}{N_x} \sum_{\sigma \in A_x} d^\sigma (\epsilon^\sigma - \epsilon^{m(\sigma)}) \quad (72.108)$$

$$\widehat{ATT}_x^{bi} = \underbrace{\frac{1}{N_x} \sum_{\sigma \in A_x} d^\sigma \left( \widehat{\mathcal{Y}}_{|1,x^\sigma} - \widehat{\mathcal{Y}}_{|0,x^\sigma} \right)}_{ATT_x^{unbi}} \quad (72.109)$$

$$+ \underbrace{\frac{1}{N_x} \sum_{\sigma \in A_x} d^\sigma \left( \widehat{\mathcal{Y}}_{|0,x^\sigma} - \widehat{\mathcal{Y}}_{|0,x^{m(\sigma)}} \right)}_{\Delta ATT_x} \quad (72.110)$$

$$+ \underbrace{\frac{1}{N_x} \sum_{\sigma \in A_x} d^\sigma (\epsilon^\sigma - \epsilon^{m(\sigma)})}_{\mathcal{E}_x} \quad (72.111)$$

$$ATT_x^{unbi} = \underbrace{\widehat{ATT}_x^{bi} - \Delta ATT_x}_{\widehat{ATT}_x^{unbi}} - \mathcal{E}_x \quad (72.112)$$

By the Central Limit Theorem, for large  $N_x$ , this sum over  $\sigma \in A_x$  of i.i.d. summands is normally distributed

$$\sqrt{N_x} ATT_x^{unbi} \sim \mathcal{N}(x; 0, var) \quad (72.113)$$

The reason for the  $\sqrt{N_x}$  normalization is that we want the variance to be proportional to  $N_x$ .

$$var = N_x \langle ATT_x^{unbi}, ATT_x^{unbi} \rangle \quad (72.114)$$

$$= N_x \left\langle \widehat{ATT}_x^{unbi}, \widehat{ATT}_x^{unbi} \right\rangle + N_x \langle \mathcal{E}_x, \mathcal{E}_x \rangle \quad (72.115)$$

QED

## 72.15 Propensities

It is often the case that the discrete vector  $\underline{x}^\sigma$  has too many possible values to make matching possible. In such cases, it is convenient to map the space of vectors  $\underline{x}^\sigma$  to the real line. One very convenient choice for that map is the **propensity score**, which is defined as

$$g(x^\sigma) = P(\underline{d}^\sigma = 1 | \underline{x}^\sigma). \quad (72.116)$$

$P(\underline{d}^\sigma = 1 | \underline{x}^\sigma)$  is easy to calculate from the dataset.  $g(x) = N_{1,x}/N_x$ .

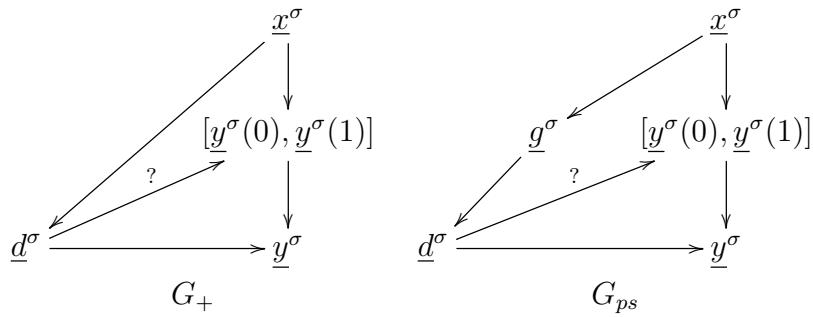


Figure 72.14: Bnet  $G_{ps}$  used when doing propensity scoring.

To use the propensity score, one replaces the bnet  $G_+$  by the bnet  $G_{ps}$  as shown in Fig.72.14. The TPMs, printed in blue, for the 2 nodes of  $G_{ps}$  that differ from the nodes of  $G_+$ , are as follows:

$$P(g^\sigma | x^\sigma) = \delta(g^\sigma, g(x^\sigma)) \quad (72.117)$$

$$P(d^\sigma | g^\sigma) = g^\sigma d^\sigma + (1 - g^\sigma)(1 - d^\sigma) \quad (72.118)$$

Note that these TPMs are self-consistent because

$$P(d|x) = \sum_g P(d|g)P(g|x) \quad (72.119)$$

$$= g(x)d + [1 - g(x)](1 - d) \quad (72.120)$$

$$= P(\underline{d} = 1|x)d + [1 - P(\underline{d} = 1|x)](1 - d) \quad (72.121)$$

$$= P(d|x) \quad (72.122)$$

We would like to do **propensity score strata-matching** by matching g-strata instead of x-strata. PO calculations for x- strata-matching use the TPMs for  $P(d|x)$ ,  $P(x)$  and  $P(y|d, x)$ . To do g- strata-matching using the same equations, but with  $x$  replaced by  $g$ , we would need to solve for  $P(d|g)$ ,  $P(g)$  and  $P(y|d, g)$  in terms of  $P(d|x)$ ,  $P(x)$  and  $P(y|d, x)$ . We solve for those next.

From the TPMs for  $G_{ps}$ , one has

$$\boxed{P(d|g) = gd + (1 - g)(1 - d)} \quad (72.123)$$

and

$$\boxed{P(g) = \sum_x \overbrace{\delta(g, g(x))}^{P(g|x)} P(x)} \quad (72.124)$$

Next, note that

$$P(y|d, g) = \sum_x P(y|d, x)P(x|g) \quad (72.125)$$

so we need to find  $P(x|g)$ . Since

$$P(x|g) = \frac{P(g|x)P(x)}{P(g)} \quad (72.126)$$

$$= \frac{\delta(g, g(x))P(x)}{P(g)} \quad (72.127)$$

we finally get

$$\boxed{P(y|d, g) = \sum_x P(y|d, x) \frac{\delta(g, g(x))P(x)}{P(g)}} \quad (72.128)$$

Eq.(72.128) looks complicated, but all it is saying is that

$$P(y|d, g)P(g) = \sum_{x \in g^{-1}(g)} P(y|d, x)P(x), \quad (72.129)$$

where  $g^{-1}(g) = \{x : g(x) = g\}$ . In general,

$$\sum_x \delta(g, g(x)) = \sum_{x \in g^{-1}(g)} \quad (72.130)$$

Recall that for any treatment effect  $\mathcal{E} \in \{ATE, ATT, ATU, SB, SDO\}$ , we can estimate  $\mathcal{E}_x$ , and then calculate  $\mathcal{E}$  from it, using

$$\mathcal{E} = \sum_x P(x)\mathcal{E}_x. \quad (72.131)$$

Hence

$$\mathcal{E} = \sum_g \sum_x \delta(g, g(x))P(x)\mathcal{E}_x \quad (72.132)$$

$$= \sum_g \sum_{x \in g^{-1}(g)} P(x)\mathcal{E}_x \quad (72.133)$$

Let

$$g_{d|x} = g_d(x) = P(d|x) \quad (72.134)$$

for  $d \in \{0, 1\}$ . Note that  $g_{0|x} + g_{1|x} = 1$ . We will refer to  $g_d(x)$  for  $d \in \{0, 1\}$  as a two **propensities** and to  $g_1(x)$  as the **propensity score**.

Define

$$\delta_{y|x} = P(y|d = 1, x) - P(y|d = 0, x) \quad (72.135)$$

Note that

$$\delta_{y|x} = \frac{P(y, d = 1|x)}{g_{1|x}} - \frac{P(y, d = 0|x)}{g_{0|x}} \quad (72.136)$$

$$= \frac{P(y, d = 1|x)g_{0|x} - P(y, d = 0|x)g_{1|x}}{g_{0|x}g_{1|x}} \quad (72.137)$$

$$= \frac{P(y, d = 1|x) - P(y|x)g(x)}{g(x)(1 - g(x))} \quad (72.138)$$

Dividing each term in a sum over  $d \in \{0, 1\}$  by  $g_d(x)$  is often called **inverse probability (or propensity) weighting** (IPW).  $g_d(x) = P(\underline{d} = d|x)$  is the likelihood of strata  $x$ , so dividing each term by this likelihood increases the contribution to the sum by less likely strata and decreases the contribution by more likely strata.

Note that the backdoor adjustment formula can be expressed as an IPW:

$$P(y|\mathcal{D}\underline{d} = d) = \sum_x P(y|d, x)P(x) \quad (72.139)$$

$$= \sum_x \frac{P(y, d, x)}{P(d|x)} \quad (72.140)$$

Note that  $ATE = ACE$  can be expressed in terms of propensities:

$$ACE = \sum_y y[P(y|\mathcal{D}\underline{d} = 1) - P(y|\mathcal{D}\underline{d} = 0)] \quad (72.141)$$

$$= \sum_x P(x) \sum_y y [P(y|d = 1, x) - P(y|d = 0, x)] \quad (72.142)$$

$$= \sum_x P(x) \sum_y \underbrace{y\delta_{y|x}}_{ACE_x} \quad (72.143)$$

Note that

$$P(y(c)|d) = \sum_x P(y(c)|d, x)P(x|d) \quad (72.144)$$

$$= \sum_x P(y(c)|c, x)P(x|d) \text{ (by CIA)} \quad (72.145)$$

$$= \sum_x P(y|c, x)P(x|d) \text{ (by SUTVA)} \quad (72.146)$$

It's instructive to express all the other treatment effects besides  $ATE$  in terms of propensities:

$$ATT = \sum_y y[P(\underline{y}(1) = y|d = 1) - P(\underline{y}(0) = y|d = 1)] \quad (72.147)$$

$$= \sum_x P(x|d = 1) \sum_y y [P(y|\underline{d} = 1, x) - P(y|\underline{d} = 0, x)] \text{ (by Eq.(72.146))} \quad (72.148)$$

$$= \sum_x P(x|d = 1) \sum_y y \delta_{y|x} \quad (72.149)$$

$$= \sum_x P(x) \underbrace{\frac{1}{P(\underline{d} = 1)} \sum_y y g_{1|x} \delta_{y|x}}_{ATT_x} \quad (72.150)$$

$$ATU = \sum_x P(x) \underbrace{\frac{1}{P(\underline{d} = 0)} \sum_y y g_{0|x} \delta_{y|x}}_{ATU_x} \quad (72.151)$$

$$SB = \sum_y y [P(\underline{y}(0) = y | d = 1) - P(\underline{y}(0) = y | d = 0)] \quad (72.152)$$

$$= \sum_y y \sum_x P(y | \underline{d} = 0, x) [P(x | d = 1) - P(x | d = 0)] \text{ (by Eq.(72.146))} \quad (72.153)$$

$$= \sum_x P(x) \underbrace{\sum_y y \frac{P(y, \underline{d} = 0 | x)}{g_{0|x}} \left[ \frac{g_{1|x}}{P(\underline{d} = 1)} - \frac{g_{0|x}}{P(\underline{d} = 0)} \right]}_{SB_x} \quad (72.154)$$

$$SDO = \sum_y y [P(\underline{y}(1) = y | d = 1) - P(\underline{y}(0) = y | d = 0)] \quad (72.155)$$

$$= \sum_x P(x) \underbrace{\sum_y y \left[ \frac{P(y, \underline{d} = 1 | x)}{P(\underline{d} = 1)} - \frac{P(y, \underline{d} = 0 | x)}{P(\underline{d} = 0)} \right]}_{SDO_x} \text{ (by SUTVA)} \quad (72.156)$$

## 72.16 Propensity based estimates of treatment effects

In the strata-matching section 72.14, we gave an estimate of  $ACE_x$ . In strata-matching, one fills in the missing counterfactual values via the map  $m()$ . This is justified because, by CIA (weak-d limit), the counterfactual distributions are assumed to equal the factual distributions (see Fig. 72.6). In this section, we give estimates of treatment effects that are based on the formulae derived in Section 72.15. The estimates given in this section do no require the map  $m()$ , because the identification of counterfactual distributions with factual ones was used to derive the formulae of Section 72.15.

Eq.(72.143) suggests the estimate

$$\widehat{ACE}_x = \frac{1}{N_x} \sum_{\sigma \in A_x} y^\sigma \left[ \frac{d^\sigma - g(x)}{g(x)(1 - g(x))} \right] \quad (72.157)$$

$$= \frac{1}{N_x} \sum_{\sigma \in A_x} \left[ \frac{d^\sigma y^\sigma}{g_{1|x}} - \frac{(1 - d^\sigma)y^\sigma}{g_{0|x}} \right] \quad (72.158)$$

This estimate is unbiased (because it doesn't have a source of noise like the strata-matching estimates do), but it is still possible to improve it. We next define another

*ACE* estimate called **Doubly Robust Estimate** (DRE) that is also unbiased and has smaller variance.

Let  $\widehat{\mathcal{Y}}_{|d,x}$  be an estimate of  $\mathcal{Y}_{|d,x} = E_{\underline{y}|d,x}[\underline{y}]$  that is obtained, for example, via Linear Regression. Define the DRE

$$\widehat{ACE}_x^{DRE} = \widehat{\mathcal{Y}}_{1|x}^{DRE} - \widehat{\mathcal{Y}}_{0|x}^{DRE} \quad (72.159)$$

where

$$\widehat{\mathcal{Y}}_{1|x}^{DRE} = \frac{1}{N_x} \sum_{\sigma \in A_x} \left[ \frac{d^\sigma(y^\sigma - \widehat{\mathcal{Y}}_{|1,x})}{g_{1|x}} + \widehat{\mathcal{Y}}_{|1,x} \right] \quad (72.160)$$

and

$$\widehat{\mathcal{Y}}_{0|x}^{DRE} = \frac{1}{N_x} \sum_{\sigma \in A_x} \left[ \frac{(1-d^\sigma)(y^\sigma - \widehat{\mathcal{Y}}_{|0,x})}{g_{0|x}} + \widehat{\mathcal{Y}}_{|0,x} \right]. \quad (72.161)$$

The DRE  $\widehat{\mathcal{Y}}_{1|x}^{DRE}$  requires first estimating 2 preparatory quantities,  $\widehat{\mathcal{Y}}_{|1,x}$  and  $g_{1|x}$ . It's called doubly robust because it remains unbiased even if one of the estimates of those 2 preparatory quantities is wrong, but not if both are wrong. Let's check this.

- Suppose the propensity  $g_{1|x}$  is slightly wrong. So what because

$$E_{\sigma|1,x} \left[ \frac{d^\sigma(y^\sigma - \widehat{\mathcal{Y}}_{|1,x})}{g_{1|x}} \right] = 0 \quad (72.162)$$

- Suppose  $\widehat{\mathcal{Y}}_{|1,x}$  is slightly wrong. So what because

$$E_{\sigma|1,x} \left[ \frac{-d^\sigma \widehat{\mathcal{Y}}_{|1,x} + g_{1|x} \widehat{\mathcal{Y}}_{|1,x}}{g_{1|x}} \right] = 0 \quad (72.163)$$

A similar argument can be used to show that  $\widehat{\mathcal{Y}}_{0|x}^{DRE}$  is doubly robust too.

## 72.17 Positivity

**Positivity** or **non-zero overlap** is defined as the requirement that for all layers  $x$ ,

$$0 < \underbrace{P(d^\sigma = 1 | \underline{x}^\sigma = x)}_{g_{1|x}} < 1 \quad (72.164)$$

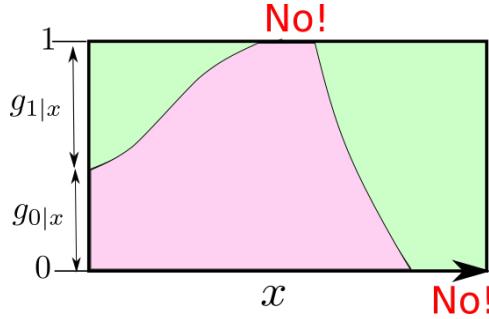


Figure 72.15: Pictorial representation of positivity.  $g_{0|x} + g_{1|x} = 1$ .  $g_{0|x} = 0$  and  $g_{1|x} = 0$  are forbidden.

or, equivalently,

$$\underbrace{P(\underline{d}^\sigma = 1 | \underline{x}^\sigma = x)}_{g_{1|x}} > 0 \quad \text{and} \quad \underbrace{P(\underline{d}^\sigma = 0 | \underline{x}^\sigma = x)}_{g_{0|x}} > 0. \quad (72.165)$$

In other words, for each layer  $x$ , there is a non-zero probability of being both treated and untreated. See Fig.72.15 for a pictorial representation of positivity.

If positivity is violated for some layer  $x$ , then

- the propensity based estimate Eq.(72.158) for  $ACE_x$  (which equals  $ATE_x$ ) is undefined.
- all strata-matching estimates of  $\mathcal{E}_x$  that use the matching function  $m()$  are undefined because that function is undefined if  $A_{0,x} = \emptyset$  or  $A_{1,x} = \emptyset$ .

If a quantity (estimand) can be estimated, it is said to be **do-identifiable** (i.e., expressible without do() operators). If positivity is violated, then  $ACE = ATE$  is not identifiable.

When  $P(d|x)$  becomes 0 or 1 for some  $x$ , the arrow  $\underline{x} \rightarrow \underline{d}$  becomes deterministic for that  $x$ . This situation is the very antithesis of RCTs, wherein the influence exerted by  $\underline{x}^\sigma$  on  $\underline{d}^\sigma$  is uniformly random and therefore ignorable. Hence, it is perhaps not too surprising that a violation of positivity makes  $ACE = ATE$  not identifiable.

## 72.18 Multi-time PO bnets (Panel Data)

In this section, we will discuss Multi-time PO bnets (MT-PO).

A **time-series** is a function  $f : D \rightarrow \mathbb{R}$  whose domain  $D$  is a discrete set of times. A time-series usually describes a single unit  $\sigma$  (i.e., an individual) in a population.

An **observational study (or analysis or model)** can be cross-sectional or longitudinal. A **cross-sectional study** collects and analyzes a **cross-sectional**

**dataset**; i.e., a dataset for a population at a single time. A **longitudinal study or panel study** collects and analyzes a **longitudinal dataset**; i.e., a dataset for a population at multiple times. Thus, a longitudinal study consists of one or more time-series.

Let  $\mathcal{T} = \{t_0, t_1, \dots, t_{nt-1}\}$ . For any time-series  $a_t : \mathcal{T} \rightarrow \mathbb{R}$ , define

$$E_t a_t = \frac{1}{nt} \sum_{t \in \mathcal{T}} a_t \quad (72.166)$$

$$\Delta_t a_t = a_t - E_t a_t \quad (72.167)$$

$$\langle a_t, b_t \rangle_t = E_t \Delta_t a_t \Delta_t b_t \quad (72.168)$$

Consider a quantity  $a_t^\sigma$  that is a function of the time  $t$  and of the particular unit  $\sigma$  in a population.  $a_t^\sigma$  is said to be a **t-constant effect** if it is  $t$ -independent.  $a_t^\sigma$  is said to be a **homogeneous effect** (antonym: **heterogeneous effect**) if it is  $\sigma$ -independent. Henceforth, we will avoid using the word "effect" for these because that word has already been used for "treatment effect" in PO theory. Instead, we will use the word "quantity".

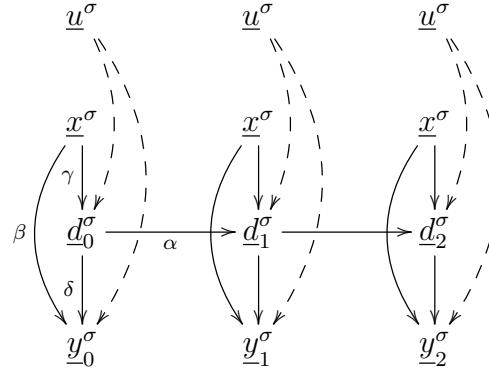


Figure 72.16: Example of multi-time PO bnet with t-constant quantities  $\underline{x}^\sigma, \underline{u}^\sigma$ . The 3 nodes  $\underline{x}^\sigma$  should be identified as a single node. Likewise, the 3 nodes  $\underline{u}^\sigma$  should be identified as a single node.

Fig.72.16 gives an example of a multi-time PO bnet (MT-PO). Note that in this example,  $\underline{x}^\sigma$  and  $\underline{u}^\sigma$  are t-constant quantities.  $\underline{u}^\sigma$  is an unobserved confounder and  $\underline{x}^\sigma$  is an observed confounder. For convenience and simplicity, we will assume linear deterministic TPMs, printed in blue, for the bnet Fig.72.16, are as follows:

$$P(x^\sigma) = P_{\underline{x}}(x^\sigma) \quad (72.169)$$

$$P(u^\sigma) = P_{\underline{u}}(u^\sigma) \quad (72.170)$$

$$P(y_t^\sigma | d_t^\sigma, x^\sigma, u^\sigma) = \mathbb{1}(y_t^\sigma = \delta d_t^\sigma + \beta x^\sigma + u^\sigma) \quad (72.171)$$

$$P(d_{t+1}^\sigma | d_t^\sigma, x^\sigma, u^\sigma) = \mathbb{1}(d_{t+1}^\sigma = \alpha d_t^\sigma + \gamma x^\sigma + u^\sigma) \quad (72.172)$$

Taking time averages of the treatment decision and treatment outcome, we get

$$E_t \underline{y}_t^\sigma = \delta E_t \underline{d}_t^\sigma + \beta \underline{x}^\sigma + \underline{u}^\sigma, \quad (72.173)$$

$$E_t \underline{d}_{t+1}^\sigma = \alpha E_t \underline{d}_t^\sigma + \gamma \underline{x}^\sigma + \underline{u}^\sigma. \quad (72.174)$$

Subtracting the time averages from the quantities being averaged, we get

$$\Delta_t \underline{y}_t^\sigma = \delta \Delta_t \underline{d}_t^\sigma, \quad (72.175)$$

$$\Delta_t \underline{d}_{t+1}^\sigma = \alpha \Delta_t \underline{d}_t^\sigma. \quad (72.176)$$

This allows us to find estimates for  $\delta$  and  $\alpha$ :

$$E_\sigma \langle \underline{y}_t^\sigma, \underline{y}_t^\sigma \rangle_t = \delta E_\sigma \langle \underline{y}_t^\sigma, \underline{d}_t^\sigma \rangle_t \quad (72.177)$$

$$\delta = \frac{E_\sigma \langle \underline{y}_t^\sigma, \underline{y}_t^\sigma \rangle_t}{E_\sigma \langle \underline{y}_t^\sigma, \underline{d}_t^\sigma \rangle_t} \quad (72.178)$$

$$E_\sigma \langle \underline{d}_{t+1}^\sigma, \underline{d}_{t+1}^\sigma \rangle_t = \alpha E_\sigma \langle \underline{d}_{t+1}^\sigma, \underline{d}_t^\sigma \rangle_t \quad (72.179)$$

$$\alpha = \frac{E_\sigma \langle \underline{d}_{t+1}^\sigma, \underline{d}_{t+1}^\sigma \rangle_t}{E_\sigma \langle \underline{d}_{t+1}^\sigma, \underline{d}_t^\sigma \rangle_t} \quad (72.180)$$

As shown in Fig.72.17, subtraction of time averages from each node removes the confounder nodes from the bnet of Fig.72.16 (However, this assumes that the confounders are t-constant and that the TPMs are linear deterministic, two very strong assumptions).

$$\begin{array}{ccc} \Delta_t \underline{d}_t^\sigma & \xrightarrow{\alpha} & \Delta_t \underline{d}_{t+1}^\sigma \\ \delta \downarrow & & \downarrow \\ \Delta_t \underline{y}_t^\sigma & & \Delta_t \underline{y}_{t+1}^\sigma \end{array}$$

Figure 72.17: time-average-subtracted (TAS) bnet for the bnet of Fig.72.16.

# Chapter 73

## Program evaluation and review technique (PERT)

This chapter is based on Refs.[68] and [147].

PERT diagrams are used for scheduling a project consisting of a series of interdependent activities and estimating how long it will take to finish the project. PERT diagrams were invented by the NAVY in 1958 to manage a submarine project. Nowadays they are taught in many business and management courses.

A **PERT diagram** is a Directed Acyclic Graph (DAG) with the following properties. (See Fig.73.2 for an example of a PERT diagram). The nodes  $\underline{E}_i$  for  $i = 1, 2, \dots, ne$  of a PERT diagram are called **events**. The edges  $i \rightarrow j$  of a PERT diagram are called **activities**. An event represents the starting (kickoff) date of one or more activities. A PERT diagram has a single root node ( $i = 1$ , start event) and a single leaf node ( $i = ne$ , end event).

The PERT diagram user must initially provide a **Duration Times (DT) table** which gives  $(DO_{i \rightarrow j}, DP_{i \rightarrow j}, DM_{i \rightarrow j})$  for each activity  $i \rightarrow j$ , where

$DO_{i \rightarrow j}$ = optimistic duration time of activity  $i \rightarrow j$

$DP_{i \rightarrow j}$ = pessimistic duration time of activity  $i \rightarrow j$

$DM_{i \rightarrow j}$ = median duration time of activity  $i \rightarrow j$

From the DT table, one calculates:

Duration time of activity  $i \rightarrow j$

$$D_{i \rightarrow j} = \frac{1}{6}(DO_{i \rightarrow j} + DP_{i \rightarrow j} + 4DM_{i \rightarrow j}) \quad (73.1)$$

Duration Variance of activity  $i \rightarrow j$

$$V_{i \rightarrow j} = \left( \frac{DO_{i \rightarrow j} - DP_{i \rightarrow j}}{DM_{i \rightarrow j}} \right)^2 \quad (73.2)$$

Often, it is convenient to define "dummy" edges with  $D_{i \rightarrow j} = 0$ . That is perfectly fine.

Define:

$TES_i$  = Earliest start time for event  $i$   
 $TLS_i$  = Latest start time for event  $i$   
 $slack_i = TLS_i - TES_i$  = slack for event  $i$   
 $TEF_{i \rightarrow j} = TES_i + D_{i \rightarrow j}$  = Earliest finish time for activity  $i \rightarrow j$ .  
 $TLF_{i \rightarrow j} = TLS_j - D_{i \rightarrow j}$  = Latest finish time for activity  $i \rightarrow j$ . See footnote below.<sup>1</sup>

A **critical path** is a directed path (i.e., a chain of connected arrows, all pointing in the same direction) going from the start to the end node, such that slack equals zero at every node visited. In a DAG, the neighbors of a node is the union of its parent and children nodes. A critical path must also have all other nodes as neighbors; i.e, the union of the neighbors of every node in the path plus the nodes in the path itself, equals all nodes in the graph.

---

**GOAL of PERT analysis:** The main goal of PERT analysis is to find, based on the data of the DT table, the interval  $[TES_i, TLS_i]$  giving a lower and an upper bound to the starting time of each node  $i$ . Another goal is to find a critical path for the PERT diagram (which represents an entire project). By adding the  $D_{i \rightarrow j}$  of each edge of the critical path, one can get the mean value of the total duration of the entire project, and by adding the variances of each edge along the critical path, one can get an estimate of the total variance of the total duration. Knowing the mean and variance of the total duration and assuming a Normal distribution, one can predict the probability that the actual duration will deviate by a certain amount from its mean.

---

To calculate the interval  $[TES_i, TLS_i]$ , one follows the following two steps.

1. Assume  $TES_1 = 0$  and solve

$$TES_i = \max_{a \in pa(i)} (\underbrace{TES_a + D_{a \rightarrow i}}_{TEF_{a \rightarrow i}}) \quad (73.3)$$

for  $i \in [2, ne]$ . This recursive equation is solved by what is called “forward propagation”, wherein one moves up the list of nodes  $i$  in order of increasing  $i$  starting at  $i = 1$  with  $TES_1 = 0$ .

2. Assume  $TLS_{ne} = TES_{ne}$  and solve

$$TLS_i = \min_{b \in ch(i)} (\underbrace{TLS_b - D_{i \rightarrow b}}_{TLF_{i \rightarrow b}}) \quad (73.4)$$

---

<sup>1</sup>In the popular educational literature, the edge variables  $TEF_{i \rightarrow j}$  and  $TLF_{i \rightarrow j}$  are sometimes associated with the nodes, but they are clearly edge variables. This makes things confusing. The reason this is done is that some software draws PERT diagrams as trees whereas other software draws them as DAGs. For trees, storing  $TEF_{i \rightarrow j}$  and  $TLF_{i \rightarrow j}$  in a node makes some sense but not for DAGs. You will notice that giving specific names to the variables  $TEF_{i \rightarrow j}$  and  $TLF_{i \rightarrow j}$  is unnecessary. It is possible to delete all mention of their names from this chapter without losing any details. I only declare their names in this chapter so as tell the reader what they are in case he/she hears them mentioned and wonders what they are equal to in our notation.

for  $i \in [1, ne - 1]$ . This recursive equation is solved by what is called “backward propagation”, wherein one moves down the list of nodes  $i$  in order of decreasing  $i$  starting at  $i = ne$  with  $TLS_{ne} = TES_{ne}$ .  $TES_{ne}$  is known from step 1.

Eqs.(73.3) and (73.4) are illustrated in Fig.73.1.

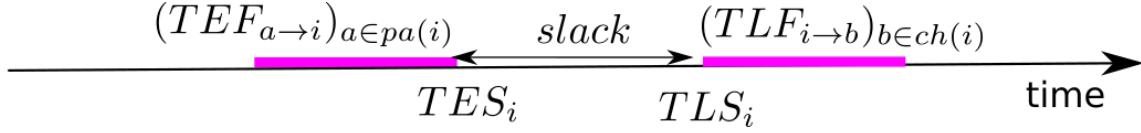


Figure 73.1:  $TES_i$  defined from info received from parents of  $i$  and  $TLS_i$  defined from info received from children of  $i$ .

## 73.1 Example

To illustrate PERT analysis, we end with an example. We present the example in the form of an exercise question and then provide the answer. This example comes from Ref.[68], except for part (e) about bnets, which is our own.

**Question:** For the PERT diagram of Fig.73.2, calculate the following:

- (a) Interval  $[TES_i, TLS_i]$  for all  $i$ .
- (b) A critical path for this PERT diagram.
- (c) The mean and variance of the total duration of the critical path.
- (d) The probability that the total duration will be 225 days or less.
- (e) A bnet interpretation of this problem.

**Answer to (a)**  $[TES_i, TLS_i]$  are given by Fig.73.3.

**Answer to (b)** The critical path is given in red in Fig.73.3. Note that this path does indeed have zero slack at each node it visits and the union of its neighborhood and the path itself encompasses all nodes.

**Answer to (c)** The mean and variance of the total duration are calculated in Table 73.1.

**Answer to (d)**

$$P(\underline{x} < 225) = P\left[\frac{\underline{x} - \mu}{\sigma} \leq \frac{225 - 220}{\sqrt{7.73}}\right] \quad (73.5)$$

$$= P[\underline{z} \leq 1.80] \quad (73.6)$$

$$= 0.9641 \quad (73.7)$$

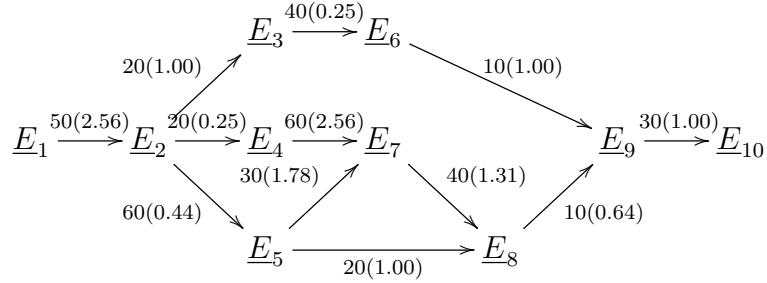


Figure 73.2: Example of a PERT diagram. The numbers attached to the arrows are the duration times  $D_{i \rightarrow j}$  in days followed by, enclosed in parentheses, the variance  $V_{i \rightarrow j}$  of that duration. The info given in this PERT diagram was derived from a DT table in Ref.[68]. The info in this PERT diagram is sufficient for calculating  $TES_i$  and  $TLS_i$  for each node  $i$ . The results of that calculation are given in Fig.73.3.

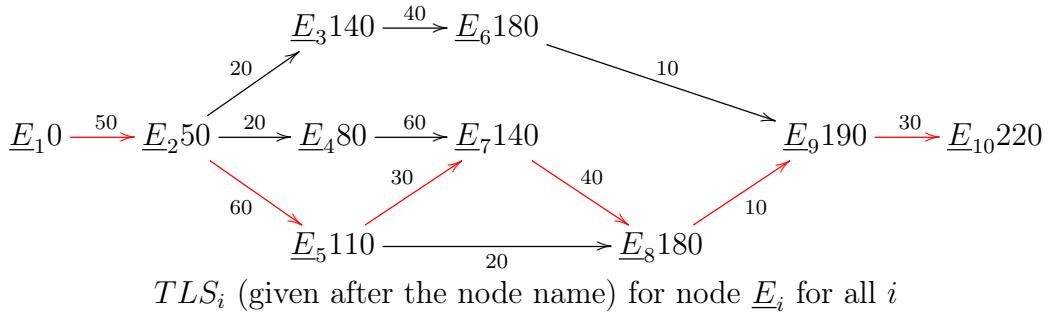
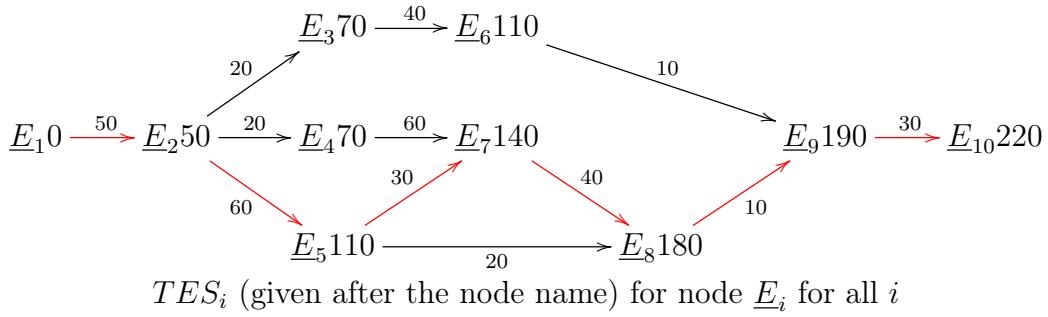


Figure 73.3: Results of calculating  $TES_i$  for all  $i$  via a forward pass, followed by calculating  $TLS_i$  for all  $i$  via a backward pass. Critical path indicated in red.

**Answer to (e)** Define 2 bnets.

1. The first PERT bnet is for calculating  $TES_i$  for all  $i$  and is given by Fig.73.4.

edge $i \rightarrow j$	duration $D_{i \rightarrow j}$	variance $V_{i \rightarrow j}$
A (1 → 2)	50	2.56
D (2 → 5)	60	0.44
G (5 → 7)	30	1.78
J (7 → 8)	40	1.31
K (8 → 9)	10	0.64
L (9 → 10)	30	1.00
Total	220	7.73

Table 73.1: Calculation of mean and variance of total duration along critical path.

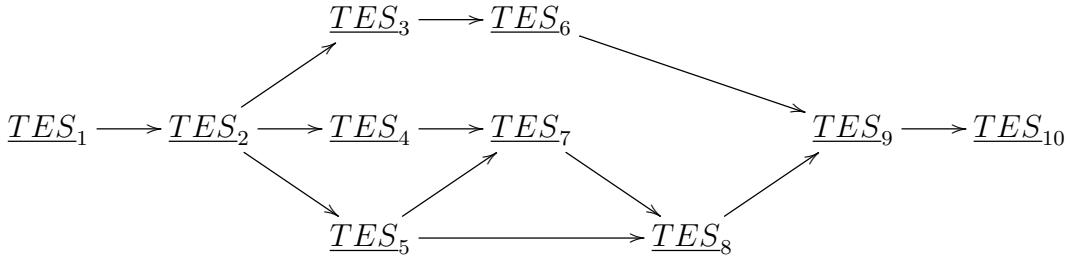


Figure 73.4: bnet for  $TES_i$  calculation.

The TPMs, printed in blue, for the bnet Fig.73.4, are as follows (this equation is to be evaluated recursively by a forward pass through the bnet):

$$P(TES_i | (TES_a)_{a \in pa(i)}) = \delta(TES_i, \max_{a \in pa(i)} (TES_a + D_{a \rightarrow i})) \quad (73.8)$$

2. The second PERT bnet is for calculating  $TLS_i$  for all  $i$  and is given by Fig.73.5. Note that the directions of all the arrows in the PERT diagram Fig.73.2 have been reversed so Fig.73.5 is a time reversed graph.

The TPMs, printed in blue, for the bnet Fig.73.5, are as follows (this equation is to be evaluate recursively by a backward pass through the bnet):

$$P(TLS_i | (TLS_b)_{b \in pa(i)}) = \delta(TLS_i, \min_{b \in pa(i)} (TLS_b - D_{b \rightarrow i}^T)) , \quad (73.9)$$

where  $D_{i \rightarrow j}^T = D_{j \rightarrow i}$ .

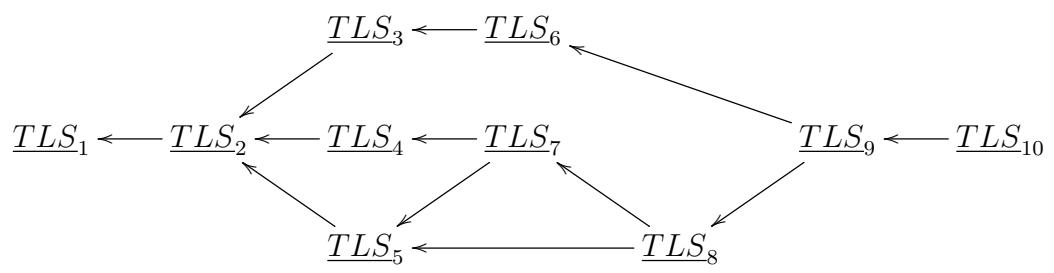


Figure 73.5: bnet for  $TLS_i$  calculation.

# Chapter 74

## Random Forest and Bagging

This chapter is based on Refs.[98] and [148].

Chapter 16 defines decision trees (dtrees) and explains how to construct them. A Random Forest (RF) is an ensemble of dtrees. The RF algorithm is a method of, given a dataset, constructing a RF and averaging over the classifier functions of the RF to produce an ensemble classifier.

The RF algo uses the method of Bootstrap Aggregating (a.k.a. Bagging), which is discussed in detail below. Bagging is a method of constructing an ensemble of datasets (called **bootstrap datasets or bags**) that are fairly uncorrelated. Each of these bags is used to train a **bag-classifier**. The bag-classifiers are averaged over to produce an **ensemble classifier, or e-classifier** for short. Bagging can be used to train any type of bag-classifier, but it was invented with dtrees in mind, and is still most commonly used to train dtrees.

Boosting (see Chapter 1 on AdaBoost and Chapter 101 on XGBoost) is another method, besides Bagging, of constructing a classifier function from an ensemble of classifier functions. These two methods are most commonly applied to dtrees: Boosting for an ensemble of small dtrees, and Bagging for a random forest (which is an ensemble of dtrees that are usually much more complicated than small dtrees).

### 74.1 Bagging (with fully-featured bags)

In this section we discuss the bagging algorithm. As already mentioned, bagging is usually used to train dtrees. In this section, we explain bagging in general, not just for dtrees.

Let  $L = [0, 1, 2, \dots, nsam - 1]$  be a list of individuals (samples) in a population. In this chapter, we will use the notation  $A^\sigma = A[\sigma]$  and  $\vec{A} = [A^\sigma : \sigma \in L]$  for a list (vector, 1-D array) indexed by  $L$ . We will refer to  $DS = (\vec{x}, \vec{y})$  where  $x^\sigma \in S_x$ ,  $y^\sigma \in S_y$ , as a dataset. If  $L_j$  is a list (possibly with duplicate items) such that  $set(L_j) \subset set(L)$ , then define  $DS_j = (\vec{x}, \vec{y})_{L_j} = ((x^\sigma)_{\sigma \in L_j}, (y^\sigma)_{\sigma \in L_j})$ . We will refer to  $DS_j$  as the **restriction of  $(\vec{x}, \vec{y})$  to  $L_j$** .

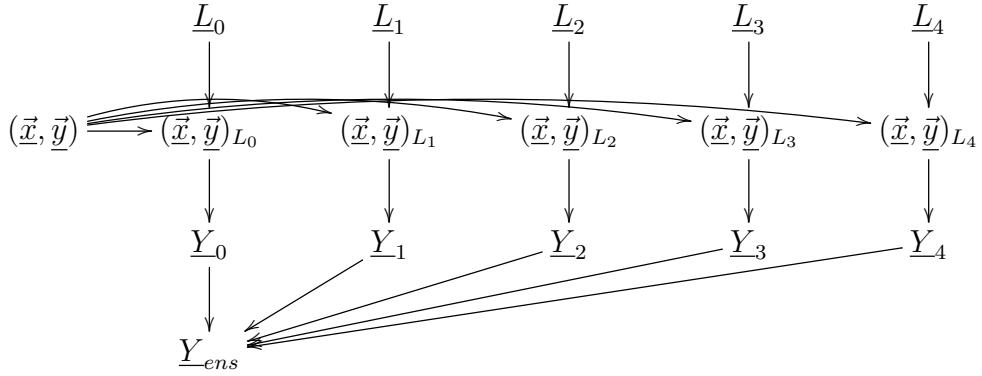


Figure 74.1: Bnet for Random Forest (RF) with 5 bags.

We will refer to a function  $Y : S_{\underline{x}} \rightarrow S_{\underline{c}}$  as a classifier. It maps vector of vector of features  $x \in S_{\underline{x}}$  to a class  $c \in S_{\underline{c}}$ . Below,  $Y_b$  for all  $b$  and  $Y_{ens}$  are classifiers.

Fig.74.1 is a bnet that encapsulates the RF algo. The TPMs, printed in blue, for the bnet Ref.74.1, are as follows.

Let  $b \in \{0, 1, 2, \dots, nbags - 1\} = B$  and  $\sigma \in L$ . Let  $L_b^\sigma \in L$  and

$$P(L_b^\sigma) = 1/nsam \quad (74.1)$$

In other words, each item in item in list  $L_b$  is chosen from the items of list  $L$ , uniformly at random with replacements.  $|L_b| = |L|$  (same size as original).  $L_b$  can have duplicate items and be missing items from  $L$ .

$$P((\vec{x}, \vec{y})_{L_b} | (\vec{x}, \vec{y}), L_b) = \mathbb{1}(\text{ } (\vec{x}, \vec{y})_{L_b} \text{ = restriction of } (\vec{x}, \vec{y}) \text{ to } L_b \text{ }) \quad (74.2)$$

We will refer to  $(\vec{x}, \vec{y})$  as the **original dataset** and to the  $(\vec{x}, \vec{y})_{L_b}$  for  $b \in B$  as the **bootstrap datasets** or **bags**.

$$P(Y_b | (\vec{x}, \vec{y})_{L_b}) = \mathbb{1}(\text{ } Y_b(\cdot) \text{ = classifier trained on dataset } (\vec{x}, \vec{y})_{L_b}. \text{ }) \quad (74.3)$$

$$P(Y_{ens} | (Y_b)_{b \in B}) = \prod_{\sigma} \mathbb{1}(\text{ } Y_{ens}(x^\sigma) = \text{majority}(\{Y_b(x^\sigma) : b \in B\}) \text{ }) \quad (74.4)$$

The **majority()** function can be replaced by an average  $\frac{1}{nbags} \sum_b$  in case the set of classes  $S_{\underline{c}}$  equals  $\mathbb{R}$  rather than a finite set. We will refer to  $Y_{ens}$  as the **ensemble classifier (e-classifier)** and to the  $Y_b$  as the **bag-classifiers**.

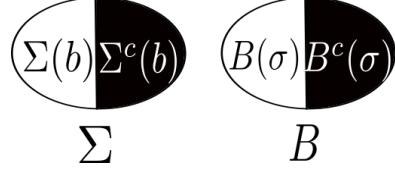


Figure 74.2:  $\Sigma(b)$  and  $\Sigma^c(b)$  are disjoint sets whose union is  $\Sigma$ .  $B(\sigma)$  and  $B^c(\sigma)$  are disjoint sets whose union is  $B$ .

Define (these definitions are illustrated in Fig.74.2)

$$\Sigma = \text{set}(L), \quad \Sigma(b) = \text{set}(L_b), \quad \Sigma^c(b) = \Sigma - \Sigma(b) \quad (74.5)$$

and

$$B(\sigma) = \{b \in B : \sigma \in \Sigma(b)\}, \quad B^c(\sigma) = B - B(\sigma) \quad (74.6)$$

$\Sigma(b)$  is the set of **in-the-b-bag individuals** and  $\Sigma^c(b)$  is the set of **out-of-the-b-bag (OOB) individuals**.  $B(\sigma)$  is the set of bags that contain individual  $\sigma$ , and  $B^c(\sigma)$  is the set of bags that don't.

The **OOB error** is defined as

$$\text{err} = \sum_{\sigma \in L} \mathbb{1}(B^c(\sigma) \neq \emptyset) \mathbb{1}(\text{ } y^\sigma \neq \text{majority}([Y_b(x^\sigma) : b \in B^c(\sigma)]) \text{ }) . \quad (74.7)$$

Empirical results supposedly show that OOB error is comparable in accuracy to the error calculated by doing cross-validation (CV) (see Chapter 13), although CV error is considered more dependable.

## 74.2 Bagging (with randomly-shortened bags)

Suppose the feature vector  $x^\sigma$  in the dataset  $DS = (\vec{x}, \vec{y})$  has  $nf$  components; i.e.,  $x^\sigma = (x_0^\sigma, x_1^\sigma, \dots, x_{nf-1}^\sigma) \in S_{\underline{x}_0} \times S_{\underline{x}_1} \times \dots \times S_{\underline{x}_{nf-1}} = S_{\underline{x}}$ .

For each bag  $DS_b$ , one chooses at random  $nf' = \sqrt{nf}$  out of the  $nf$  features, and discards the remaining features from  $DS_b$ , thus producing a new, **randomly-shortened-bag (rs-bag)**  $DS'_b$ . Each rs-bag is then used to train a bag-classifier, usually a dtree, using the methods for dtree SL described in Chapter 16. Using rs-bags is called the **random subspace method**. The reason for using rs-bags is that they further decorrelate the set of bags used to train bag-classifiers.

# Chapter 75

## Recurrent Neural Networks

This chapter is mostly based on Ref.[43].

This chapter assumes you are familiar with the material and notation of Chapter 64 on plain Neural Nets.

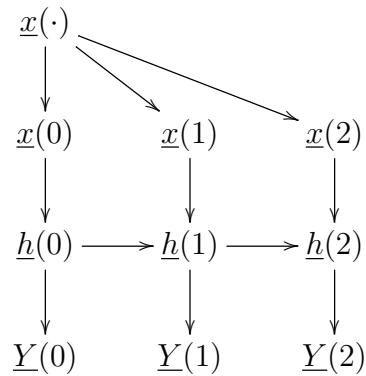


Figure 75.1: Simple example of RNN with  $T = 3$

Suppose

$T$  is a positive integer.

$t = 0, 1, \dots, T - 1$ ,

$\underline{x}_i(t) \in \mathbb{R}$  for  $i = 0, 1, \dots, nx - 1$ ,

$\underline{h}_i(t) \in \mathbb{R}$  for  $i = 0, 1, \dots, nh - 1$ ,

$\underline{Y}_i(t) \in \mathbb{R}$  for  $i = 0, 1, \dots, ny - 1$ ,

$W^{h|x} \in \mathbb{R}^{nh \times nx}$ ,

$W^{h|h} \in \mathbb{R}^{nh \times nh}$ ,

$W^{y|h} \in \mathbb{R}^{ny \times nh}$ ,

$b^y \in \mathbb{R}^{ny}$ ,

$b^h \in \mathbb{R}^{nh}$ .

Henceforth,  $x(\cdot)$  will mean the array of  $x(t)$  for all  $t$ .

The simplest kind of recurrent neural network (RNN) has the bnet Fig.75.1 with arbitrary  $T$ . The node TPMs, printed in blue, for this bnet, are as follows.

$$P(x(\cdot)) = \text{given} \quad (75.1)$$

$$P(x(t)) = \delta(x(t), [x(\cdot)]_t) \quad (75.2)$$

$$P(h(t) | h(t-1), x(t)) = \delta(h(t), \mathcal{A}(W^{h|x}x(t) + W^{h|h}h(t-1) + b^h)) , \quad (75.3)$$

where  $h(-1) = 0$ .

$$P(Y(t) | h(t)) = \delta(Y(t), \mathcal{A}(W^{y|h}h(t) + b^y)) \quad (75.4)$$

Define

$$W^h = [W^{h|x}, W^{h|h}, b^h] , \quad (75.5)$$

and

$$W^y = [W^{y|h}, b^y] . \quad (75.6)$$

The bnet of Fig.75.1 can be used for classification once its parameters  $W^h$  and  $W^y$  have been optimized. To optimize those parameters via gradient descent, one can use the bnet of Fig.75.2.

Let  $\sigma = 0, 1, \dots, nsam(\vec{x}) - 1$  be the labels for a batch of samples. Below, we will write  $A^\sigma = A[\sigma]$  for the  $\sigma$  component of any vector  $\vec{A}$ . The TPMs, printed in blue, for bnet Fig.75.2, are as follows.

$$P(x(\cdot)^\sigma) = \text{given} \quad (75.7)$$

$$P(x(t)^\sigma) = \delta(x(t)^\sigma, [x(\cdot)]_t^\sigma) \quad (75.8)$$

$$P(h(t)^\sigma | h(t-1)^\sigma, x(t)^\sigma) = \delta(h(t)^\sigma, \mathcal{A}(W^{h|x}x(t)^\sigma + W^{h|h}h(t-1)^\sigma + b^h)) \quad (75.9)$$

$$P(Y(t)^\sigma | h(t-1)^\sigma) = \delta(Y(t)^\sigma, \mathcal{A}(W^{y|h}h(t-1)^\sigma + b^y)) \quad (75.10)$$

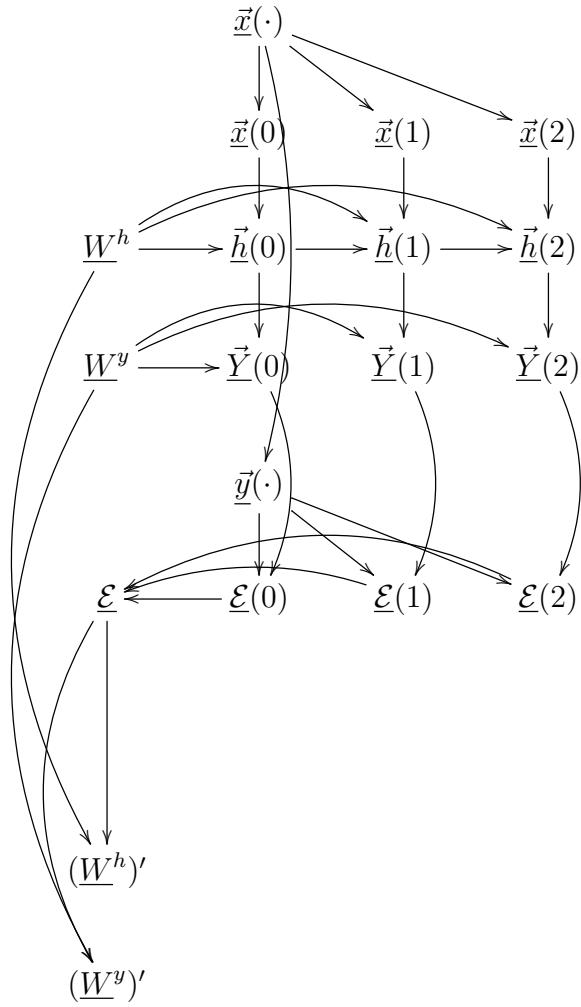


Figure 75.2: RNN bnet used to optimize parameters  $W^h$  and  $W^y$  of RNN bnet Fig.75.1.

$$P(y(\cdot)^\sigma | x(\cdot)^\sigma) = \text{given} \quad (75.11)$$

$$P(\mathcal{E}(t) | \vec{y}(t), \vec{Y}(t)) = \frac{1}{nsam(\vec{x})} \sum_{\sigma} d(y(t)^\sigma, Y(t)^\sigma) , \quad (75.12)$$

where

$$d(y, Y) = |y - Y|^2 . \quad (75.13)$$

If  $y, Y \in [0, 1]$ , one can use this instead

$$d(y, Y) = XE(y \rightarrow Y) = -y \ln Y - (1 - y) \ln(1 - Y). \quad (75.14)$$

$$P(\mathcal{E} | \mathcal{E}(\cdot)) = \delta(\mathcal{E}, \sum_t \mathcal{E}(t)) \quad (75.15)$$

For  $a = h, y$ ,

$$P(W^a) = \text{given}. \quad (75.16)$$

The first time it is used,  $W^a$  is arbitrary. Afterwards, it is determined by previous horizontal stage.

$$P((W^a)' | \mathcal{E}, W^a) = \delta((W^a)', W^a - \eta^a \partial_{W^a} \mathcal{E}). \quad (75.17)$$

$\eta^a > 0$  is the learning rate for  $W^a$ .

## 75.1 Language Sequence Modeling

Estimate  $P(x(\cdot))$  empirically. We can use this to:

- predict the probability of a sentence,  
example: Get  $P(x(0), x(1), x(2))$ .
- predict the most likely next word in a sentence,  
example: Get  $P(x(2)|x(0), x(1))$ .
- generate fake sentences.  
example:  
Get  $x(0) \sim P(x(0))$ .  
Next get  $x(1) \sim P(x(1)|x(0))$ .  
Next get  $x(2) \sim P(x(2)|x(0), x(1))$ .

## 75.2 Other types of RNN

Let  $\mathcal{T} = \{0, 1, \dots, T - 1\}$ , and  $\mathcal{T}^x, \mathcal{T}^y \subset \mathcal{T}$ . Above, we assumed that  $\underline{x}(t)$  and  $\underline{Y}(t)$  were both defined for all  $t \in \mathcal{T}$ . More generally, they might be defined only for subsets of  $\mathcal{T}$ :  $\underline{x}(t)$  for  $t \in \mathcal{T}^x$  and  $\underline{Y}(t)$  for  $t \in \mathcal{T}^y$ . If  $|\mathcal{T}^x| = 1$  and  $|\mathcal{T}^y| > 1$ , we say the RNN bnet is of the **1 to many** kind. In general, can have **1 to 1**, **1 to many**, **many to 1**, **many to many** RNN bnets.

Plain RNNs can suffer from the **vanishing or exploding gradients problem**. There are various ways to mitigate this (e.g., good choice of initial  $W^h$  and

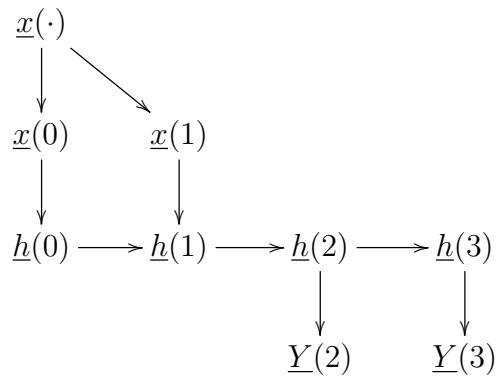


Figure 75.3: RNN bnet of the many to many kind. This one can be used for translation.  $x(0)$  and  $x(1)$  might denote two words of an English sentence, and  $Y(2)$  and  $Y(3)$  might be their Italian translation.

$W^y$ , good choice of activation functions, regularization). Or by using GRU or LSTM (discussed below). **GRU and LSTM** were designed to mitigate the vanishing or exploding gradients problem. They are very popular in NLP (Natural Language Processing).

### 75.2.1 Long Short Term Memory (LSTM) unit (1997)

This section is based on Wikipedia article Ref.[135]. In this section,  $\odot$  will denote the Hadamard matrix product (elementwise product).

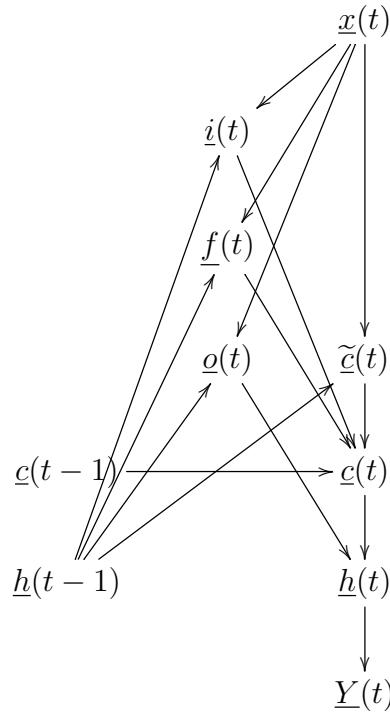


Figure 75.4: bnet for a Long Short Term Memory (LSTM) unit.

Let

$\underline{x}(t) \in \mathbb{R}^{nx}$ : **input state vector** to the LSTM unit

$\underline{f}(t) \in \mathbb{R}^{nh}$ : **forget activation vector**

$\underline{i}(t) \in \mathbb{R}^{nh}$ : **input activation vector**

$\underline{o}(t) \in \mathbb{R}^{nh}$ : **output activation vector**

$\underline{h}(t) \in \mathbb{R}^{nh}$ : **hidden state vector**

$\underline{\tilde{c}}(t) \in \mathbb{R}^{nh}$ : **cell activation vector**

$\underline{c}(t) \in \mathbb{R}^{nh}$ : **cell state vector**

$\underline{Y}(t) \in \mathbb{R}^{ny}$ : **classification** of  $\underline{x}(t)$ .

$\underline{W} \in \mathbb{R}^{nh \times nx}$ ,  $\underline{U} \in \mathbb{R}^{nh \times nh}$  and  $\underline{b} \in \mathbb{R}^{nh}$ : weight matrices and bias vectors, parameters learned by training.

$\mathcal{W}^{y|h} \in \mathbb{R}^{ny \times nh}$ : weight matrix

Fig.75.4 is a bnet for a LSTM unit. The TPMs, printed in blue, for this bnet, are as follows.

$$P(f(t)|x(t), h(t-1)) = \mathbb{1}(\quad f(t) = \text{smoid}(W^{f|x}x(t) + U^{f|h}h(t-1) + b^f) \quad ) , \quad (75.18)$$

where  $h(-1) = 0$ .

$$P(i(t)|x(t), h(t-1)) = \mathbb{1}(\quad i(t) = \text{smoid}(W^{i|x}x(t) + U^{i|h}h(t-1) + b^i) \quad ) \quad (75.19)$$

$$P(o(t)|x(t), h(t-1)) = \mathbb{1}(\quad o(t) = \text{smoid}(W^{o|x}x(t) + U^{o|h}h(t-1) + b^o) \quad ) \quad (75.20)$$

$$P(\tilde{c}(t)|x(t), h(t-1)) = \mathbb{1}(\quad \tilde{c}(t) = \tanh(W^{c|x}x(t) + U^{c|h}h(t-1) + b^c) \quad ) \quad (75.21)$$

$$P(c(t)|f(t), c(t-1), i(t), \tilde{c}(t)) = \mathbb{1}(\quad c(t) = f(t) \odot c(t-1) + i(t) \odot \tilde{c}(t) \quad ) \quad (75.22)$$

$$P(h(t)|o(t), c(t)) = \mathbb{1}(\quad h(t) = o(t) \odot \tanh(c(t)) \quad ) \quad (75.23)$$

$$P(Y(t)|h(t)) = \mathbb{1}(\quad Y(t) = \mathcal{A}(\mathcal{W}^{y|h}h(t) + b^y) \quad ) \quad (75.24)$$

### 75.2.2 Gated Recurrence Unit (GRU) (2014)

This section is based on Wikipedia article Ref.[116]. In this section,  $\odot$  will denote the Hadamard matrix product (elementwise product).

GRU is a more recent (17 years later) attempt at simplifying LSTM.

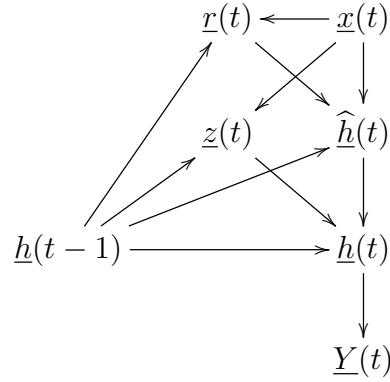


Figure 75.5: bnet for a Gated Recurrent Unit (GRU).

Let

$x(t) \in \mathbb{R}^{nx}$ : **input state** vector

$h(t) \in \mathbb{R}^{nh}$ : **hidden state** vector

$\hat{h}(t) \in \mathbb{R}^{nh}$ : **hidden activation** vector

$z(t) \in \mathbb{R}^{nh}$ : **update activation** vector

$r(t) \in \mathbb{R}^{nh}$ : **reset activation** vector

$Y(t) \in \mathbb{R}^{ny}$ : **classification** of  $x(t)$ .

$W \in \mathbb{R}^{nh \times nx}$ ,  $U \in \mathbb{R}^{nh \times nh}$  and  $b \in \mathbb{R}^{nh}$ : weight matrices and bias vectors, parameters learned by training.

$\mathcal{W}^{y|h} \in \mathbb{R}^{ny \times nh}$ : weight matrix

Fig.75.5 is a bnet for a GRU. The TPMs, printed in blue, for this bnet, are as follows.

$$P(z(t)|x(t), h(t-1)) = \mathbb{1}(\quad z(t) = \text{smoid}(W^{z|x}x(t) + U^{z|h}h(t-1) + b^z) \quad) , \quad (75.25)$$

where  $h(-1) = 0$ .

$$P(r(t)|x(t), h(t-1)) = \mathbb{1}(\quad r(t) = \text{smoid}(W^{r|x}x(t) + U^{r|h}h(t-1) + b^r) \quad) \quad (75.26)$$

$$P(\hat{h}(t)|x(t), r(t), h(t-1)) = \mathbb{1}(\quad \hat{h}(t) = \tanh(W^{h|x}x(t) + U^{h|h}(r(t) \odot h(t-1)) + b^h) \quad) \quad (75.27)$$

$$P(h(t)|z(t), h(t-1), \widehat{h}(t)) = \mathbb{1}(\quad h(t) = (1 - z(t)) \odot h(t-1) + z(t) \odot \widehat{h}(t) \quad ) \quad (75.28)$$

$$P(Y(t)|h(t)) = \mathbb{1}(\quad Y(t) = \mathcal{A}(\mathcal{W}^{y|h}h(t) + b^y) \quad ) \quad (75.29)$$

# Chapter 76

## Regression Discontinuity Design

This chapter is based on Ref.[12].

This chapter assumes that the reader has read Chapter 72 on Potential Outcomes (PO).

In Regression Discontinuity Design (RDD), one switches the treatment dose  $d$  from 0 when  $\underline{x} < \xi$  to 1 where  $\underline{x} > \xi$ , where  $\underline{x}$  is an observed confounder (call it the **switch confounder**) and  $\xi$  is a threshold value for  $\underline{x}$ . One measures the jump  $\delta$  in the treatment outcome  $y$  as  $\underline{x}$  passes through  $\underline{x} = \xi$ . Then one makes the very reasonable assumption that  $\delta$  equals<sup>1</sup>  $\mathcal{Y}_{1|x=\xi} - \mathcal{Y}_{0|x=\xi} = ATE|_{x=\xi}$  for an imaginary experiment in which the confounder  $\underline{x}$  acts as a normal confounder that doesn't switch the treatment dose  $d$ .

For example,  $d^\sigma$  might be whether an individual is admitted to Harvard Univ.,  $y^\sigma$  might be how much money the individual earns for the first 20 years after graduating from Harvard, and  $x^\sigma$  might be his SAT scores. We assume Harvard only admits students with an SAT score higher than  $\xi$ .

### 76.1 PO analysis

The TPMs, printed in blue, for the bnet  $G_{disc}$  shown in Fig.76.1, are as follows. Note that the TPMs for the bnet  $G_{disc}$  are defined in terms of the TPMs for the bnet  $G$ .

$$P(x^\sigma) = \delta(x^\sigma, x) \quad (76.1)$$

$$P(d^\sigma|x^\sigma = x) = \begin{cases} \delta(d^\sigma, 1) & \text{for } x > \xi \\ \delta(d^\sigma, 0) & \text{for } x < \xi \end{cases} \quad (76.2)$$

$$P(y^\sigma|y^\sigma(0), y^\sigma(1), d^\sigma) = \mathbb{1}(y^\sigma = y^\sigma(d^\sigma)) \quad (76.3)$$

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<sup>1</sup>ATE, which stands for “average treatment effect”, is defined in Chapter 72.

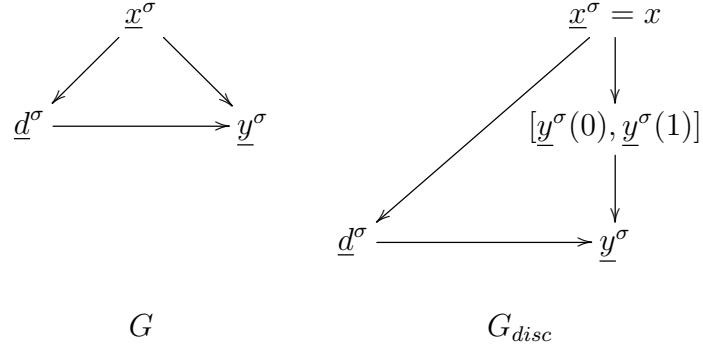


Figure 76.1: 2 bnets used in the PO analysis of RDD. The TPMs for  $G_{disc}$  are defined in terms of the TPMs for  $G$ . The TPM  $P(d^{\sigma}|x^{\sigma})$  for  $G_{disc}$  is discontinuous in  $x^{\sigma}$ .

$$P(y^{\sigma}(c)|x) = P(y^{\sigma}(c)|d^{\sigma}, x) = \text{given} \quad (76.4)$$

Define

$$E_{\sigma|x}[y^{\sigma}(c)] = E_{y(c)|x}[y(c)] = \mathcal{Y}_{c|x} \quad (76.5)$$

and

$$\xi^{\pm} = \xi \pm \epsilon \quad (76.6)$$

for some infinitesimal  $\epsilon > 0$ .

See Fig.76.2. In RDD, we assume that if we define the following 2  $\delta$ 's, one for bnet  $G$  and the other for bnet  $G_{disc}$ , then the two  $\delta$ 's are equal, and they equal a conditional ATE.

$$\delta_{G_{disc}} = \mathcal{Y}_{1|x=\xi+} - \mathcal{Y}_{0|x=\xi-} \quad (76.7)$$

$$\delta_G = \mathcal{Y}_{1|x=\xi} - \mathcal{Y}_{0|x=\xi} \quad (76.8)$$

$$\delta_G = \delta_{G_{disc}} = \delta \quad (76.9)$$

$$\delta = ATE|_{x=\xi} \quad (76.10)$$

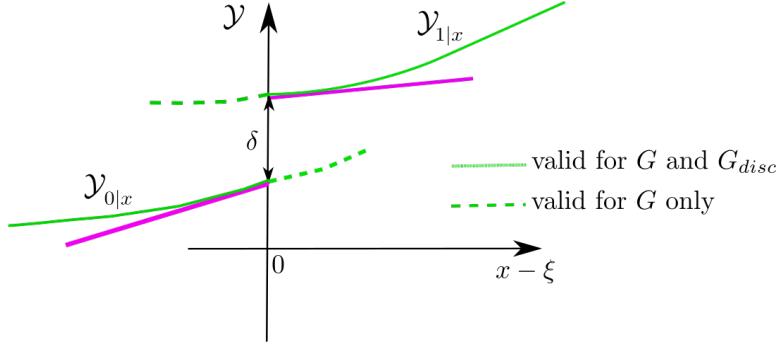


Figure 76.2: The jump  $\delta$  between  $\mathcal{Y}_{1|x}$  and  $\mathcal{Y}_{0|x}$  is the same for  $G$  and  $G_{disc}$ .

## 76.2 Linear Regression

In this section, we show how to apply linear regression (LR) to the PO analysis of RDD.

$y^\sigma$  can be fitted as a function of  $x \in \mathbb{R}$ , for  $c^\sigma \in \{0, 1\}$ , as follows. Here  $\epsilon^\sigma$  is the residual for individual  $\sigma$  and  $b_0, m_0, b_1, m_1 \in \mathbb{R}$  are the fit parameters.

$$y^\sigma = [b_0 + m_0(x - \xi)](1 - c^\sigma) + [b_1 + m_1(x - \xi)]c^\sigma + \epsilon^\sigma. \quad (76.11)$$

Note that Eq.(76.11) yields a straight line in the  $y^\sigma - x$  plane for  $c^\sigma = 0$ , and another straight line for  $c^\sigma = 1$ . These 2 lines are colored magenta in Fig.76.2. We are using the standard symbols  $b$  to denote the y-intercept, and  $m$  to denote the slope of a straight line.

Taking the expected value of Eq.(76.11), we get

$$\mathcal{Y}_{c|x} = [b_0 + m_0(x - \xi)](1 - c) + [b_1 + m_1(x - \xi)]c. \quad (76.12)$$

Hence,

$$\mathcal{Y}_{1|x=\xi+} = b_1, \quad \mathcal{Y}_{0|x=\xi-} = b_0 \quad (76.13)$$

$$\delta = b_1 - b_0 \quad (76.14)$$

# Chapter 77

## Regularization of Loss Functions

The topic of this chapter is Regularization of Loss functions (ROLF).

ROLF is the practice of adding a convex function  $\mathcal{R} : \mathbb{R}^n \rightarrow \mathbb{R}$  (called the **regulator function**<sup>1</sup>) to a convex function  $\mathcal{L} : \mathbb{R}^n \rightarrow \mathbb{R}$  (called the **loss function**<sup>2</sup>), when one wishes to minimize the loss function. In Machine Learning, the variable being minimized over is often the weights of a Neural Net, so we will denote it by  $w \in \mathbb{R}^n$ , and use  $w^* \in \mathbb{R}^n$  to represent the minimum of  $\mathcal{L}^+(w) = \mathcal{L}(w) + \mathcal{R}(w)$ .

In some cases (like in  $L^p$  norm ROLF, which we discuss below), the minimum of  $\mathcal{L}^+(w)$  and that of  $\mathcal{L}(w)$  are not the same but very close. In such cases, displacing the minimum of  $\mathcal{L}(w)$  might be done in order to avoid overfitting, or to spread out degenerate solutions, or to produce sparse solutions.

In other cases (like in proximal ROLF, which we discuss below), the minimum of  $\mathcal{L}^+(w)$  and that of  $\mathcal{L}(w)$  are the same. In such cases, ROLF might be done to improve the convergence properties of a sequence of points  $\{w_k\}_{k=0}^\infty$  such that  $w_k \rightarrow w^*$  as  $k \rightarrow \infty$ .

There are many methods of biasing the minimum of a convex function that don't involve adding a regulator function. For example, Early Stopping of training and Cross Validation for Neural Nets, or adding Latent Variables to a Bayesian Network. Or Constraint Optimization where hard equality and/or inequality constraints are imposed (as in Linear Programming, Lagrange multipliers, Khun-Tucker conditions, method of simple substitution of constraints). We won't discuss those types of ROLFs in this chapter<sup>3</sup>, except for a brief section on latent nodes at the end.

Loss functions commonly used in Statistics and Machine Learning (ML) are of the form

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<sup>1</sup>This function is also commonly called a **penalty function**. It can also be thought of, from a Bayesian perspective, as the log of a prior probability, and the loss function can be thought of as a log likelihood function.

<sup>2</sup>This function is also commonly called the **cost or error function**.

<sup>3</sup>ROLF that adds a regulator function (resp., doesn't add) is sometimes called **Explicit** (resp., **Implicit**) **regularization**.

$$\mathcal{L}(w) = \sum_{\sigma=1}^{nsam} \widehat{\mathcal{L}}(\widehat{y}_\sigma(x_\sigma, w), y_\sigma) \quad (77.1)$$

where the sum is over  $nsam$  samples. A common, more specific type of  $\mathcal{L}(w)$  is the **mean square error** which is given by

$$\mathcal{L}(w) = \frac{1}{nsam} \sum_{\sigma=1}^{nsam} \| \widehat{y}_\sigma(x_\sigma, w) - y_\sigma \|_2 \quad (77.2)$$

This loss function is convex, so it has a minimum:

$$\begin{cases} w^* = \underset{w}{\operatorname{argmin}} \mathcal{L}(w) \\ Loss = \min_w \mathcal{L}(w) = \mathcal{L}(w^*) \end{cases} \quad (77.3)$$

In ROLF, we add a regulator  $\mathcal{R}(w)$  to  $\mathcal{L}(w)$ :

$$\mathcal{L}^+(w) = \mathcal{L}(w) + \mathcal{R}(w) \quad (77.4)$$

## 77.1 $L^p$ norm ROLF

See C.5 for the definition of  $L^p$  norms. Let

$$\mathcal{L}^+(w) = \mathcal{L}(w) + \mathcal{R}(w) \quad (77.5)$$

Then, for  $\lambda, \lambda_1, \lambda_2 > 0$ ,

- $L^1$  norm ROLF (called LASSO or Basis Pursuit)

$$\mathcal{R}(w) = \lambda \| w \|_1 \quad (77.6)$$

- $L^2$  norm ROLF (called Ridge or Tikhonov Regression) (note that the  $L^2$  norm is squared)

$$\mathcal{R}(w) = \lambda \| w \|_2^2 \quad (77.7)$$

- $L^1 + L_2$  norm ROLF (called Elastic Net)

$$\mathcal{R}(w) = \lambda_1 \| w \|_1 + \lambda_2 \| w \|_2^2 \quad (77.8)$$

### 77.1.1 $L^1$ norm ROLF can lead to sparsity

The obvious way to induce sparsity in the minimum  $w^*$  is to use the  $L^0$  norm of  $w$  as regulator. However, calculating  $\| w \|_0$  is hard (NP-hard, in fact). In this section, we will show that using the  $L^1$  norm of  $w$  as regulator can also induce sparsity (not as well as the  $L^0$  norm, but still significant.)

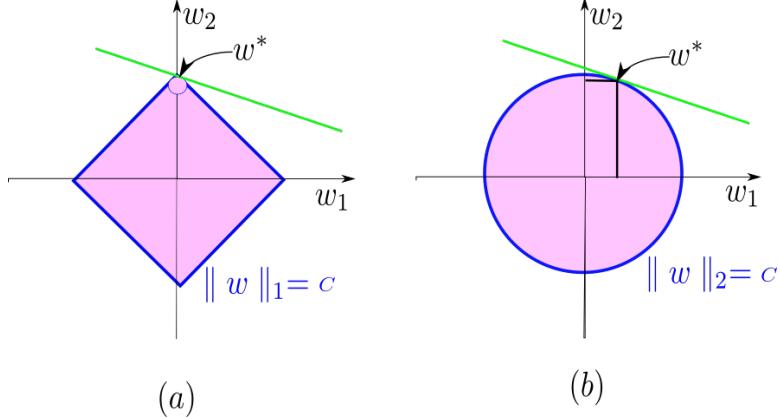


Figure 77.1: Pictorial explanation of why  $L^1$  norm ROLF can lead to sparsity and  $L^2$  norm ROLF can help avert it. Sometimes you want sparsity and sometimes you don't.  $c$  in this figure is some fixed constant.

Assume  $\mathcal{L}(w)$  is linear in  $w$ .<sup>4</sup> For example,

$$\mathcal{L}(w) = Xw - y \quad (77.9)$$

where  $w \in \mathbb{R}^n$ ,  $X \in \mathbb{R}^{nsam \times n}$ , and  $y \in \mathbb{R}^{nsam}$ .  $nsam$  is often the number of samples. That's why we name it that way. The set  $A = \{w : Xw - y = c\}$  for some fixed constant  $c$  might be empty, or contain a single point or a line or a plane, or a hyperplane. Let  $dof = n - nsam$  be the degrees of freedom in  $w$ . Barring some exceptional cases, if  $dof \leq 0$ , we expect  $A$  to be empty. If  $dof = 1$ , we expect  $A$  to trace out a line, if  $dof = 2$ , we expect  $A$  to trace out a plane, and so forth.

In Fig.77.1, we imagine what would happen if  $w \in \mathbb{R}^2$ ,  $X \in \mathbb{R}^{1 \times 2}$  and  $y \in \mathbb{R}$  so  $A$  traces a line, represented in green. In Fig.77.1 (a), we imagine that  $\mathcal{R}(w) = \|w\|_1$  and in Fig.77.1 (b), that  $\mathcal{R}(w) = \|w\|_2^2$ . For points  $w$  such that  $\mathcal{R}(w)$  has a well defined gradient, minimization of

$$\mathcal{L}^+(w) = \mathcal{L}(w) + \mathcal{R}(w) \quad (77.10)$$

requires that the  $w$ -gradients of  $\mathcal{L}$  and  $\mathcal{R}$  be equal in magnitude but opposite in direction.

$$\nabla_w \mathcal{L} = -\nabla_w \mathcal{R} \quad (77.11)$$

But when  $\mathcal{R}(w)$  is the  $L^1$  norm,  $\nabla_w \mathcal{R}$  is not defined along the  $w_1$  and  $w_2$  axes. To avoid this, we can approximate the diamond contour  $\|w\|_1 = c$  by rounding out its corners by an infinitesimal amount. If the green line had slope of  $-1$ , there would be a diamond contour  $\|w\|_1 = c$  that would coincide with the green line along the

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<sup>4</sup>What we say here about sparsity also applies in some cases when  $\mathcal{L}(w)$  is not linear in  $w$ . For example, it applies sometimes when  $\mathcal{L}(w)$  is quadratic in  $w$  as occurs in Least Squares.

segment connecting points  $(0, c)$  and  $(c, 0)$ . However, this is an exceptional case. Usually, the slope of the green line is not  $\pm 1$ . In that case, the only way for  $\mathcal{L}$  and  $\mathcal{R}$  to have opposite gradients is if the diamond contour and the green line kiss at one of the (rounded) corners of the diamond contour. Call that kissing point  $w^*$ . Note from Fig.77.1 (a) that that kissing point  $w^* = (0, c)$  would be sparse. In going from the Fig.77.1 (a) to Fig.77.1 (b), we have replaced the diamond contour  $\|w\|_1 = c$  by a circular contour  $\|w\|_2 = c$ , but we have kept the same green line. Note that with the circular contour, the kissing point  $w^*$  is no longer sparse; both of its components are non-zero.

The moral of Fig.77.1 is that  $L^1$  norm ROLF can lead to sparsity and  $L^2$  norm ROLF can help avert it. Sometimes we want the vector of weights  $w$  to be sparse so as to give a succinct description. At other times, we want solutions in set  $A$  to be spread out over many dimensions instead of being sparse and clumped together in a small number of dimensions.

### 77.1.2 $L^2$ norm ROLF for Least Squares

As in Section C.27 on Linear Regression, suppose  $w \in \mathbb{R}^n$ ,  $X \in \mathbb{R}^{nsam \times n}$ , and  $y \in \mathbb{R}^{nsam}$ . Let

$$\mathcal{L}^+(w) = \mathcal{L}(w) + \mathcal{R}(w) \quad (77.12)$$

where

$$\mathcal{L}(w) = \frac{1}{n}(Xw - y)^T(Xw - y) \quad (77.13)$$

and

$$\mathcal{R}(w) = \lambda \|w\|_2^2. \quad (77.14)$$

If we vary the vector  $w$  by an infinitesimal amount  $\delta w^T$ , we get

$$0 = \delta \mathcal{L}^+(w) = \delta w^T \left[ \frac{2X^T}{n}(Xw - y) + 2\lambda w \right] \quad (77.15)$$

Hence

$$X^T(Xw - y) + \lambda nw = 0 \quad (77.16)$$

$$(X^T X + \lambda n)w = X^T y \quad (77.17)$$

$$w = (X^T X + \lambda n I)^{-1} X^T y \quad (77.18)$$

$$= \frac{1}{\lambda n} (I + \frac{X^T X}{\lambda n})^{-1} X^T y \quad (77.19)$$

Note that for  $\lambda = 0$ , the minimum  $w^*$  of  $\mathcal{L}^+(w)$  is

$$w^* = (X^T X)^{-1} X^T y \quad (\text{valid for } \lambda = 0) \quad (77.20)$$

When  $\lambda \gg 1$ , we can express  $w^*$  as a Taylor expansion in  $w$ . Recall that if  $|\epsilon| < 1$ ,

$$\frac{1}{1 - \epsilon} = 1 + \epsilon + \epsilon^2 + \dots \quad (77.21)$$

Define  $n_0 = 1/\lambda$ , and assume that  $\frac{n_0}{n}|X^T X| < 1$ . Then

$$w^* = \frac{n_0}{n} \sum_{i=0}^{\infty} \left( -\frac{n_0 X^T X}{n} \right)^i X^T y \quad (77.22)$$

$$= - \sum_{i=0}^{\infty} \left( -\frac{n_0 X^T X}{n} \right)^{i+1} (X^T X)^{-1} X^T y \quad (\text{valid for } \lambda = \frac{1}{n_0} \gg 1) \quad (77.23)$$

Truncating this series is itself a kind of regularization.

## 77.2 Proximal functions

For  $v \in \mathbb{R}^n$ ,  $w \in \mathbb{W} \subset \mathbb{R}^n$  and  $\alpha > 0$ , we define the **proximal function**  $w^{prox} : \mathbb{R}^n \rightarrow \mathbb{W}$  by

$$w^{prox}(v; \alpha \mathcal{L}, \mathbb{W}) = \underset{w \in \mathbb{W}}{\operatorname{argmin}} \underbrace{\left( \mathcal{L}(w) + \underbrace{\frac{1}{2\alpha} \|w - v\|^2}_{\mathcal{R}(w, v)} \right)}_{\mathcal{L}^+(w, v)} \quad (77.24)$$

$w^{prox}(v)$  can be viewed as a projection of  $v \in \mathbb{R}^n$  onto  $w$  in the subspace  $\mathbb{W} \subset \mathbb{R}^n$ . Henceforth we assume  $\mathbb{W} = \mathbb{R}^n$ , so the projected vector  $v$  and its projection  $w$  are in the same vector space  $\mathbb{R}^n$ .

See Fig.77.2 for a numerical example of a proximal function  $w^{prox} : \mathbb{R} \rightarrow \mathbb{R}$ .

Next, we will discuss an analytical rather a numerical example of proximal functions. We begin by defining the shrinking function<sup>5</sup>  $sh_0 : \mathbb{R} \rightarrow \mathbb{R}$  and its inverse  $sh_0^{-1} : \mathbb{R} \rightarrow \mathbb{R}$  for any  $\alpha > 0$ :

$$sh_0(v; \alpha) = (v - \alpha)\mathbb{1}(v > \alpha) + (v + \alpha)\mathbb{1}(v < -\alpha) \quad (77.25)$$

---

<sup>5</sup>We call it a **shrinking function** because it shrinks a neighborhood-of-zero to zero. Another common name for this function is a **soft-threshold function**, because it makes the transition from negative to positive y axis values occur over the interval of  $x \in [-\alpha, \alpha]$  instead of  $x \in [0, 0]$ .

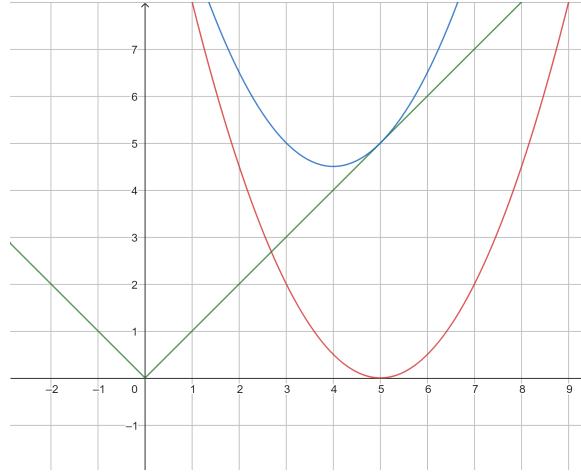


Figure 77.2: Example of a proximal function. x-axis is  $w$  and  $v = 5$ . Green curve:  $\mathcal{L}(w) = |w|$ . Red curve:  $\mathcal{R}(w, 5) = \frac{1}{2}(w-5)^2$ , Blue curve:  $\mathcal{L}^+(w, 5) = \mathcal{L}(w) + \mathcal{R}(w, 5)$ . Note that we are adding 2 convex functions so the minimum of the sum is somewhere in between the minima of the two summands.  $w^{prox}(5) = \operatorname{argmin}_w \mathcal{L}^+(w, 5) = 4$ .

$$sh_0^{-1}(w; \alpha) = (w + \alpha)\mathbb{1}(w > 0) + (w - \alpha)\mathbb{1}(w < 0) \quad (77.26)$$

Fig.77.3 shows a plot of  $sh_0$  and  $sh_0^{-1}$ .

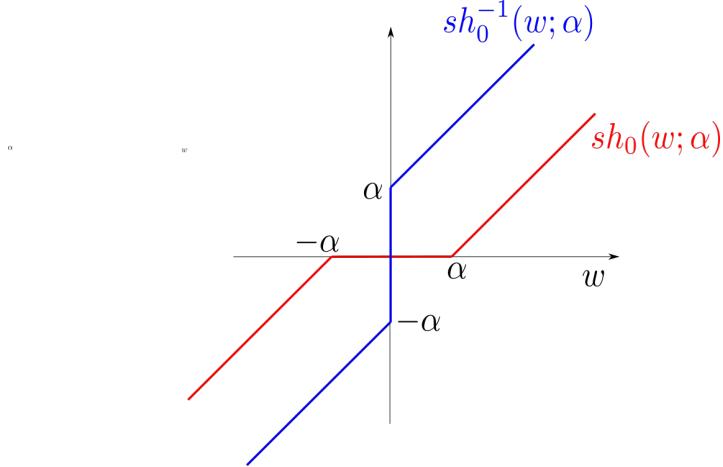


Figure 77.3: Plot of the functions  $sh_0(w; \alpha)$  and  $sh_0^{-1}(w; \alpha)$ .

**Claim 124** For  $\mathbb{W} = \mathbb{R}$  and  $w, v \in \mathbb{R}$ , if

$$\mathcal{L}(w) = |w|, \quad (77.27)$$

then

$$w^{prox}(v) = sh_0(v; \alpha) \quad (77.28)$$

and

$$\mathcal{L}^+(w^{prox}(v), v) = |sh_0(v; \alpha)| + \frac{\alpha}{2} \quad (77.29)$$

**proof:**

$$0 = \frac{d\mathcal{L}^+}{dw} = \alpha[\mathbb{1}(w > 0) - \mathbb{1}(w < 0)] + (w - v) \quad (77.30)$$

So

$$v = w + \alpha[\mathbb{1}(w > 0) - \mathbb{1}(w < 0)] \quad (77.31)$$

$$= (w + \alpha)\mathbb{1}(w > 0) + (w - \alpha)\mathbb{1}(w < 0) \quad (77.32)$$

$$= sh_0^{-1}(w; \alpha) \quad (77.33)$$

Hence

$$w^{prox}(v; \alpha) = sh_0(v; \alpha) \quad (77.34)$$

Note that

$$|w - v| = |\alpha| \quad (77.35)$$

so

$$\mathcal{L}^+(w^{prox}(v), v) = |w^{prox}(v; \alpha)| + \frac{\alpha}{2} \quad (77.36)$$

$$= |sh_0(v; \alpha)| + \frac{\alpha}{2} \quad (77.37)$$

**QED**

### 77.3 Proximal ROLF

Proximal functions can be used to do ROLF as follows. For  $w, v \in \mathbb{R}^n$  and  $\alpha > 0$ , let

$$\mathcal{R}(w, v) = \frac{1}{2\alpha} \|w - v\|_2^2 \quad (77.38)$$

and<sup>6</sup>

$$\mathcal{L}^+(w) = \mathcal{L}(w) + \mathcal{R}(w, w^*) , \quad (77.39)$$

---

<sup>6</sup>Note that  $\mathcal{L}$  here could be the mean square error plus an  $L^p$  norm. A loss function plus a regulator function gives a new loss function to which a new regulator may be added.

where  $w^*$  is the  $w$ -minimum of both  $\mathcal{L}(w)$  and  $\mathcal{R}(w, w^*)$ :

$$w^* = \operatorname{argmin}_w \mathcal{L}(w) = \operatorname{argmin}_w \mathcal{R}(w, w^*) \quad (77.40)$$

Hence,

$$w^* = \operatorname{argmin}_w [\mathcal{L}(w) + \mathcal{R}(w, w^*)] . \quad (77.41)$$

Now assume the sequence of points  $\{w_k\}_{k=0}^\infty$  satisfies  $w_k \rightarrow w^*$  as  $k \rightarrow \infty$ . Then

$$w_{k+1} = \underbrace{\operatorname{argmin}_w \left( \mathcal{L}(w) + \frac{1}{2\alpha} \|w - w_k\|_2^2 \right)}_{w^{prox}(w_k)} \quad (77.42)$$

If we differentiate the argument of  $\operatorname{argmin}()$  to find its minimum, we find

$$0 = \alpha \underbrace{\nabla_w \mathcal{L}(w_{k+1})}_{\approx \nabla_w \mathcal{L}(w_k)} + w_{k+1} - w_k \quad (77.43)$$

Thus, the following 3 recursion relations<sup>7</sup> can be used to calculate  $w_k$ :

$$\boxed{w_{k+1} = w_k - \alpha \nabla_w \mathcal{L}(w_k)} \quad (77.44a)$$

$$\boxed{w_{k+1} = w^{prox}(w_k)} \quad (77.44b)$$

$$\boxed{w_{k+1} = w^{prox}(w_k - \alpha \nabla_w \mathcal{L}(w_k))} \quad (77.44c)$$

Eq.(77.44a) is the familiar recursion relation for gradient descent (See Chapter 35). Eq.(77.44c) combines gradient descent and a proximal projection, so it is expected to converge faster than simple gradient descent.

## 77.4 Unobserved Nodes of a bnet

Nodes of a bnet for which the CPT is unknown are called unobserved nodes. In this book, Unobserved (a.k.a. hidden, latent) nodes are indicated in a bnet by enclosing their label in a dashed circle. For example,  $(\bar{u})$ . Alternatively, they are indicated by using dashed arrows for all arrows emanating from the unobserved node.

**Unobserved nodes (UN)** represent what are called **latent random variables** in Statistics.

---

<sup>7</sup>Some people use a sequence  $\alpha_k \in \mathbb{R}_+$  instead of the constant  $\alpha > 0$ . This is called an **adaptive step size** and can yield faster convergence rates.

UN make an appearance in many places throughout this book. For example, they are essential to the methods of Kalman Filtering (see Chapter 44) and Hidden Markov Model (see Chapter 37).

This being a book about bnets and a chapter about ROLF, we would like to stress that UN can be viewed as a very natural and powerful way of doing (implicit) ROLF when using bnets.

# Chapter 78

## Reinforcement Learning (RL)

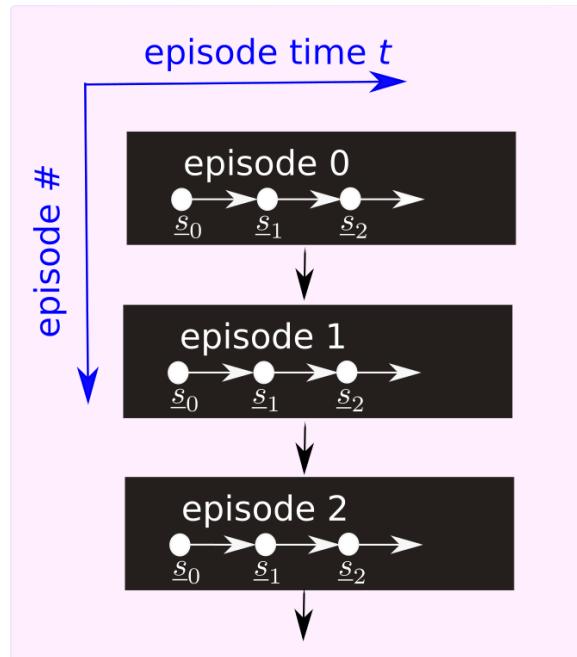


Figure 78.1: Axes for episode time and episode number.

I based this chapter on the following references. Refs.[16][33]

In RL, we consider an “agent” or robot that is learning.

Let  $T \in \mathbb{Z}_{>0}$  be the duration time of an **episode** of learning. If  $T = \infty$ , we say that the episode has an infinite time horizon. A learning episode will evolve towards the right, for times  $t = 0, 1, \dots, T - 1$ . We will consider multiple learning episodes. The episode number will evolve from top to bottom. This is illustrated in Fig.78.1.

Let  $\underline{s}_t \in S_s$  for  $t \in \mathbb{Z}_{[0,T-1]}$  be random variables that record the **state** of the agent at various times  $t$ .

Let  $\underline{a}_t \in S_a$  for  $t \in \mathbb{Z}_{[0,T-1]}$  be random variables that record the **action** of the agent at various times  $t$ .

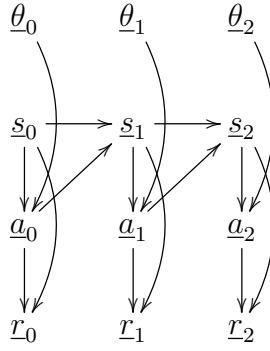


Figure 78.2: State-Action-Reward dynamical bnet

Let  $\underline{\theta}_t \in S_\theta$  for  $t \in \mathbb{Z}_{[0,T-1]}$  be random variables that record the **policy parameters** at various times  $t$ .

For  $\underline{X} \in \{\underline{s}, \underline{a}, \underline{\theta}\}$ , define  $\underline{X}$  followed by a dot to be the vector

$$\underline{X}_\cdot = [\underline{X}_0, \underline{X}_1, \dots, \underline{X}_{T-1}] . \quad (78.1)$$

Also let

$$\underline{X}_{\geq t} = [\underline{X}_t, \underline{X}_{t+1}, \dots, \underline{X}_{T-1}] . \quad (78.2)$$

Fig.78.2 shows the basic State-Action-Reward bnet for an agent that is learning. The TPMs, printed in blue, for the bnet Fig.78.2, are as follows.

$$P(a_t|s_t, \theta_t) = \text{given.} \quad (78.3)$$

$P(a_t|s_t, \theta_t)$  is called a **policy with parameter**  $\theta_t$ .

$$P(s_t|s_{t-1}, a_{t-1}) = \text{given.} \quad (78.4)$$

$P(s_t|s_{t-1}, a_{t-1})$  is called the **TPM of the model**.  $P(s_t|s_{t-1}, a_{t-1})$  reduces to  $P(s_0)$  when  $t = 0$ .

$$P(r_t|s_t, a_t) = \delta(r_t, r(s_t, a_t)) . \quad (78.5)$$

$r : S_s \times S_a \rightarrow \mathbb{R}$  is a given **one-time reward function**.

Note that

$$P(s_\cdot, a_\cdot | \theta_\cdot) = \prod_{t=0}^{T-1} \{P(s_t|s_{t-1}, a_{t-1})P(a_t|s_t, \theta_t)\} . \quad (78.6)$$

Define the **all times reward**  $\Sigma$  by

$$\Sigma(s., a.) = \sum_{t=0}^{T-1} \gamma^t r(s_t, a_t) . \quad (78.7)$$

Here  $0 < \gamma < 1$ .  $\gamma$ , called the **discount rate**, is included to assure convergence of  $\Sigma$  when  $T \rightarrow \infty$ . If  $r(s_t, a_t) < K$  for all  $t$ , then  $\Sigma < K \frac{1}{1-\gamma}$ .

Define the **objective (i.e., goal) function**  $E\Sigma(\theta.)$  by

$$E\Sigma(\theta.) = E_{\underline{s}.,\underline{a}.|\theta.} \Sigma(\underline{s}.,\underline{a}.) = \sum_{s.,a.} P(s.,a.|\theta.) \Sigma(s.,a.) \quad (78.8)$$

The goal of RL is to maximize the objective function over its parameters  $\theta..$ . The parameters  $\theta^*$ . that maximize the objective function are the optimum strategy:

$$\theta.^* = \operatorname{argmax}_{\theta.} E\Sigma(\theta.) \quad (78.9)$$

Define a **future reward** for times  $\geq t$  as:

$$\Sigma_{\geq t}((s_{t'}, a_{t'})_{t' \geq t}) = \sum_{t'=t}^{T-1} \gamma^{t'-t} r(s_{t'}, a_{t'}) \quad (78.10)$$

Define the following **expected conditional future rewards** (rewards for times  $\geq t$ , conditioned on certain quantities having given values):

$$v_t = v(s_t, a_t; \theta.) = E_{\underline{s}.,\underline{a}.|s_t,a_t,\theta.} [\Sigma_{\geq t}] \quad (78.11)$$

$$V_t = V(s_t; \theta.) = E_{\underline{s}.,\underline{a}.|s_t,\theta.} [\Sigma_{\geq t}] = E_{\underline{a}_t|s_t,\theta.} [v(s_t, \underline{a}_t; \theta.)] \quad (78.12)$$

$v$  is usually called  $Q$  in the literature. We will refer to  $Q$  as  $v$  in order to follow a convention wherein an  $\underline{a}_t$ -average changes a lower case letter to an upper case one.

We will sometimes write  $v(s_t, a_t)$  instead of  $v(s_t, a_t; \theta.).$

Since  $E\Sigma_{\geq t}$  only depends on  $\theta_{\geq t}$ ,  $v(s_t, a_t; \theta.) = v(s_t, a_t; \theta_{\geq t})$ , and  $V(s_t; \theta.) = V(s_t; \theta_{\geq t})$ .

Note that the objective function  $E\Sigma$  can be expressed in terms of  $v_0$  by averaging over its unaveraged parameters:

$$E\Sigma(\theta.) = E_{\underline{s}_0,\underline{a}_0|\theta_0} v(\underline{s}_0, \underline{a}_0; \theta.) \quad (78.13)$$

Define a **one-time reward** and an **expected conditional one-time reward** as:

$$r_t = r(s_t, a_t) \quad (78.14)$$

$$R_t = R(s_t; \theta_t) = E_{\underline{a}_t|s_t,\theta_t} [r(s_t, \underline{a}_t)] . \quad (78.15)$$

Note that

$$\Sigma_{\geq t} = r_t + \gamma r_{t+1} + \gamma^2 r_{t+2} + \dots + \gamma^{T-1-t} r_{t+(T-1-t)} \quad (78.16)$$

$$= r_t + \gamma \Sigma_{\geq t+1}; \quad (78.17)$$

If we take  $E_{s., a.|s_t, a_t, \theta.}[\cdot]$  of both sides of Eq.(78.17), we get

$$v_t = r_t + \gamma E_{s_{t+1}, a_{t+1} | \theta.}[v_{t+1}] . \quad (78.18)$$

If we take  $E_{s., a.|s_t, \theta.}[\cdot]$  of both sides of Eq.(78.17), we get

$$V_t = R_t + \gamma E_{s_{t+1} | \theta.}[V_{t+1}] . \quad (78.19)$$

Note that

$$\Delta r_t = r_t - R_t \quad (78.20)$$

$$= r_t - (V_t - \gamma E_{s_{t+1} | \theta.}[V_{t+1}]) \quad (78.21)$$

$$= r_t + \gamma E_{s_{t+1} | \theta.}[V_{t+1}] - V_t . \quad (78.22)$$

Define

$$\Delta v_t = v_t - V_t . \quad (78.23)$$

Note that

$$\Delta v_t = \Delta r_t . \quad (78.24)$$

Next, we will discuss 3 RL bnets

- exact RL bnet (exact, assumes policy is known)
- Actor-Critic RL bnet (approximate, assumes policy is known)
- Q function learning RL bnet (approximate, assumes policy is NOT known)

## 78.1 Exact RL bnet

An exact RL bnet is given by Fig.78.3.

Fig.78.3 is the same as Fig.78.2 but with more nodes added in order to optimize the policy parameters. The TPMs, printed in blue, for the nodes not already discussed in connection to bnet Fig.78.2, are as follows.

$$P(\theta_t | \theta.) = \delta(\theta_t, (\theta.)_t) \quad (78.25)$$

$$\forall (s_t, a_t) : P(v_t(s_t, a_t) | r_t, v_{t+1}(\cdot), \theta.) = \delta(v_t(s_t, a_t), r_t + \gamma E_{s_{t+1}, a_{t+1} | \theta.}[v_{t+1}]) \quad (78.26)$$

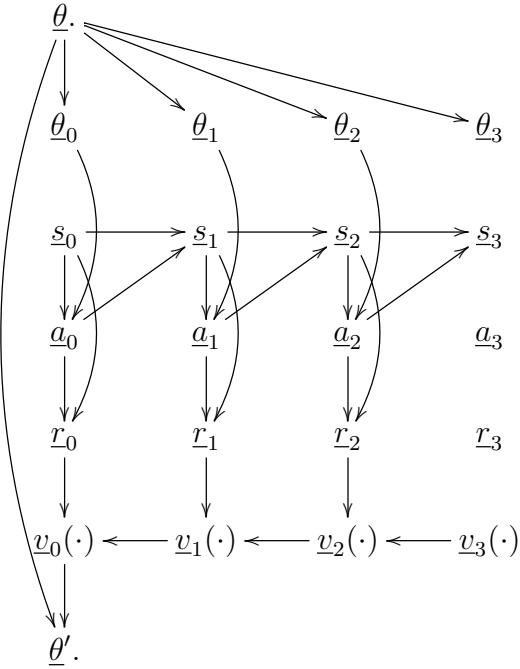


Figure 78.3: Exact RL bnet.  $v_t(\cdot)$  means the array  $[v_t(s_t, a_t)]_{\forall s_t, a_t}$  The following arrows are implicit: for all  $t$ , arrow from  $\underline{\theta}.$   $\rightarrow \underline{v}_t(\cdot)$ . We did not draw those arrows so as not to clutter the diagram.

$$P(\theta' | \theta, v_0(\cdot)) = \delta(\theta', \theta + \alpha \partial_{\theta} \underbrace{E_{\underline{s}_0, \underline{a}_0 | \theta_0} v(\underline{s}_0, \underline{a}_0; \theta)}_{E\Sigma(\theta)}) \quad (78.27)$$

$\alpha > 0$  is called the **learning rate**. This method of improving  $\theta$ . is called gradient ascent.

Concerning the gradient of the objective function, note that

$$\partial_{\theta_t} E\Sigma(\theta) = \sum_{s., a.} \partial_{\theta_t} P(s., a. | \theta.) \Sigma(s., a.) \quad (78.28)$$

$$= \sum_{s., a.} P(s., a. | \theta.) \partial_{\theta_t} \ln P(s., a. | \theta.) \Sigma(s., a.) \quad (78.29)$$

$$= E_{\underline{s}, \underline{a} | \theta.} \{ \partial_{\theta_t} \ln P(a_t | s_t, \theta_t) \Sigma(s., a.) \} . \quad (78.30)$$

If we run the agent  $nsam(\vec{s}_t)$  times and obtain samples  $s_t[i], a_t[i]$  for all  $t$  and for  $i = 0, 1, \dots, nsam(\vec{s}_t) - 1$ , we can express this gradient as follows:

$$\partial_{\theta_t} E\Sigma(\theta) \approx \frac{1}{nsam(\vec{s}_t)} \sum_i \sum_{t=0}^{T-1} \partial_{\theta_t} \ln P(a_t[i] | s_t[i], \theta_t) r(s_t[i], a_t[i]) . \quad (78.31)$$

The exact RL bnet Fig.78.3 is difficult to use to calculate the optimum parameters  $\theta^*$ . The problem is that  $\underline{s}_t$  propagates towards the future and the  $\underline{v}_t(\cdot)$  propagates towards the past, so we don't have a Markov Chain with a chain link for each  $t$  (i.e., a dynamical bnet) in the episode time direction. Hence, people have come up with approximate RL bnets that are doubly dynamical (i.e., dynamical along the episode time and episode number axes.) We discuss some of those approximate RL bnets next.

## 78.2 Actor-Critic RL bnet

For the actor-critic RL bnet, we approximate Eq.(78.31) by

$$\partial_{\theta_t} E\Sigma(\theta) \approx \frac{1}{nsam(\vec{s})} \sum_i \sum_{t=0}^{T-1} \underbrace{\partial_{\theta_t} \ln P(a_t[i] | s_t[i], \theta_t)}_{Actor} \underbrace{\Delta r_t(s_t[i], a_t[i])}_{Critic} \quad (78.32)$$

The actor-critic RL bnet is given by Fig.78.4. This bnet is approximate and assumes that the policy is known. The TPMs, printed in blue, for this bnet, are as follows.

$$P(\theta_t) = \text{given} \quad (78.33)$$

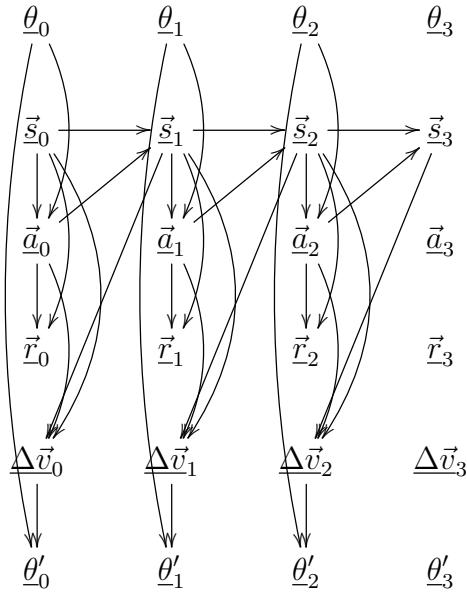


Figure 78.4: Actor-Critic RL bnet.

$$P(s_t[i] | s_{t-1}[i], a_{t-1}[i]) = \text{ given} \quad (78.34)$$

$$P(a_t[i] | s_t[i], \theta_t) = \text{ given} \quad (78.35)$$

$$P(r_t[i] | s_t[i], a_t[i]) = \delta(r_t[i], r(s_t[i], a_t[i])) \quad (78.36)$$

$r : S_{\underline{s}} \times S_{\underline{a}} \rightarrow \mathbb{R}$  is given.

$$P(\Delta v_t[i] | s_t[i], a_t[i], s_{t+1}[i]) = \delta(\Delta v_t[i], r(s_t[i], a_t[i]) + \gamma \widehat{V}(s_{t+1}[i]; \phi') - \widehat{V}(s_t[i]); \phi) . \quad (78.37)$$

$$P(\theta'.) = \delta(\theta', \theta_t + \alpha \partial_{\theta_t} \sum_i \ln P(a_t[i] | s_t[i], \theta_t) \Delta v_t[i]) \quad (78.38)$$

$\widehat{V}(s_t[i]; \phi)$  is obtained by curve fitting (see Chapter 35) using samples  $(s_t[i], a_t[i])$   $\forall t, i$  with

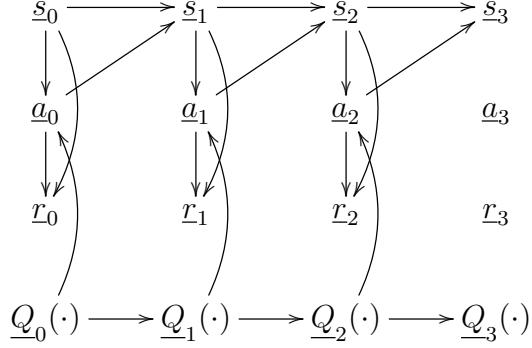


Figure 78.5: Q function learning RL bnet.

$$y[i] = \sum_{t'=t}^T r(s_{t'}[i], a_{t'}[i]) \quad (78.39)$$

and

$$\hat{y}[i] = \hat{V}(s_t[i]; \phi) . \quad (78.40)$$

Eq.(78.39) is an approximation because  $(s_{t'}, a_{t'})_{t'>t}$  are averaged over in the exact expression for  $V(s_t)$ .  $\hat{V}(s_{t+1}[i]); \phi'$  is obtained in the same way as  $\hat{V}(s_t[i]); \phi$  but with  $t$  replaced by  $t + 1$  and  $\phi$  by  $\phi'$ .

### 78.3 Q function learning RL bnet

The Q-function learning RL bnet is given by Fig.78.5. This bnet is approximate and assumes that the policy is NOT known. The TPMs, printed in blue, for this bnet, are as follows. (Remember that  $Q = v$ ).

$$P(s_t | s_{t-1}, a_{t-1}) = \text{given} \quad (78.41)$$

$$P(a_t | s_t, v_t(\cdot)) = \delta(a_t, \operatorname{argmax}_a v_t(s_t, a)) \quad (78.42)$$

$$P(r_t | s_t, a_t) = \delta(r_t, r(s_t, a_t)) \quad (78.43)$$

$r : S_s \times S_a \rightarrow \mathbb{R}$  is given.

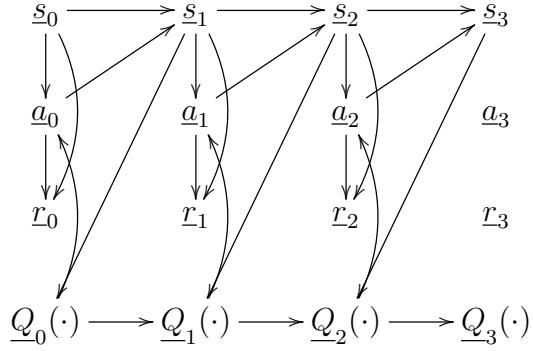


Figure 78.6: Q function learning RL bnet. Same as Fig.78.5 but with new arrow passing \$s\_t\$ to \$\underline{Q}\_{t-1}\$.

$$\begin{aligned} \forall(s_t, a_t) : P(v_t(s_t, a_t) | v_{t-1}(\cdot)) = \\ = \delta(v_t(s_t, a_t), r(s_t, a_t) + \gamma \max_a E_{s_{t+1}|s_t, a_t} v_{t-1}(s_{t+1}, a)) \end{aligned} \quad (78.44)$$

This value for \$v\_t(s\_t, a\_t)\$ approximates \$v\_t = r\_t + \gamma E\_{s\_{t+1}|s\_t, a\_t} v\_{t+1}\$.

Some people use the bnet of Fig.78.6 instead of Fig.78.5 and replace Eq.(78.44) by

$$\begin{aligned} \forall(s_t, a_t) : P(v_t(s_t, a_t) | s_{t+1}, v_{t-1}(\cdot)) = \\ = \delta(v_t(s_t, a_t), r(s_t, a_t) + \gamma \max_a v_{t-1}(s_{t+1}, a)) . \end{aligned} \quad (78.45)$$

# Chapter 79

## Reliability Box Diagrams and Fault Tree Diagrams

This chapter is based on Refs.[59] and [82].

In this chapter, we assume that reader is familiar with Boolean Algebra. See Chapter C for a quick review of what we recommend that you know about Boolean Algebra to fully appreciate this chapter.

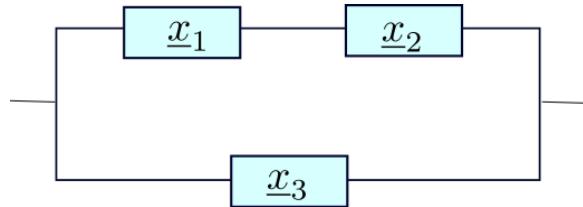


Figure 79.1: Example of rbox diagram.

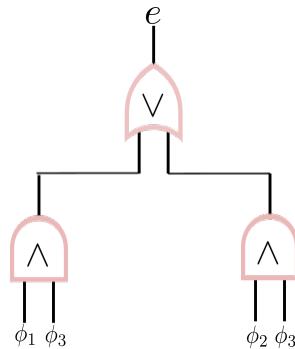


Figure 79.2: An ftree diagram equivalent to Fig.79.1. It represents  $e = (\phi_1 \wedge \phi_3) \vee (\phi_2 \wedge \phi_3)$ .

Complicated devices with a large number of components such as airplanes or rockets can fail in many ways. If their performance depends on some components

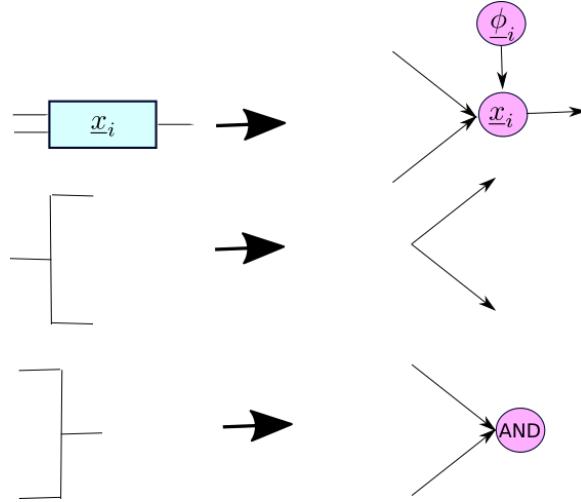


Figure 79.3: How to map an rbox diagram to a bnet.

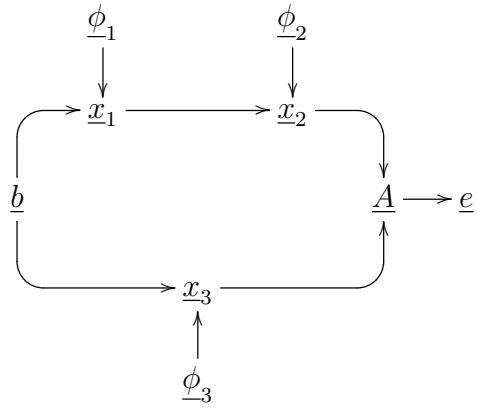


Figure 79.4: bnet corresponding the rbox diagram Fig.79.1.

working in series and one of the components in the series fails, this may lead to catastrophic failure. To avert such disasters, engineers use equivalent components connected in parallel instead of in series, thus providing multiple backup systems. They analyze the device to find its weak points and add backup capabilities there. They also estimate the average time to failure for the device.

The two most popular diagrams for finding the failure modes and their rates for large complicated devices are

- rbox diagrams = Reliability Box diagrams. See Fig.79.1 for an example.
- ftree diagrams = Fault Tree Diagrams. See Fig.79.2 for an example.

In an ftree diagram, several nodes might stand for the same component of a physical

device. In an rbox diagram, on the other hand, each node represents a distinct component in a device. Hence, rbox diagrams resemble the device they are addressing whereas ftree diagrams don't. Henceforth, we will refer to this desirable property as **physical resemblance**.

As we will show below with an example, it is pretty straightforward to translate an rbox to an ftree diagram. Going the other way, translating an ftree to an rbox diagram is much more difficult.

Next we will define a new kind of bnet that we will call a failure bnet that has physical resemblance. Then we will describe a simple method of translating (i.e., mapping) any rbox diagram to a failure bnet. Then we will show how a failure bnet can be used to do all the calculations that are normally done with an rbox or an ftree diagram. In that sense, failure bnets seem to afford all the benefits of both ftree and rbox diagrams.

A **failure bnet** contains nodes of 5 types, labeled  $\underline{b}$ ,  $\underline{e}$ ,  $\underline{x}_i$ ,  $\underline{\phi}_i$ , and  $\underline{A}_i$ . All nodes have only two possible states  $S = Success = 0$ ,  $F = Failure = 1$ .

1. The bnet has a beginning node labeled  $\underline{b}$  which is always set to success. The  $\underline{b}$  node and the  $\underline{\phi}_i$  nodes are the only root nodes of the bnet.
2. The bnet has a single leaf node, the end node, labeled  $\underline{e}$ .  $\underline{e}$  is fixed. In rbox diagrams,  $\underline{e} = S$  whereas in ftree diagrams,  $\underline{e} = F$ .
3.  $\underline{x}^{nx} = (\underline{x}_0, \underline{x}_1, \dots, \underline{x}_{nx-1})$ .  $\underline{x}_i \in \{S, F\}$  for all  $i$ .

Suppose  $\underline{x}_i$  has parents  $\underline{\phi}_i$  and  $\underline{a}^{na} = (a_0, a_1, \dots, a_{na-1})$ . Then the TPM of node  $\underline{x}_i$  is defined to be

$$P(x_i | \phi_i, a^{na}) = \delta(x_i, \phi_i \vee \vee_{i=0}^{na-1} a_i) \quad (79.1)$$

4. For each node  $\underline{x}_i$ , the bnet has a "performance" root node  $\underline{\phi}_i \in \{0, 1\}$  with an arrow pointing from it to  $\underline{x}_i$  (i.e.,  $\underline{\phi}_i \rightarrow \underline{x}_i$ ). For all  $i$ ,

$$P(\phi_i) = \epsilon_i \delta(\phi_i, F) + \bar{\epsilon}_i \delta(\phi_i, S). \quad (79.2)$$

$\epsilon_i$  is the failure probability and  $\bar{\epsilon}_i = 1 - \epsilon_i$  is the success probability. We name the failure probability  $\epsilon_i$  because it is normally very small. It is usually set to  $1 - e^{-\lambda_i t} \approx \lambda_i t$  when  $\lambda_i t \ll 1$ , where  $\lambda_i$  is the failure rate for node  $\underline{x}_i$  and  $t$  stands for time. The rblock literature usually calls  $\bar{\epsilon}_i = R_i$  the **reliability** of node  $\underline{x}_i$ , and  $\epsilon_i = (1 - R_i) = F_i$  its **unreliability**.

5. The nodes  $\underline{A}_i \in \{0, 1\}$  are simply AND gates. If  $\underline{A}_i$  has inputs  $\underline{y}^{ny} = (\underline{y}_0, \underline{y}_1, \dots, \underline{y}_{ny-1})$ , then the TPM of  $\underline{A}_i$  is

$$P(A_i|y^{ny}) = \delta(A_i, \wedge_{i=0}^{ny-1} y_i) . \quad (79.3)$$

An instance (instantiation) of a bnet is the bnet with all nodes set to a specific state. A **realizable instance (r-instance)** of a bnet is one which has non-zero probability.

Fig.79.3 shows how to translate any rbox diagram to a failure bnet. To illustrate this procedure, we translated the rbox diagram Fig.79.1 into the failure bnet Fig.79.4.

For the failure bnet Fig.79.4, one has:

$$\begin{aligned} P(b) &= \mathbb{1}(b = 0) \\ P(x_1|\phi_1, b) &= \mathbb{1}(x_1 = \phi_1 \vee b) \\ P(x_2|\phi_2, x_1) &= \mathbb{1}(x_2 = \phi_2 \vee x_1) \\ P(x_3|\phi_3, b) &= \mathbb{1}(x_3 = \phi_3 \vee b) \\ P(A|x_2, x_3)e &= \mathbb{1}(x_2 \wedge x_3) \\ P(e|A) &= \mathbb{1}(e = A) \end{aligned} . \quad (79.4)$$

Therefore, all r-instances of this bnet must satisfy

$$e = (\phi_1 \vee \phi_2) \wedge \phi_3 \quad (79.5)$$

$$= (\phi_1 \wedge \phi_3) \vee (\phi_2 \wedge \phi_3) . \quad (79.6)$$

Eq.(79.6) proves that Fig.79.2 is indeed a representation of Fig.79.1.

Next, we consider r-instances of this bnet for two cases:  $e = S$  and  $e = F$ .

- **rblock analysis:**  $e = S = 0$ .

Table 79.1 shows the probability of all possible r-instances that end in success for the failure bnet Fig.79.4. (These r-instances are the main focus of rblock analysis). The first 4 of those probabilities (those with  $\phi_3 = 0$ ) sum to  $\bar{\epsilon}_3$  so the sum  $P(e = S)$  of all 5 is

$$P(e = S) = \bar{\epsilon}_3 + \bar{\epsilon}_1 \bar{\epsilon}_2 \epsilon_3 , \quad (79.7)$$

or, expressing it in reliability language in which  $\bar{\epsilon} = R$ ,

$$P(e = S) = R_3 + R_1 R_2 \bar{R}_3 . \quad (79.8)$$

- **ftree analysis:**  $e = F = 1$ .

Table 79.2 shows the probability of all possible r-instances that end in failure for the failure bnet Fig.79.4. (These r-instances are the main focus of ftree analysis). If we set  $\epsilon_i = \epsilon$  and  $\bar{\epsilon}_i \approx 1$  for  $i = 1, 2, 3$ , then the first two of

instance	probability
	$\bar{\epsilon}_1 \epsilon_2 \bar{\epsilon}_3$
	$\epsilon_1 \bar{\epsilon}_2 \bar{\epsilon}_3$
	$\epsilon_1 \epsilon_2 \bar{\epsilon}_3$
	$\bar{\epsilon}_1 \bar{\epsilon}_2 \bar{\epsilon}_3$
	$\bar{\epsilon}_1 \bar{\epsilon}_2 \epsilon_3$

Table 79.1: Probabilities of all possible r-instances with  $e = S = 0$  for failure bnet Fig.79.4.

instance	probability
	$\bar{\epsilon}_1 \epsilon_2 \epsilon_3$
	$\epsilon_1 \bar{\epsilon}_2 \epsilon_3$
	$\epsilon_1 \epsilon_2 \epsilon_3$

Table 79.2: Probabilities of all possible r-instances with  $e = F = 1$  for the failure bnet Fig.79.4.

those r-instances have probabilities of  $order(\epsilon^2)$  and the third has probability of  $order(\epsilon^3)$ . The two lowest order ( $order(\epsilon^2)$ ) r-instances are called the “minimal cut sets” of the ftree. We will have more to say about minimal cut sets later on. For now, just note from Eq.(79.6) that the ftree Fig.79.2 is just the result of joining together with ORs two expressions, one for each of the two minimal cut sets.

---

### More general $\underline{x}_i$ .

Failure bnets can actually accommodate  $\underline{x}_i$  nodes of a more general kind than what we first stipulated. Here are some possibilities:

For any  $a^n \in \{0, 1\}^n$ , let

$$len(a^n) = \sum_i a_i \quad (79.9)$$

- **OR gate**

$$P(x_i|\phi_i, a^{na}) = \delta(x_i, \phi_i \vee \vee_j a_j) \quad (79.10)$$

$$= \delta(x_i, \phi_i \vee \mathbb{1}(\text{len}(a^{na}) > 0)) \quad (79.11)$$

- **AND gate**

$$P(x_i|\phi_i, a^{na}) = \delta(x_i, \phi_i \vee \wedge_j a_j) \quad (79.12)$$

$$= \delta(x_i, \phi_i \vee \mathbb{1}(\text{len}(a^{na}) = na)) \quad (79.13)$$

- **Fail if least  $K$  failures (less than  $K$  successes)**

$$P(x_i|\phi_i, a^{na}) = \delta(x_i, \phi_i \vee \mathbb{1}(\text{len}(a^{na}) \geq K)) \quad (79.14)$$

- **Fail if less than  $K$  failures (at least  $K$  successes)**

$$P(x_i|\phi_i, a^{na}) = \delta(x_i, \phi_i \vee \mathbb{1}(\text{len}(a^{na}) < K)) \quad (79.15)$$

- **Fail if exactly one failure**

$$P(x_i|\phi_i, a^{na}) = \delta(x_i, \phi_i \vee \mathbb{1}(\text{len}(a^{na}) = 1)) \quad (79.16)$$

This equals an XOR (exclusive OR) gate when  $na = 2$ .

- **General gate**

$$f : \{0, 1\}^{na} \rightarrow \{0, 1\}$$

$$P(x_i|\phi_i, a^{na}) = \delta(x_i, \phi_i \vee f(a^{na})) \quad (79.17)$$

## 79.1 Minimal Cut Sets

Suppose  $x \in \{0, 1\}$  and  $f : \{0, 1\} \rightarrow \{0, 1\}$ . Then by direct evaluation, we see that

$$f(x) = [\bar{x}f(0)] \vee [xf(1)]. \quad (79.18)$$

Let

$$\begin{aligned} !x &= 1 - x, \\ !^0 x &= x, \\ !^1 x &= !x \end{aligned} \tag{79.19}$$

Then Eq.(79.18) can be rewritten as

$$f(x) = \vee_{a \in \{0,1\}} [(!^{\bar{a}} x) f(a)] . \tag{79.20}$$

Now suppose  $x^n \in \{0,1\}^n$  and  $f : \{0,1\}^n \rightarrow \{0,1\}$ . Eq.(79.20) generalizes to

$$f(x^n) = \vee_{a^n \in \{0,1\}^n} \left[ \prod_i (!^{\bar{a}_i} x_i) f(a^n) \right] . \tag{79.21}$$

Eq.(79.21) is called an **ors-of-ands** normal form expansion. There is also an **ands-of-orss** normal form expansion obtained by swapping multiplication and  $\vee$  in Eq.(79.21), but we won't need it here.

A **cut set** is a set of  $\phi_i$ 's such that if they are all equal to  $F$ , then  $e = F$  for all the r-instances. A **minimal cut set** is a cut set such that there are no larger cut sets that contain it. From the failure bnet, we can always find a function  $f : \{0,1\}^{nx} \rightarrow \{0,1\}$  such that  $e = f(\phi^{nx})$  for all the r-instances. We did that for our example failure bnet and obtained Eq.(79.6). We can then express  $f(\phi^{nx})$  as an ors-of-ands expansion to find all the minimal cut sets. The ands terms in that ors-of-ands expansion each gives a different minimal cut set, after some simplification. The ors-of-ands expression is not unique and it may be necessary to simplify (using the Boolean Algebra identities given in Chapter C) to remove those redundancies.

# Chapter 80

## Restricted Boltzmann Machines

In what follows, we will abbreviate "restricted Boltzmann machine" by rebo.

Let

$$v \in \{0, 1\}^{nv}$$

$$h \in \{0, 1\}^{nh}$$

$b \in \mathbb{R}^{nv}$  (mnemonic,  $v$  and  $b$  sound the same)

$$a \in \mathbb{R}^{nh}$$

$$W^{v|h} \in \mathbb{R}^{nv \times nh}$$

Energy:

$$E(v, h) = -(b^T v + a^T h + v^T W^{v|h} h) \quad (80.1)$$

Boltzmann distribution:

$$P(v, h) = \frac{e^{-E(v, h)}}{Z} \quad (80.2)$$

Partition function:

$$Z = \sum_{v, h} e^{-E(v, h)} = Z(a, b, W^{v|h}) \quad (80.3)$$

$$P(v|h) = \frac{e^{b^T v + a^T h + v^T W^{v|h} h}}{\sum_v e^{b^T v + a^T h + v^T W^{v|h} h}} \quad (80.4)$$

$$= \frac{e^{b^T v + v^T W^{v|h} h}}{\sum_v e^{b^T v + v^T W^{v|h} h}} \quad (80.5)$$

$$= \prod_i \frac{e^{v_i(b_i + \sum_j W_{i,j}^{v|h} h_j)}}{\sum_{v_i=0,1} e^{v_i(b_i + \sum_j W_{i,j}^{v|h} h_j)}} \quad (80.6)$$

$$= \prod_i P(v_i|h) \quad (80.7)$$

$$P(v_i|h) = \frac{e^{v_i(b_i + \sum_j W_{i,j}^{v|h} h_j)}}{Z_i(h)} \quad (80.8)$$

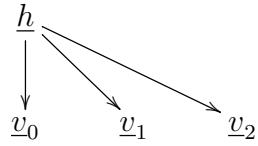


Figure 80.1: bnet for a Restricted Boltzmann Machine (rebo) with  $nv = 3$

Eq.(80.8) implies that a rebo can be represented by the bnet Fig.80.1.

Let

$$x_i = b_i + \sum_j W_{ij}^{vh} h_j . \quad (80.9)$$

Then

$$P(v_i = 1|h) = \frac{e^{x_i}}{1 + e^{x_i}} \quad (80.10)$$

$$= \frac{1}{1 + e^{-x_i}} \quad (80.11)$$

$$= \text{smoid}(x_i) . \quad (80.12)$$

One could also expand the node  $h$  in Fig.80.1 into  $nh$  nodes. But note that  $P(h) \neq \prod_j P(h_j)$  so there would be arrows among the  $h_j$  nodes.

Note that the rebo bnet is a special case of Naive Bayes (See Chapter 63) with  $v_i, h_i \in \{0, 1\}$  and specific  $P(h)$  and  $P(v_i|h)$  node matrices.

# Chapter 81

## ROC curves

This chapter is based on Ref.[149].

ROC stands for **Receiver Operating Characteristic**. ROC curves are used in binary classification (BC).

To do BC, we are given the value  $x \in \mathbb{R}$  for an individual. From this, we want to decide whether that individual has  $a = 0$  or  $a = 1$ . The decision will depend on the value of a **threshold parameter**  $\tau \in \mathbb{R}$ .

$$\underline{x} \longleftarrow \underline{a}$$

Figure 81.1: bnet for BC.

Fig.81.1 shows the bnet used for BC.

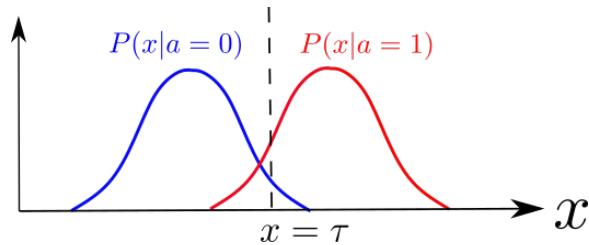


Figure 81.2:  $x$ -distribution for two hypotheses  $a = 0, 1$ .

Fig.81.2 is a plot of  $P(x|a)$ , i.e., the TPM for node  $\underline{x}$  of the bnet in Fig.81.1. Whereas  $a$  is binary,  $x$  is continuous. But we can replace  $x$  by a binary variable

$$b = \mathbb{1}(x > \tau). \quad (81.1)$$

$P(b|a)$  for  $b, a \in \{0, 1\}$  is called the **confusion matrix** or **contingency table** for BC. The confusion matrix can be calculated from the TPM  $P(x|a)$ . Fig.81.3 illustrates

		Actual Value (a)	
		0	1
Predicted Value (x)	0	$TNR \triangleleft$	$FNR \nwarrow$
	1	$FPR \nearrow$	$TPR \blacktriangleleft$

Figure 81.3: The confusion matrix  $P(b|a)$  for BC.

the confusion matrix  $P(b|a)$  for BC. In that figure, the rates  $R$  are defined as follows.<sup>1</sup>

- **True Negative Rate (TNR)**

$$R_{0|0}(\tau) = P(x < \tau | a = 0) = \int_{x < \tau} dx P(x | a = 0) \quad (81.2)$$

- **False Positive Rate (FPR)**

$$R_{1|0}(\tau) = 1 - R_{0|0}(\tau) \quad (81.3)$$

$$= P(x > \tau | a = 0) = \int_{x > \tau} dx P(x | a = 0) \quad (81.4)$$

In Hypothesis Testing,  $R_{1|0}$  is called the **p-value that  $x > \tau$  assuming curve 0 is the null hypothesis**.

- **False Negative Rate (FNR)**

$$R_{0|1}(\tau) = P(x < \tau | a = 1) = \int_{x < \tau} dx P(x | a = 1) \quad (81.5)$$

In Hypothesis Testing,  $R_{0|1}$  is called the **p-value that  $x < \tau$  assuming curve 1 is the null hypothesis**.

- **True Positive Rate (TPR)**

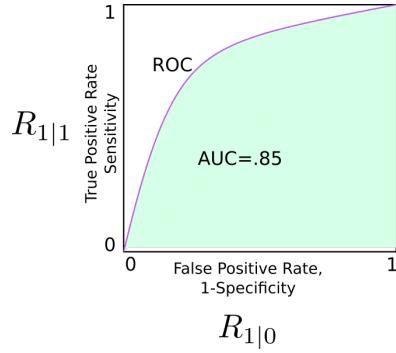
$$R_{1|1}(\tau) = 1 - R_{0|1}(\tau) \quad (81.6)$$

$$= P(x > \tau | a = 1) = \int_{x > \tau} dx P(x | a = 1) \quad (81.7)$$

The **Receiver Operating Characteristic (ROC)** is a parametric plot with  $X = R_{1|0}(\tau)$  and  $Y = R_{1|1}(\tau)$ , where  $\tau \in \mathbb{R}$ . The **Area Under the Curve (AUC)** is the area under the ROC. Fig.81.4 shows an example of a ROC and its AUC.

---

<sup>1</sup>I find the notation  $x|a$  where  $x, a \in \{0, 1\}$  much clearer than  $\alpha\beta$  where  $\alpha = T, F$  and  $\beta = N, P$ . Note that  $\alpha = \mathbb{1}(x = a)$  and  $\beta = x$ , if we identify  $0 = F = N$  and  $1 = T = P$ .



$$R_{1|0}$$

Figure 81.4: Example of ROC. Green shaded area is the AUC of the ROC.

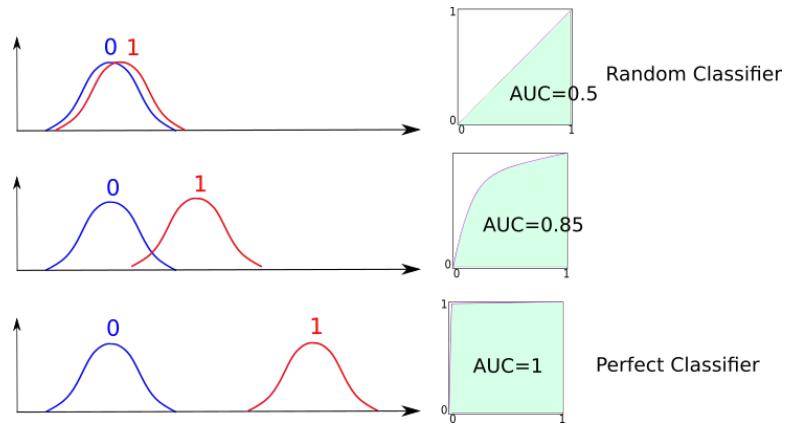


Figure 81.5: ROC curves for 3 different separations between the 0 and 1 x-distributions.

Fig.81.5 shows situations that give  $AUC=.5$  (random classifier),  $AUC=.85$ , and  $AUC=1$  (perfect classifier). It's also possible to get an  $AUC \in [0, 0.5]$ , but we will ignore those models because they are useless for BC.

Note that

$$AUC = \int_{x=0}^1 d\tau R_{1|1}(\tau) \frac{dR_{1|0}(\tau)}{d\tau} \quad (81.8)$$

$$= \int_{-\infty}^{-\infty} d\tau \left\{ \int_{-\infty}^{\infty} dx \mathbb{1}(x > \tau) P(x|a=1) \right\} (-1) P(x = \tau|a=0) \quad (81.9)$$

$$= \int_{-\infty}^{\infty} dx' \int_{-\infty}^{\infty} dx \mathbb{1}(x > x') P(x|a=1) P(x'|a=0) . \quad (81.10)$$

See Fig.81.6 for an example of False Positive and False Negative predictions.

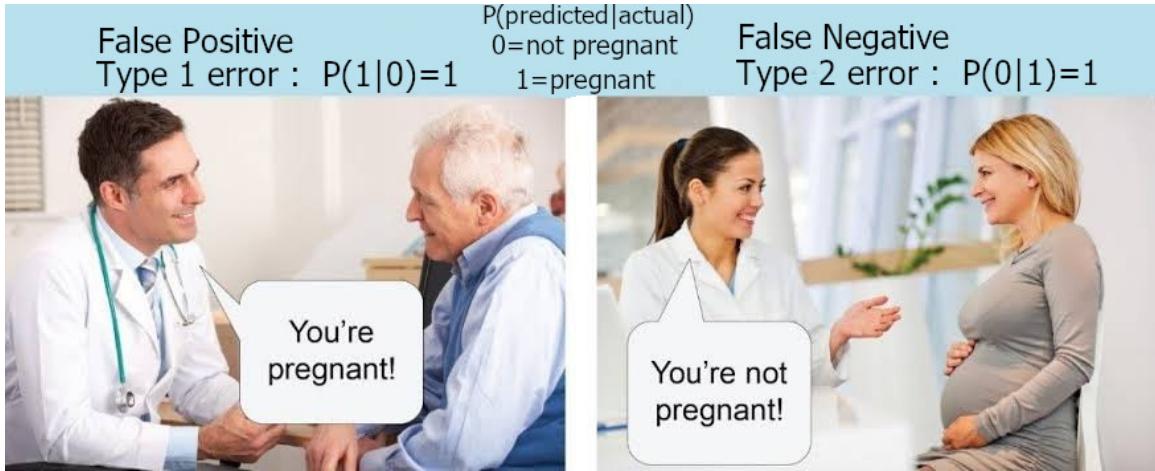


Figure 81.6: Example of False Positive and False Negative predictions.

## 81.1 Terminology Table Adapted from Wikipedia Ref.[149]

Let  $N_{x|a}$  be numbers (counts) so that

$$P(x|a) = \frac{N_{x|a}}{\sum_{x'} N_{x'|a}} \quad (81.11)$$

for all  $x, a \in \{0, 1\}$ .

condition positive (P):  $N_{|1} = \sum_x N_{x|1}$ , the number of real positive cases in the data

condition negative (N):  $N_{|0} = \sum_x N_{x|0}$ , the number of real negative cases in the data

true positive (TP):  $N_{1|1}$ , hit

true negative (TN):  $N_{0|0}$ , correct rejection

false positive (FP):  $N_{1|0}$ , false alarm, type I error or overestimation

false negative (FN):  $N_{0|1}$ , miss, type II error or underestimation

sensitivity, recall, hit rate, or true positive rate (TPR):

$$TPR = R_{1|1} = \frac{N_{1|1}}{N_{|1}} = \frac{N_{1|1}}{N_{1|1} + N_{0|1}} = 1 - R_{0|1} \quad (81.12)$$

specificity, selectivity or true negative rate (TNR):

$$TNR = R_{0|0} = \frac{N_{0|0}}{N_{|0}} = \frac{N_{0|0}}{N_{0|0} + N_{1|0}} = 1 - R_{1|0} \quad (81.13)$$

precision or positive predictive value (PPV):

$$PPV = \frac{N_{1|1}}{N_{1|1} + N_{1|0}} = 1 - FDR \quad (81.14)$$

negative predictive value (NPV):

$$NPV = \frac{N_{0|0}}{N_{0|0} + N_{0|1}} = 1 - FOR \quad (81.15)$$

miss rate or false negative rate (FNR):

$$FNR = R_{0|1} = \frac{N_{0|1}}{N_{|1}} = \frac{N_{0|1}}{N_{0|1} + N_{1|1}} = 1 - R_{1|1} \quad (81.16)$$

fall-out or false positive rate (FPR):

$$FPR = R_{1|0} = \frac{N_{1|0}}{N_{|0}} = \frac{N_{1|0}}{N_{1|0} + N_{0|0}} = 1 - R_{0|0} \quad (81.17)$$

false discovery rate (FDR):

$$FDR = \frac{N_{1|0}}{N_{1|0} + N_{1|1}} = 1 - PPV \quad (81.18)$$

false omission rate (FOR):

$$FOR = \frac{N_{0|1}}{N_{0|1} + N_{0|0}} = 1 - NPV \quad (81.19)$$

accuracy (ACC):

$$ACC = \frac{N_{1|1} + N_{0|0}}{N_{|1} + N_{|0}} = \frac{N_{1|1} + N_{0|0}}{N_{1|1} + N_{0|0} + N_{1|0} + N_{0|1}} \quad (81.20)$$

balanced accuracy (BA):

$$BA = \frac{R_{1|1} + R_{0|0}}{2} \quad (81.21)$$

F1 score is the harmonic mean of precision and sensitivity:

$$F_1 = 2 \times \frac{PPV \times R_{1|1}}{PPV + R_{1|1}} = \frac{2N_{1|1}}{2N_{1|1} + N_{1|0} + N_{0|1}} \quad (81.22)$$

# Chapter 82

## Scoring the Nodes of a Learned Bnet

Chapter 88 discusses how to learn a bnet from data. Many algorithms for doing this require scoring how well a particular bnet fits the data. This chapter is an introduction to such scoring.

Normally, each node of a bnet is scored separately, and then those node scores are summed to get the bnet score.

In this chapter, scores are defined so that a higher score means a better fit. By taking the negative of such a score, one can always get a score such that a lower score means a better fit.

There are 2 main types of bnet scores: Maximum Likelihood (ML) scores, and Shannon Information Theory (SIT) scores. ML scores consist of the log of a maximum likelihood function  $P(\vec{x}|\theta)$  for i.i.d. samples  $\vec{x} = (x^\sigma)_{\sigma=0,1,\dots,nsam-1}$ , where  $x^\sigma \sim P_{\underline{x}|\theta}(x|\theta)$ :

$$\text{ML-score} = \ln(P(\vec{x}|\theta)) \quad (82.1)$$

$$= \ln \prod_{\sigma} P(x^\sigma | \theta) \quad (82.2)$$

$$= \sum_{\sigma} \ln P(x^\sigma | \theta) \quad (82.3)$$

$$\approx nsam \sum_x P(x|\theta) \ln P(x|\theta) \quad (82.4)$$

$$= -nsam H(P_{\underline{x}|\theta}) , \quad (82.5)$$

and SIT scores consist of a negative entropy:

$$\text{Info-score} = -H(P_{\underline{x}|\theta}) . \quad (82.6)$$

Thus, up to a factor of  $nsam$ , they are the same thing. Maximizing a log likelihood function for i.i.d. samples or minimizing the corresponding entropy, are the same thing, and they both yield a good estimate of the hidden parameters  $\theta$ .

## 82.1 Probability Distributions and Special Functions

While writing this chapter, I briefly consulted the following Wikipedia articles about the definitions and properties of certain probability distributions and special functions.

- Categorical Distribution, Ref.[99]
- Multinomial Distribution, Ref.[141]
- Dirichlet Distribution, Ref.[108]
- Multivariate Normal Distribution, Ref.[143]
- Beta function, Ref.[95]
- Multinomial Coefficients, Ref.[142]
- Gamma Function Ref.[115]

Here are a few results from those Wikipedia articles that we will use later on in this chapter.

Below, we will abbreviate  $q_+ = \sum_i q_i$ , and  $q_\cdot = (q_0, q_1, \dots, q_{nq-1})$  for various quantities  $q$

**Gamma function.** If  $n > 0$  is an integer,

$$\Gamma(n + 1) = n! \quad (82.7)$$

The **multivariate Beta function** is defined by

$$B(\alpha_\cdot) = \frac{\prod_k \Gamma(\alpha_k)}{\Gamma(\alpha_+)} \quad (82.8)$$

where  $\alpha_k > 0$  for all  $k$ .

The **multinomial coefficient** is defined by

$$C(N_\cdot) = \frac{N_+!}{\prod_k N_k!} \quad (82.9)$$

where  $N_k$  are non-negative integers.

The **inverse of the multinomial coefficient** will be denoted by

$$CI(N_\cdot) = \frac{1}{C(N_\cdot)} = \frac{\prod_k N_k!}{N_+!} \quad (82.10)$$

The **Categorical Distribution** is defined by

$$Cat(x; \pi_\cdot) = \pi_x = \prod_k \pi_k^{\mathbb{1}(k=x)} \quad (82.11)$$

for  $k, x \in S_x$ , where  $\pi.$  is a probability dist.(i.e.,  $\pi_k \geq 0$  for all  $k$ , and  $\pi_+ = 1$ ).

The **Multinomial Distribution** is defined by

$$Mul(N.; \pi., N) = C(N.) , \quad (82.12)$$

where  $N_k$  is a non-negative integer for all  $k$ ,  $N_+ = N$ , and  $\pi.$  is a probability dist.  $Mul()$  satisfies:

$$E[N_k] = N\pi_k . \quad (82.13)$$

The **Dirichlet Distribution** is defined by

$$Dir(\pi.; \alpha.) = \frac{1}{B(\alpha.)} \prod_k \pi_k^{\alpha_k - 1} \quad (82.14)$$

where  $\alpha_k > 0$  for all  $k$ , and  $\pi.$  is a probability dist. The  $\alpha.$  are called **concentration parameters** or **hyperparameters**.  $Dir()$  satisfies:

$$E[\underline{\pi}_k] = \frac{N_k}{N_+} . \quad (82.15)$$

$Dir()$  is **conjugate prior** of  $Mul()$

Note that

$$Mul(N.; \pi., N) Dir(\pi.; \alpha.) = \mathcal{K}(N., \alpha.) Dir(\pi.; N. + \alpha.) , \quad (82.16)$$

where

$$\mathcal{K}(N., \alpha.) = \frac{B(N. + \alpha.)}{CI(N.)B(\alpha.)} . \quad (82.17)$$

$Dir()$  is replaceable by a  $Mul()$  for large concentration parameters

Note that if  $N_k$  is a positive integer and  $\alpha_k = N_k + 1$  for all  $k$ , then

$$Dir(\pi.; \alpha_k = N_k + 1) = C(N.) \prod_k \pi_k^{N_k} \quad (82.18)$$

$$= Mul(N.; \pi., N_+) . \quad (82.19)$$

## 82.2 Single node with no parents

In this section, we consider a learned bnet consisting of a single node with no parents. We will consider arbitrary learned bnets in the next section. But we start with this simplified case so as to reduce the number of indices in most quantities from 3 to 1. All the results that we derive in this section will be used in the next section after adding the extra indices. This way, we will avoid carrying the extra indices throughout the intermediate steps of many derivations.

For state  $k \in \{0, 1, \dots, nk - 1\}$  of a single node  $\underline{x}$ , let  
 $\underline{N}_k$  = current count number (an integer, data)  
 $\underline{\pi}.$  = a probability dist, the TPM for the node  
 $\underline{\alpha}_k$  = prior count number

$$\underline{N}. \longleftarrow \underline{\pi}. \longleftarrow \underline{\alpha}.$$

Figure 82.1: For a bnet consisting of a single node with no parents, this is a Markov chain of current counts ( $\underline{N}.$ ), TPM ( $\underline{\pi}.$ ), and prior counts ( $\underline{\alpha}.$ ) .

Consider the Markov chain bnet of Fig.82.1 with the following TPMs, printed in blue.

$$P(N.| \underline{\pi}. ) = Mul(N.; \underline{\pi}., N_+) \quad (82.20)$$

$$P(\underline{\pi}. | \underline{\alpha}. ) = Dir(\underline{\pi}.; \underline{\alpha}. ) \quad (82.21)$$

It follows that

$$P(N., \underline{\pi}. | \underline{\alpha}. ) = P(N.| \underline{\pi}. )P(\underline{\pi}. | \underline{\alpha}. ) \quad (82.22)$$

$$= Mul(N.; \underline{\pi}., N_+) Dir(\underline{\pi}.; \underline{\alpha}. ) \quad (82.23)$$

$$= \mathcal{K}(N., \underline{\alpha}. ) Dir(\underline{\pi}.; N. + \underline{\alpha}. ) . \quad (82.24)$$

From Eq.(82.15) for the expected value of  $Dir()$ , we get

$$\hat{\pi}. = E[\underline{\pi}.] = \frac{N. + \underline{\alpha}.}{N_+ + \alpha_+} . \quad (82.25)$$

Integrating both sides of Eq.(82.24) over  $\underline{\pi}.$ , we find that

$$P(N.| \underline{\alpha}. ) = \mathcal{K}(N., \underline{\alpha}. ) . \quad (82.26)$$

If  $N_k >> 1$  for all  $k$ , then the  $Dir()$  in Eq.(82.24) can be replaced by a  $Mul()$

$$P(N., \underline{\pi}. | \underline{\alpha}. ) \approx \mathcal{K}(N., \underline{\alpha}. ) Mul(N. + \underline{\alpha}. ; \underline{\pi}., N_+ + \alpha_+ ) . \quad (82.27)$$

Therefore,

$$P(N.| \underline{\pi}., \underline{\alpha}. ) = \frac{P(N., \underline{\pi}. | \underline{\alpha}. )}{P(N.| \underline{\alpha}. )} \quad (82.28)$$

$$= Mul(N. + \underline{\alpha}. ; \underline{\pi}., N_+ + \alpha_+ ) . \quad (82.29)$$

**Claim 125**

$$\ln P(N_{\cdot} | \widehat{\pi}_{\cdot}, \alpha_{\cdot}) = -(N_{+} + \alpha_{+})H\left(\frac{N_{\cdot} + \alpha_{\cdot}}{N_{+} + \alpha_{+}}\right) + \ln C(N_{\cdot} + \alpha_{\cdot}) \quad (82.30)$$

$$> -(N_{+} + \alpha_{+})H\left(\frac{N_{\cdot} + \alpha_{\cdot}}{N_{+} + \alpha_{+}}\right) - \frac{1}{2}(nk - 1)\ln N_{+} \quad (82.31)$$

**proof:**

$$\ln P(N_{\cdot} | \widehat{\pi}_{\cdot}, \alpha_{\cdot}) = \sum_k (N_k + \alpha_k) \ln \widehat{\pi}_k + \ln C(N_{\cdot} + \alpha_{\cdot}) \quad (82.32)$$

$$= \sum_k (N_k + \alpha_k) \ln \frac{N_k + \alpha_k}{N_{+} + \alpha_{+}} + \ln C(N_{\cdot} + \alpha_{\cdot}) \quad (82.33)$$

$$= -(N_{+} + \alpha_{+})H\left(\frac{N_{\cdot} + \alpha_{\cdot}}{N_{+} + \alpha_{+}}\right) + \ln C(N_{\cdot} + \alpha_{\cdot}) \quad (82.34)$$

Recall Stirling's approximation of a factorial, valid for large integers  $n$ :

$$\ln n! \approx (n + \frac{1}{2}) \ln n - n . \quad (82.35)$$

Assume  $N_k \gg 1$  for all  $k$ . Applying Stirling's approximation to all factorials in  $C(N)$ , we get

$$\ln C(N_{\cdot}) \approx (N_{+} + \frac{1}{2}) \ln N_{+} - N_{+} - \sum_k \left[ (N_k + \frac{1}{2}) \ln N_k - N_k \right] \quad (82.36)$$

$$= (N_{+} + \frac{1}{2}) \ln N_{+} - \sum_k (N_k + \frac{1}{2}) \ln N_k . \quad (82.37)$$

Next assume that

$$N_k \approx \frac{N_{+}}{nk} . \quad (82.38)$$

Then

$$\ln C(N_{\cdot}) = (N_{+} + \frac{1}{2}) \ln N_{+} - nk\left(\frac{N_{+}}{nk} + \frac{1}{2}\right)[\ln N_{+} - \ln nk] \quad (82.39)$$

$$= -\frac{1}{2}(nk - 1)\ln N_{+} + (N_{+} + \frac{nk}{2})\ln nk \quad (82.40)$$

$$> -\frac{1}{2}(nk - 1)\ln N_{+} . \quad (82.41)$$

**QED**

## 82.3 Multiple nodes with any number of parents

In the previous section, we considered a bnet consisting of a single node with no parents, so we only needed a single index  $k$  for the states of the single node. In this section, we consider an arbitrary bnet with multiple nodes each of which may have multiple parents. Most of the results in the previous section are valid for the general case if we make the following replacements:  $\pi_{\cdot} \rightarrow \pi_{\cdot|\mu}^i$ ,  $N_{\cdot} \rightarrow N_{\cdot,\mu}^i$ ,  $\alpha_{\cdot} \rightarrow \alpha_{\cdot,\mu}^i$ . Upon this replacement, Fig.82.1 becomes Fig.82.2. The TPMs, printed in blue, of the new Markov chain, are as follows:

$$\underline{N_{\cdot,\mu}^i} \longleftarrow \underline{\pi_{\cdot|\mu}^i} \longleftarrow \underline{\alpha_{\cdot,\mu}^i}$$

Figure 82.2: Generalization of Fig.82.1. For a bnet with multiple nodes each of which may have multiple parents, this is a Markov chain of current counts ( $\underline{N_{\cdot,\mu}^i}$ ), TPM ( $\underline{\pi_{\cdot|\mu}^i}$ ), and prior counts ( $\underline{\alpha_{\cdot,\mu}^i}$ ) .

$$P(N_{\cdot,\mu}^i | \pi_{\cdot|\mu}^i) = \text{Mul}(N_{\cdot,\mu}^i; \pi_{\cdot|\mu}^i, N_{\cdot,\mu}^i) \quad (82.42)$$

$$P(\pi_{\cdot|\mu}^i | \alpha_{\cdot,\mu}^i) = \text{Dir}(\pi_{\cdot|\mu}^i; \alpha_{\cdot,\mu}^i) \quad (82.43)$$

In these TPMs,

$i \in S_i = \{0, 1, \dots, ni - 1\}$  = node index

$\underline{x}_{\cdot} = (\underline{x}_i)_{i \in S_i}$  = the nodes of the learned bnet.

$k \in S_k^i = \{0, 1, \dots, nk^i - 1\}$  = states of node  $\underline{x}_i$

$\mu \in S_{\mu}^i = \{0, 1, \dots, n\mu^i - 1\}$  = states of parents of node  $\underline{x}_i$ .

In the previous section, we assumed a single node ( $ni = 1$ ) with no parents ( $n\mu^0 = 1$ ) so that we could drop the  $i, \mu$  indices. In this section, we eliminate that restriction.

It is convenient to define the magnitude of a bnet  $B$  to equal the sum over nodes of the number of free parameters in each TPM:

$$|B| = \sum_i (nk^i - 1)n\mu^i. \quad (82.44)$$

Suppose that we are given  $nsam$  samples  $\vec{x}_i = (\underline{x}_i^{\sigma})_{\sigma=0,1,\dots,nsam-1}$  of our learned bnet. The count numbers  $N_{k,\mu}^i$  are defined in terms of those samples as follows:

$$N_{k,\mu}^i = \sum_{\sigma} \mathbb{1}(\underline{x}_i^{\sigma} = k, pa(\underline{x}_i^{\sigma}) = \mu). \quad (82.45)$$

It is also convenient to define count number ratios

$$N_{k|\mu}^i = \frac{N_{k,\mu}^i}{N_{+, \mu}^i}. \quad (82.46)$$

Note that  $N_{k,\mu}^i$  is a positive integer whereas  $N_{k|\mu}^i \in [0, 1]$ .

Let's denote the components of the TPMs by  $\pi_{k|\mu}^i$ :

$$\pi_{k|\mu}^i = P(\underline{x}_i = k \mid pa(\underline{x}_i) = \mu) \approx N_{k|\mu}^i. \quad (82.47)$$

The rest of this section lists equations that we obtained from the previous section, by adding the new indices  $i, \mu$ :

$$\mathcal{K}(N_{\cdot, \mu}^i, \alpha_{\cdot, \mu}^i) = \frac{B(N_{\cdot, \mu}^i + \alpha_{\cdot, \mu}^i)}{CI(N_{\cdot, \mu}^i)B(\alpha_{\cdot, \mu}^i)} \quad (82.48)$$

$$\widehat{\pi}_{k|\mu}^i = \frac{N_{k,\mu}^i + \alpha_{k,\mu}^i}{N_{+, \mu}^i + \alpha_{+, \mu}^i} \quad (82.49)$$

$$P(N_{\cdot, \mu}^i | \alpha_{\cdot, \mu}^i) = \mathcal{K}(N_{\cdot, \mu}^i, \alpha_{\cdot, \mu}^i) \quad (82.50)$$

$$P(N_{\cdot, \mu}^i | \pi_{\cdot|\mu}^i, \alpha_{\cdot, \mu}^i) \approx Mul(N_{\cdot, \mu}^i + \alpha_{\cdot, \mu}^i; \pi_{\cdot|\mu}^i, N_{+, \mu}^i + \alpha_{+, \mu}^i) \quad (82.51)$$

### Claim 126

$$\ln P(N_{\cdot, \mu}^i | \widehat{\pi}_{\cdot|\mu}^i, \alpha_{\cdot, \mu}^i) = \sum_k (N_{k,\mu}^i + \alpha_{k,\mu}^i) \ln \left( \frac{N_{k,\mu}^i + \alpha_{k,\mu}^i}{N_{+, \mu}^i + \alpha_{+, \mu}^i} \right) + \ln C(N_{\cdot, \mu}^i + \alpha_{\cdot, \mu}^i) \quad (82.52)$$

$$> \sum_k (N_{k,\mu}^i + \alpha_{k,\mu}^i) \ln \left( \frac{N_{k,\mu}^i + \alpha_{k,\mu}^i}{N_{+, \mu}^i + \alpha_{+, \mu}^i} \right) - \frac{1}{2}(nk^i - 1) \ln N_{+, \mu}^i \quad (82.53)$$

## 82.4 Bayesian Scores

- Bayesian Information Criterion (BIC)

$$\text{BIC-score} = - \sum_i \sum_{k, \mu} N_{k,\mu}^i \ln \left( \frac{N_{k,\mu}^i}{N_{+, \mu}^i} \right) + \underbrace{\left[ - \frac{|B|}{2} \ln N_{+, +}^+ \right]}_{\sum_i \sum_\mu \ln C(N_{\cdot, \mu}^i) \text{ would be more accurate}} \quad (82.54)$$

$$\approx \sum_i \sum_\mu \ln P(N_{\cdot, \mu}^i | \widehat{\pi}_{\cdot|\mu}^i, \alpha_{\cdot, \mu}^i = 0) \quad (82.55)$$

- Bayesian Dirichlet (BD)

$$\text{BD-score} = \sum_i \sum_{\mu} \ln \frac{B(N_{\cdot,\mu}^i + \alpha_{\cdot,\mu}^i)}{B(N_{\cdot,\mu}^i)} \quad (82.56)$$

$$= \sum_i \sum_{\mu} \ln [CI(N_{\cdot,\mu}^i) P(N_{\cdot,\mu}^i | \alpha_{\cdot,\mu}^i)] \quad (82.57)$$

- BD equivalent (BDe)

$$\text{BDe-score} = \text{BD-score} (\alpha_{k,\mu}^i = \alpha' N_{k,\mu}^i) , \quad (82.58)$$

where  $\alpha'$  is a free parameter.

- BD equivalent unified (BDeu)

$$\text{BDeu-score} = \text{BD-score} \left( \alpha_{k,\mu}^i = \frac{\alpha'}{n k^i n \mu^i} \right) , \quad (82.59)$$

where  $\alpha'$  is a free parameter. The BDeu score satisfies **score equivalence**; i.e., it is the same for all DAGs in an equivalence class of observational equivalent DAGs. See Chapter 67 for more information about observational equivalence.

## 82.5 Information Theoretic scores

- Maximum likelihood

$$\text{ML-score} = \sum_i \sum_{k,\mu} N_{k,\mu}^i \ln N_{k|\mu}^i \quad (82.60)$$

$$= - \sum_i H(\underline{k}^i | \underline{\mu}^i) , \quad (82.61)$$

where  $P_{\underline{k}^i | \underline{\mu}^i}(k | \mu) = N_{k|\mu}^i$  and  $P_{\underline{k}^i, \underline{\mu}^i}(k, \mu) = N_{k,\mu}^i$ .

- Bayesian Information Criterion (BIC), a.k.a. Minimum Description Length (MDL)

$$\text{BIC-score} = \text{ML-score} - \frac{|B|}{2} \ln N_{+,+}^+ \quad (82.62)$$

$$\approx \sum_i \sum_{k,\mu} N_{k,\mu}^i \ln \frac{N_{k|\mu}^i}{\sqrt{N_{+,+}^+}} \quad (82.63)$$

- Akaike Information Criterion (AIC)

$$\text{AIC-score} = \text{ML-score} - |B| \quad (82.64)$$

$$\approx \sum_i \sum_{k,\mu} N_{k,\mu}^i [\ln N_{k|\mu}^i - 1] \quad (82.65)$$

# Chapter 83

## Selection Bias Removal

This chapter is based on Ref.[3].

Selection bias (SB) occurs when one samples from an atypical subset of a population, producing a biased dataset. Are such biased datasets useless? Not necessarily. It is possible to add auxiliary features to the biased dataset, and to sample those new features in an unbiased way, from the whole population. Then one can merge the original biased dataset with the auxiliary, unbiased one, to obtain an enhanced dataset. It is sometimes possible to do this so that the enhanced dataset is provably unbiased. It's like making horizontal the surface of a table that was not initially horizontal. The theory of Bayesian Networks and Causal Inference tells us WHEN this is possible, and HOW to do it when it is possible.

Consider the bnet Fig.83.1.

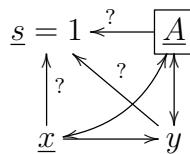


Figure 83.1: Bnet considered for selection bias (SB) removal. Arrows with question marks may or may not be present.

Let

$\underline{s} \in \{0, 1\}$  be the **switch node**.  $\underline{s} = 1$  means there is SB in the parent nodes.

$\underline{x}$  = **class features**.<sup>1</sup>

$\underline{y}$  = **target feature**.

$\underline{A}$  = **auxiliary features**. This is a set of nodes that may contain arrows entering or exiting it, as indicated by the double arrows.

$\underline{E} = \{\underline{y}, \underline{x}\} \cup \underline{A}$  = **Enhanced feature set**.

---

<sup>1</sup>A feature is the same as a node in a bnet.

$\Sigma$  = unbiased population of individuals  $\sigma$

$\Sigma_o$  = biased sub-population of individuals,  $\Sigma_o \subset \Sigma$ .

$OD = \{(\sigma_o, \underline{x}^{\sigma_o}, \underline{y}^{\sigma_o}, \underline{s}^{\sigma_o} = 1) : \sigma_o \in \Sigma_o\}$  = **Original Dataset**, dataset for  $(\underline{x}, \underline{y})$  features with  $\underline{s} = 1$ . Gives empirical distribution  $P(\underline{y}|\underline{x}, \underline{s} = 1)$ . (Ref.[3] calls this dataset the **biased study**.)

$AD = \{(\sigma, \underline{x}^\sigma, \underline{A}^\sigma) : \sigma \in \Sigma\}$  = **Auxiliary Dataset**, dataset for  $(\underline{x}, \underline{A})$  features. Gives empirical distribution  $P(\underline{A}|\underline{x})$ . (Ref.[3] calls this dataset the **population level study**.)

$ED = \{(\sigma_o, \underline{x}^{\sigma_o}, \underline{A}^{\sigma_o}, \underline{y}^{\sigma_o}, \underline{s}^{\sigma_o} = 1) : \sigma_o \in \Sigma_o\}$  = **Enhanced Dataset**, dataset for  $(\underline{x}, \underline{y}, \underline{A})$  features for  $\underline{s} = 1$ . Obtained by merging  $OD$  and  $AD$ . Gives empirical distribution  $P(\underline{y}|\underline{x}, \underline{A}, \underline{s} = 1)$ .

## 83.1 Pre and Post Switch Nodes

This book uses 2 types of switch nodes: pre-switch nodes and post-switch nodes.

**Pre-switch nodes** are used in Chapter 96 entitled “Transportability of Causal Knowledge”. Pre-switch nodes are **root** nodes. They are usually binary, and indicate whether the nodes pointed to belong to a set or not.

Most of the DAG literature, including Ref.[3], on which this chapter is based, define SB using a **post-switch node**. A post-switch node is a **leaf** node of the graph. Like pre-switch nodes, post-switch nodes are usually binary.

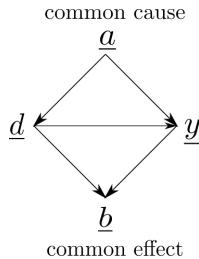


Figure 83.2: Common Cause and Effect for nodes  $\underline{d}, \underline{y}$ .

Note that in Potential Outcomes (PO) theory (see Chapter 72), pre-switch nodes such as  $a$  in Fig.83.2 are called **common cause (confounder, fork) nodes for nodes  $\underline{d}, \underline{y}$** . Furthermore, post-switch nodes such as  $b$  in Fig.83.2 are called **common effect (selection bias (SB), collider) nodes for nodes  $\underline{d}, \underline{y}$** . Hence, in PO theory, SB is indicated by a leaf node, just as we do in this chapter.

Note that **Simpson's paradox** (see Chapter 87) arises from an indirect effect caused by not conditioning on a confounder, whereas **Berkson's paradox** (see Chapter 7) arises from an indirect effect caused by conditioning on a collider.

It's possible to replace a pre-switch node by a post switch node, or vice versa, as follows. Suppose that we start with a bnet  $G_0$  that is fully connected, and we add to it a switch node  $s$  that is a root node that points to all nodes of  $G_0$ . Call the

resulting bnet  $\underline{s} \rightarrow G_0$ . We can use Bayes rule to reverse the direction of the arrows emanating from  $\underline{s}$  so that they enter node  $\underline{s}$  rather than exit it. Call the resulting bnet  $\underline{s} \leftarrow G_0$ . In general, Bayes rule allows us to translate from  $\underline{s} \rightarrow G_0$  to  $\underline{s} \leftarrow G_0$ , or in the opposite direction, without having to change the directions of any of the arrows in  $G_0$ . If  $G_0$  is not fully connected, then going from  $\underline{s} \rightarrow G_0$  to  $\underline{s} \leftarrow G'_0$  will often require that  $G'_0$  have the same arrows in the same directions as  $G_0$  plus some extra arrows new to  $G_0$ . Likewise, going from  $\underline{s} \leftarrow G_0$  to  $\underline{s} \rightarrow G''_0$  may require that  $G''_0$  have the same arrows as  $G_0$  plus some new arrows.

So far, we have been intentionally vague in specifying the graphs  $G'_0$  and  $G''_0$ . In Fig.83.3 we give a trick for determining possible candidates for graphs  $G'_0$  and  $G''_0$ . In Fig.83.3, we consider 3 panels going from left to right, depicting the cases where  $\underline{s}$  has either 1,2 or 3 neighbors. The top graph  $G_{post\text{-}sel}$ , which has a post-switch node  $\underline{s}$ , is converted to a graph which is numerically equal to it, namely the bottom graph  $G_{pre\text{-}sel}$ , which has a pre-switch node  $\underline{s}$ . The magenta arrows represent any number of arrows exiting (but none entering) a node. If we start with a graph  $\underline{s} \leftarrow G_0$ , we find the biggest subset  $X$  of the nodes of  $G_0$  such that  $\underline{s} \leftarrow X$  only has nodes exiting it (i.e., only magenta nodes). Then we add enough arrows to  $\underline{s} \leftarrow X$  to make it a fully connected graph  $\underline{s} \leftarrow X'$ . Now we can reverse the incoming arrows to  $\underline{s}$  and make them all outgoing and call the resulting graph  $\underline{s} \rightarrow X'$ .

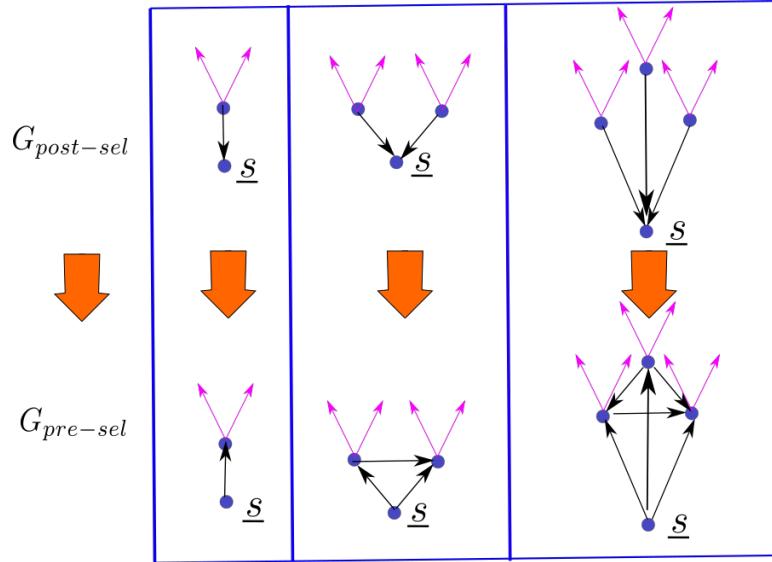


Figure 83.3: Switching from a post-switch node to a pre-switch node.

Recall that in Chapter D, we made a distinction between a good CF bnet a bad CF bnet, and we pointed out that bad CF bnets are often useful as a numerical tool. Recall also from Chapter 67 that two bnets can be “observationally equivalent”. That is what is happening here. We are faced with the choice of making switch nodes either leaf nodes or root nodes. Both choices lead to observationally equivalent bnets.

One of the two choices leads to a good CF bnet, and the other to a bad CF bnet. Both choices are numerically correct.

In this chapter, we will consider first a DAG  $G_{post\text{-}sel}$  with a post-switch node, then we will transform that DAG to a numerically equal DAG  $G_{pre\text{-}sel}$  with a pre-switch node. The latter DAG is more convenient for our needs. Why? Because in the SB theory that we present in this chapter, the  $\underline{s} = 1$  appears as a condition in a conditional probability, as in  $P(\cdots | \cdots, \underline{s} = 1)$ . Such probabilities are represented in a more straightforward manner if arrows exit rather than enter node  $\underline{s}$ .

## 83.2 Removing SB from passive query $P(y|x)$

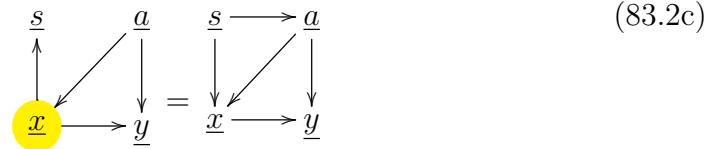
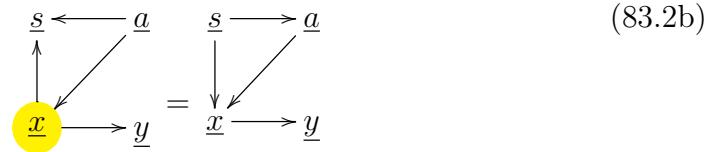
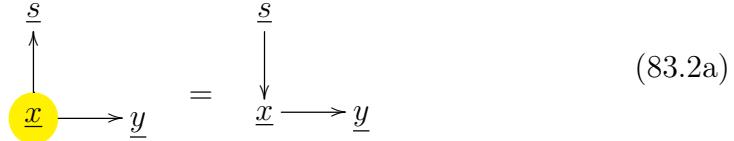
The **passive query**  $Q = P(y|x, \underline{s} = 1)$  is **SB-recoverable** if it is independent of  $\underline{s}$ .

1. **Query  $P(y|x)$  is SB-recoverable** with  $\underline{A} = \emptyset$ ; SB can be removed by conditioning on  $\underline{x}$ .

If  $\underline{y} \perp \underline{s} | \underline{x}$ , then

$$P(y|x, \underline{s} = 1) = P(y|x). \quad (83.1)$$

For example,



The bnets on the left hand sides of Eqs.(83.2) satisfy  $\underline{y} \perp \underline{s} | \underline{x}$ .

2. **Query  $P(y|x)$  is SB-recoverable** via  $\underline{a}$ ; SB can be removed by conditioning on  $\underline{x}$  and  $\underline{a}$ . Here  $\underline{a}$  is a nonempty subset of  $\underline{A}$

**Claim 127** There exists  $\underline{a} \subset \underline{A}$  such that  $\underline{y} \perp \underline{s}|(\underline{x}, \underline{a})$  and  $\underline{a} \perp \underline{s}|\underline{x}$  iff

$$P(y|x, \underline{s} = 1) = \sum_a \underbrace{P(y|x, a, \underline{s} = 1)}_{P(y|x,a)} \underbrace{P(a|x, \underline{s} = 1)}_{P(a|x)} = P(y|x) \quad (83.3)$$

$$\begin{array}{c} \underline{s} = 1 \\ \searrow \quad \nearrow \sum a \\ x \longrightarrow y = x \longrightarrow y \downarrow = x \longrightarrow y \end{array} \quad (83.4)$$

**proof:**

The  $\Rightarrow$  part of this claim is obvious. For a proof of the  $\Leftarrow$  part, see Ref.[3].  
**QED**

For example,

$$\begin{array}{c} \underline{s} \quad \underline{a} \\ \uparrow \quad \downarrow \\ x \longrightarrow y \end{array} = \begin{array}{c} \underline{s} \quad \underline{a} \\ \downarrow \quad \downarrow \\ x \longrightarrow y \end{array} \quad (83.5a)$$

The bnets on the left hand sides of Eqs.(83.5) satisfy  $\underline{y} \perp \underline{s}|(\underline{x}, \underline{a})$  and  $\underline{a} \perp \underline{s}|\underline{x}$ .

### 3. Query $P(y|x)$ is not SB-recoverable; SB cannot be removed.

For example,

$$\begin{array}{c} \underline{s} \\ \swarrow \quad \searrow \\ x \longrightarrow y \end{array} = \begin{array}{c} \underline{s} \\ \downarrow \quad \searrow \\ x \longrightarrow y \end{array} \quad (83.6)$$

$$\begin{array}{c} \underline{s} \\ \uparrow \quad \searrow \\ x \longrightarrow y \end{array} = \begin{array}{c} \underline{s} \\ \downarrow \quad \searrow \\ x \longrightarrow y \end{array} \quad (83.7)$$

$$\begin{array}{c} \underline{s} \leftarrow \underline{a} \\ \uparrow \quad \nearrow \\ x \longrightarrow y \\ \uparrow \\ w \end{array} = \begin{array}{c} \underline{s} \longrightarrow \underline{a} \\ \downarrow \quad \nearrow \\ x \longrightarrow y \\ \uparrow \\ w \end{array} \quad (83.8)$$

### 83.3 Removing SB from active query $P(y|\mathcal{D}\underline{x})$

The **active query (i.e., do query)**  $Q = P(y|\mathcal{D}\underline{x} = \underline{x}, \underline{s} = 1)$  is

- (a) **SB-recoverable** if it equals  $P(y|\mathcal{D}\underline{x} = \underline{x})$ ,
- (b) **do-identifiable** if it equals  $P(y|\underline{x}, \underline{s} = 1)$ .
- (c) both **SB-recoverable and do-identifiable** if it equals  $P(y|\underline{x})$ .

Examples

•

$$\begin{array}{ccc} \begin{array}{c} \underline{s} \leftarrow \underline{a} \\ \swarrow \quad \downarrow \\ \underline{x} \longrightarrow \underline{y} \end{array} & = & \begin{array}{c} \underline{s} \longrightarrow \underline{a} \\ \swarrow \quad \downarrow \\ \underline{x} \longrightarrow \underline{y} \end{array} \end{array} \quad \begin{array}{l} \text{SB-recoverable: NO} \\ \text{do-identifiable: YES} \end{array} \quad (83.9)$$

$Q = P(y|\mathcal{D}\underline{x} = \underline{x}, \underline{s} = 1)$  is do-identifiable because the bnet contains no hidden variables. It's s-recoverable because the bnet on the left hand side of Eq.(83.9) satisfies  $\underline{y} \perp \underline{s}|(\underline{x}, \underline{a})$  but Not  $\underline{a} \perp \underline{s}|\underline{x}$ .

•

$$\begin{array}{ccc} \begin{array}{c} \underline{s} \\ \uparrow \\ \underline{x} \longrightarrow \overset{(\underline{a})}{\underset{\top}{\swarrow}} \underline{y} \end{array} & = & \begin{array}{c} \underline{s} \\ \downarrow \\ \underline{x} \longrightarrow \overset{(\underline{a})}{\underset{\top}{\swarrow}} \underline{y} \end{array} \end{array} \quad \begin{array}{l} \text{SB-recoverable: YES} \\ \text{do-identifiable: NO} \end{array} \quad (83.10)$$

Let

$V$  = set of nodes in graph

$V^{<\underline{x}}$  = non-descendants of  $\underline{x}$  (excluding  $\underline{x}$ )

$V^{>\underline{x}}$  = descendants of  $\underline{x}$  (excluding  $\underline{x}$ )

$\underline{z}^{<\underline{x}} = \underline{z} \cap V^{<\underline{x}}$

$\underline{z}^{>\underline{x}} = \underline{z} \cap V^{>\underline{x}}$

Suppose  $\underline{z} \cup \{\underline{x}, \underline{y}\} \subset E$  and  $\underline{z} \subset \underline{A}$ . We say  $\underline{z}$  satisfies the **selection bias (SB) backdoor criterion** with respect to  $(\underline{x}, \underline{y})$  if

1. all backdoor paths from  $\underline{x}$  to  $\underline{y}$  are blocked by conditioning on  $\underline{z}^{<\underline{x}}$
2.  $\underline{z}^{>\underline{x}} \perp \underline{y}|(\underline{x}, \underline{z}^{<\underline{x}})$
3.  $\underline{y} \perp \underline{s}|(\underline{x}, \underline{z})$

**Claim 128** (*SB Backdoor Adjustment Formula*)

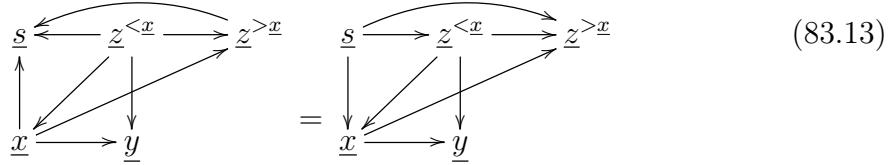
If  $\underline{z}$  satisfies the SB backdoor criterion relative to  $(\underline{x}, \underline{y})$ , then

$$P(y|\mathcal{D}\underline{x} = \underline{x}, \underline{s} = 1) = \sum_z P(y|x, z)P(z) = P(y|x) \quad (83.11)$$

$$\begin{array}{ccc} \underline{s} = 1 & & \sum z \\ \searrow & & \downarrow \\ \mathcal{D}\underline{x} = \underline{x} \longrightarrow y & = & x \longrightarrow y = x \longrightarrow y \end{array} \quad (83.12)$$

**proof:**

If  $z$  satisfies the SB backdoor criterion relative to  $(\underline{x}, \underline{y})$ , then  $\underline{x}, \underline{y}, \underline{z}$  might have the following structure.



See Claim 58 for a proof of this claim for the special case Eq.(83.13).

**QED**

# Chapter 84

## Sentence Splitting with SentenceAx

The Openie6 (O6) software (at github repo Ref.[2]) splits complex or compound sentences into simple ones.<sup>1</sup> Sentence splitting is a necessary step when doing DAG extraction from text (DEFT) (See Chapter 14).

The O6 software is described by its creators in the paper Ref.[30], which we will henceforth refer to as the O6 paper.

The SentenceAx (Sax) software (at github repo Ref.[78]) is a complete rewrite of the O6 software. Sax is 95% identical algorithmically to O6, but it has been rewritten in what we hope is a friendlier form.

Sax is a fine tuning of the BERT model. What this means in the language of Bayesian Networks is that we use BERT as a prior probability. The BERT model is the encoder part of the vanilla Transformer network which we discuss in Chapter 95.

This chapter describes the technical aspects of Sax. Although this chapter can be read without reading the O6 paper, we highly recommend to our readers that they read the O6 paper also. Some parts of this chapter are taken almost verbatim from the O6 paper. Other parts try to fill-in gaps in the explanations provided by the O6 paper or to improve those explanations. Yet others parts describe small changes that we made to the O6 software, in an effort to improve its clarity.

In this chapter, we will use the Numpy-like tensor notation discussed in Section C.48. In particular, note that  $[n] = [0 : n] = \{0, 1, \dots, n - 1\}$  and that  $T^{[n], [m]}$  is an  $n \times m$  matrix.

### 84.1 Preliminary Conventions

#### 84.1.1 Tensor Notation

Our tensor notation is discussed in Section C.48. Here is a quick review of some of the more salient facts in that section on tensors. Below, we will often accompany

---

<sup>1</sup>Simple sentences are essentially the same as the triples (subject, relationship, object) which, when visualized as a directed or undirected graph, is called a “knowledge graph”.

an equation in tensor component notation with the equivalent matrix equation, in parenthesis.

We use Greek letters for tensor indices.

Let  $\alpha \in [a]$ ,  $\beta \in [b]$ ,  $\gamma \in [c]$ ,  $\delta \in [d]$ ,  $\nu \in [n]$ ,  $\Delta \in [D]$ .

- **reshaping**

$$T^{\nu, \delta} \rightarrow T^\Delta \quad (T^{[n_h], [d]} \rightarrow T^{[D]}) \quad (84.1)$$

$$T^\Delta \rightarrow T^{\nu, \delta} \quad (T^{[D]} \rightarrow T^{[n_h], [d]}) \quad (84.2)$$

- **concatenation**

$$T^{[n]} = (T^0, T^1, \dots, T^{n-1}) = (T^\nu)_{\nu \in [n]} \quad (84.3)$$

- **Hadamard product (element-wise, entry-wise multiplication)**

$$T^{[n]} * S^{[n]} = (T^\nu S^\nu)_{\nu \in [n]} \quad (84.4)$$

- **Matrix multiplication**

$T^{[n]} = T^{[n], [1]}$  is a column vector.

$$(T^{[n]})^T S^{[n]} = \text{scalar} \quad (84.5)$$

$$T^{[a], [b]} S^{[b], [c]} = \left[ \sum_{\beta \in [b]} T^{\alpha, \beta} S^{\beta, \gamma} \right]_{\alpha \in [a], \gamma \in [c]} \quad (84.6)$$

Most treatments of Transformer Networks (tranets), including the O6 paper and PyTorch, order the operations chronologically from left to right (L2R). So if  $A$  occurs before  $B$ , they write  $AB$ . This is contrary to what is done in Linear Algebra, where one orders the operations chronologically from right to left (R2L), and one writes  $BA$ . In Chapter 95 on tranets, we followed the Linear Algebra convention. In this chapter, we will follow the PyTorch convention, because Sax is written with PyTorch so it uses the PyTorch convention.

### 84.1.2 PyTorch conventions

- **Linear**

Some pseudo-code

```

lin = nn.Linear(b, a)
y[n],[b] = lin(x[n],[a])

```

In the L2R (left to right) convention followed by PyTorch

$$x^{\nu,[a]} \rightarrow y^{\nu,[b]} = x^{\nu,[a]} W^{[a],[b]} \quad (84.7)$$

for all  $\nu \in [n]$ . Alternatively, in the R2L convention followed in Linear Algebra,

$$x^{[a],\nu} \rightarrow y^{[b],\nu} = W^{[b],[a]} x^{[a],\nu} \quad (84.8)$$

Note that in PyTorch, the rightmost index of the input is the one that is summed over.

The weights matrix  $W^{[b],[a]}$  is learned by training.

- **Dropout**

Some pseudo-code

```

dropo = nn.Dropout(pdrop)
y[n],[a] = dropo(x[n],[a])

```

$$x^{\nu,[a]} \rightarrow y^{\nu,[a]} = x^{\nu,[a]} \mathcal{W}_R^{[a],[a]} \quad (\text{in L2R}) \quad (84.9)$$

$$x^{\nu,[a]} \rightarrow y^{\nu,[a]} = \mathcal{W}_L^{[a],[a]} x^{\nu,[a]} \quad (\text{in R2L}) \quad (84.10)$$

for all  $\nu \in [n]$ .

Dropout learns a weight matrix  $W$  just like `Linear`. But at the end of the training, Dropout flips a coin for each row of  $W_L^{[a],[a]}$  (resp., column of  $W_R^{[a],[a]}$ ), with

$$P(\text{Heads}) = p_{drop}, \text{ and } P(\text{Tails}) = 1 - p_{drop} = p_{keep}.$$

If the coin lands on T, it keeps that row of  $W_L^{[a],[a]}$  (resp., column of  $W_R^{[a],[a]}$ ), whereas if lands on H, it sets that row (resp., column) to zero. Then the matrix is divided by  $p_{keep}$ . The final matrix after all these operations is denoted by  $\mathcal{W}_L$  (resp.,  $\mathcal{W}_R$ ).

- **Embedding**

Some pseudo-code

```

emb = nn.Embedding(num_embeddings=L, embedding_dim=d)
Y[n1],[n2],[d] = emb(λ[n1],[n2])

```

In Sax, we use  $L = 100$  and  $d = 768$  (for BERT base). The  $d$  is the “hidden dimension” of BERT. The  $L$  could be as large as the vocab size of BERT, but since we consider only sentences with 100 words at most, we may set  $L = 100$ .  $L$  doesn’t appear in the final answer because we sum over  $λ ∈ [L]$ .

Next, we explain in more detail the meaning of the tensors  $λ$  and  $Y$ .

Let

$L$  = number of embeddings

$d$  = embedding dimension

$λ ∈ [L]$ ,  $α ∈ [ℓ]$ ,  $ν_1 ∈ [n_1]$ ,  $ν_2 ∈ [n_2]$

$ℓ = ν_1 ν_2$ .

Consider matrices  $Y, E, X$  such that

$$Y^{δ,α} = \sum_{λ} E^{δ,λ} X^{λ,α} \quad (Y^{[d],[ℓ]} = E^{[d],[L]} X^{[L],[ℓ]}) \quad (84.11)$$

Assume that matrix  $X$  has 1-hot columns

$$X^{λ,α} = δ(λ, λ(α)) \quad (84.12)$$

where  $λ() : [ℓ] → [L]$ .

Hence,

$$Y^{δ,α} = E^{δ,λ(α)} \quad (84.13)$$

If we define

$$Λ^α = λ(α) \quad (84.14)$$

then `emb()` maps

$$Λ^α → Y^{δ,α} = E^{δ,λ(α)} \quad (Λ^{[ℓ]} → Y^{[d],[ℓ]}) \quad (84.15)$$

Now replace  $α$  by  $(ν_1, ν_2)$ . `emb()` also maps

$$Λ^{ν_1,ν_2} → Y^{δ,ν_1,ν_2} = E^{δ,λ(ν_1,ν_2)} \quad (Λ^{[n_1],[n_2]} → Y^{[d],[n_1],[n_2]}) \quad (84.16)$$

Actually, `emb()` orders the tensor indices of the output so that the  $δ$  index is on the right side rather than the left side of the input indices. Thus,

$$Y^{[n_1],[n_2],[d]} = emb(Λ^{[n_1],[n_2]}) \quad (84.17)$$

- **Cross Entropy Loss**

Some pseudo-code

```
loss = nn.CrossEntropyLoss()
output = loss(input=x[n_c], target=t[n_s])
```

**Cross Entropy** in Information Theory:

$$H(P_{tar}^\sigma, P_{in}^\sigma) = - \sum_{\gamma \in [n_c]} P_{tar}(\gamma|\sigma) \ln P_{in}(\gamma|\sigma) \quad (84.18)$$

$$= - \sum_{\gamma \in [n_c]} P_{tar}(\gamma|\sigma) \ln \left[ \frac{P_{in}(\gamma|\sigma)}{P_{tar}(\gamma|\sigma)} P_{tar}(\gamma|\sigma) \right] \quad (84.19)$$

$$= H(P_{tar}^\sigma) + D_{KL}(P_{in}^\sigma \| P_{tar}^\sigma) \quad (84.20)$$

**Cross Entropy Loss** in PyTorch:

Let

$n_s$  = total number of samples being considered (usually batch size).  $\sigma \in [n_s]$

$n_c$  = number of classes in classification.  $\gamma \in [n_c]$

$x^{[n_c], [n_s]}$  = input samples

$t^{[n_s]}$  = target samples

Define

$$P_{in}(\gamma|\sigma) = \frac{\exp(x^{\gamma, \sigma})}{\sum_{\gamma' \in [n_c]} \exp(x^{\gamma', \sigma})} \quad (84.21)$$

$$= \text{softmax}(x^{[n_c], \sigma})(\gamma|\sigma) \quad (84.22)$$

Suppose  $W^\gamma : values(t) \rightarrow [0, 1]$  for all  $\gamma \in [n_c]$ .

Define

$$P_{tar}(\gamma|\sigma) = \frac{W^\gamma(t^\sigma) \mathbb{1}(t^\sigma \neq -100)}{\sum_{\gamma \in [n_c]} \text{numerator}} \quad (84.23)$$

The -100 on the right side of the last equation can be replaced by any other integer in  $values(t)$  for which we want the loss to be zero (for example, it could be an integer used for padding)

Now define the cross entropy loss  $\mathcal{L}_{CE}$  by

$$\mathcal{L}_{CE}^\sigma(t^\sigma, x^{[n_c], \sigma}) = H(P_{tar}(\cdot | \sigma), P_{in}(\cdot | \sigma)) \quad (84.24)$$

$$\mathcal{L}_{CE} = \frac{1}{n_s} \sum_{\sigma \in [n_s]} \mathcal{L}_{CE}^\sigma \quad (84.25)$$

For example, if  $W^\gamma = 1$ , and  $n_c = 2$ ,

$$\mathcal{L}_{CE} = \frac{1}{n_s} \sum_{\sigma \in [n_s]} [P_{tar}(0|\sigma) \ln P_{in}(0|\sigma) + P_{tar}(1|\sigma) \ln P_{in}(1|\sigma)] \quad (84.26)$$

- **unsqueeze-repeat-gather**

Some pseudo-code

```
lll_loc = ll_loc0.unsqueeze(2).\
    repeat(1, 1, lll_state.shape[2])
lll_out = torch.gather(
    input=lll_state, dim=1, index=lll_loc)
```

Sax uses the trio of operations unsqueeze-repeat-gather in the manner of the above pseudo-code. We have already discussed in Section C.48 how each of these 3 operations acts individually. Here we will discuss how they act jointly, when used as in the above pseudo-code.

Let

```
lll_state= S^{[s_{ba}], [a], [d]}
ll_loc0= L_0^{[s_{ba}], [a]}
ll_loc= L^{[s_{ba}], [b], [d]}
lll_out= O^{[s_{ba}], [b], [d]}
σ ∈ s_{ba}, α ∈ [a], β ∈ [b], δ ∈ [d]
unsqueeze(2) takes
```

$$L_0^{[s_{ba}], [a]} \rightarrow L_0^{[s_{ba}], [a], 0} \quad (84.27)$$

`lll_state.shape[2]` equals  $d$ , and `repeat(1, 1, d)` takes

$$L_0^{[s_{ba}], [a], 0} \rightarrow L^{[s_{ba}], [a], [d]} = (\underbrace{L_0^{[s_{ba}], [a], 0}, \dots, L_0^{[s_{ba}], [a], 0}}_{d \text{ times}}) \quad (84.28)$$

Now define

$$\lambda(\sigma, \alpha) = L^{\sigma, \alpha, \delta} = L_0^{\sigma, \alpha} \quad (84.29)$$

Then the `gather()` with `dim=1` outputs.

$$O^{\sigma, \alpha, \delta} = S^{\sigma, \lambda(\sigma, \alpha), \delta} \quad (84.30)$$

## 84.2 Bayesian Network for this model

Let

$\ell_{pad} = 86$ , padding length, for this batch  
 $\ell_{enc} = 121$ , encoded length, for this batch,  $\ell_{enc} \geq \ell_{pad}$   
 $n_{dep} = 5$ , number of copies of solid box connected in series, number of depths  
 $n_{att} = 2$ , number of copies of dashed box connected in series, number of iterative (attention) layers.

$d = 768$ , hidden dimension per head  
 $n_h$ , number of heads (BERT base)  
 $D = dn_h$ , hidden dimension for all heads  
 $s_{ba} = 24$ , batch size  
 $n_{il} = 6$ , number of ilabels  
 $d_{me} = 300$ , merge dimension

Fig.84.1 shows the bnet for Sax.<sup>2</sup>. The structural equations, printed in blue, for that bnet, are as follows.

$$\begin{aligned}
\underline{a}^{[86]} &: 11\_greedy\_ilabel \\
\underline{B}^{[121],[768]} &: 111\_hidstate \\
\underline{d}^{[121],[768]} &: 111\_hidstate \\
\underline{E}^{[86],[768]} &: 111\_pred\_code \\
\underline{G}^{[86],[768]} &: 111\_word\_hidstate \\
\underline{I}^{[121],[768]} &: 111\_hidstate \\
\underline{L}^{[86],[6]} &: 111\_word\_score \\
\underline{M}^{[86],[300]} &: 111\_word\_hidstate \\
\underline{S}^{[86],[768]} &: 111\_word\_hidstate \\
\underline{X}^{[86],[6]} &: 111\_word\_score \\
a^{[86]} &= \text{argmax}(X^{[86],[6]}; dim = -1) \\
&\quad : 11\_greedy\_ilabel
\end{aligned} \tag{84.31a}$$

$$\begin{aligned}
B^{[121],[768]} &= \text{BERT}() \\
&\quad : 111\_hidstate
\end{aligned} \tag{84.31b}$$

---

<sup>2</sup>The bnet of Fig.84.1 was drawn with the help of the texnn software (Ref.[80])

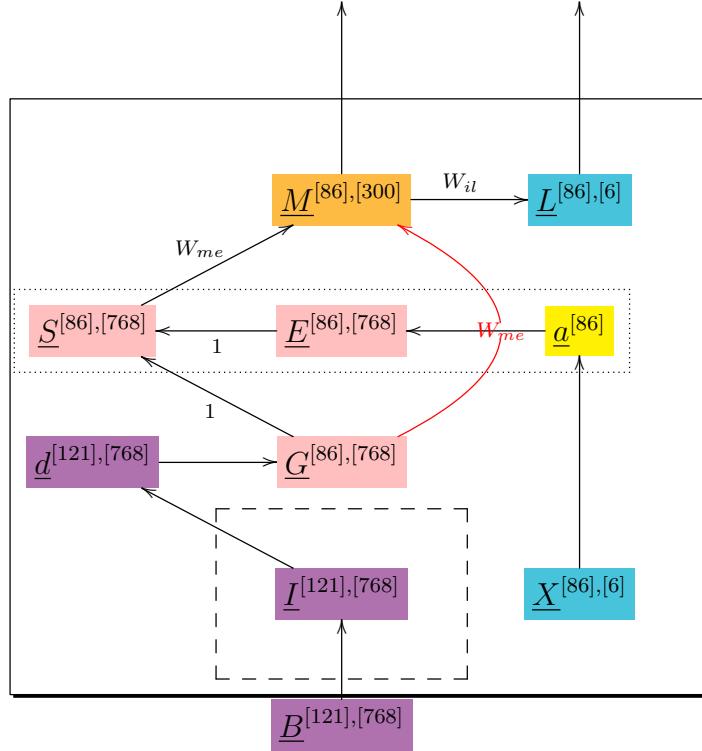


Figure 84.1: Sax bnet. 2 copies of dashed box are connected in series. 5 copies (5 depths) of plain box are connected in series. However, in the first of those 5 plain box copies, the dotted box is omitted and node  $G$  feeds directly into node  $M$  (indicated by red arrow). We display the tensor shape superscripts in the PyTorch L2R order. All tensor shape superscripts have been simplified by omitting a  $[s_{ba}]$  from their left side, where  $s_{ba} = 24$  is the batch size.

$$d^{[121],[768]} = \text{dropout}(I^{[121],[768]}) \quad : \text{111\_hidstate} \quad (84.31c)$$

$$E^{[86],[768]} = \text{embedding}(a^{[86]}) \quad : \text{111\_pred\_code} \quad (84.31d)$$

$$G^{[86],[768]} = \text{gather}(d^{[121],[768]}; \dim = -2) \quad : \text{111\_word\_hidstate} \quad (84.31e)$$

$$I^{[121],[768]} = [B^{[121],[768]} \mathbb{1}(depth = 0) + M^{[86],[300]} \mathbb{1}(depth > 0)] \quad (84.31f)$$

: l11\_hidstate

$$L^{[86],[6]} = M^{[86],[300]} W_{il}^{[300],[6]} \quad (84.31g)$$

: l11\_word\_score

$$M^{[86],[300]} = [G^{[86],[768]} \mathbb{1}(depth = 0) + S^{[86],[768]} \mathbb{1}(depth > 0)] W_{me}^{[768],[300]} \quad (84.31h)$$

: l11\_word\_hidstate

$$S^{[86],[768]} = E^{[86],[768]} + G^{[86],[768]} \quad (84.31i)$$

: l11\_word\_hidstate

$$X^{[86],[6]} = L^{[86],[6]} \mathbb{1}(depth > 0) \quad (84.31j)$$

: l11\_word\_score

### 84.3 Loss $\mathcal{L}$ for this model

The Loss  $\mathcal{L}$  is the sum of the Cross Entropy Loss  $\mathcal{L}_{CE}$  and 4 penalty losses  $\mathcal{L}_i$  for  $i \in PL$  where  $PL = \{POSC, HVC, HVE, EC\}$ .

$$\mathcal{L} = \mathcal{L}_{CE} + \sum_{i \in PL} \lambda_i \mathcal{L}_i \quad (84.32)$$

where the  $\lambda_i$  are hyper-parameters to be determined heuristically.

In an earlier section, we discussed the Cross Entropy Loss at length. In this section, we will discuss the 4 penalty losses.

Below, we will use the standard notation for the **positive-part function** (a.k.a. the **ReLU** function)

$$(x)_+ = \begin{cases} x & \text{if } x \geq 0 \\ 0 & \text{if } x < 0 \end{cases} \quad (84.33)$$

$$= \max(0, x) \quad (84.34)$$

Since loss is supposed to be bounded below (usually it is defined to be greater or equal to zero), the positive-part function comes in handy when defining a loss.

Let

$\ell$  = number of words, length of sentence.  $\alpha \in [\ell]$

$M$  = number of depths.  $\mu \in [M]$

$w^\alpha$  = word at position  $\alpha$

$T_{pos} = \{N, V, JJ, RB\}$ , POS tags, POS=Part Of Speech, N=Noun, V=Verb, JJ=Adjective, RB=Adverb

$T_{ex} = \{S, R, O, N\}$ <sup>3</sup>. extraction tags (extags), S=Subject, R=Relation, O=Object, N=None

$T_{ex} \setminus N = T_{ex} - \{N\}$

$POS^\alpha \in T_{pos}$ , Part Of Sentence of  $w^\alpha$ .

**Importance indicator function.**

$$IMP^\alpha = \mathbb{1}(POS^\alpha \in T_{pos}) \quad (84.35)$$

**Head verb indicator function.** A **head verb** is any verb that isn't a **light verb** (do, be, is, has, etc.).

$$HV^\alpha = \mathbb{1}(w^\alpha \text{ is a head verb}) \quad (84.36)$$

Let  $P(t^{\mu, \alpha} = t)$  denote an empirical probability for a table element  $t^{\mu, \alpha} \in T_{ex}$ , for all  $\mu \in [M]$  and  $\alpha \in [\ell]$ .

The O6 paper uses the following sentence to exemplify the 4 types of penalty losses.

Obama gained popularity after Oprah endorsed him for the presidency.

Henceforth, we will refer to this sentence as the red-sent.

For the red-sent, the head verbs are **gained**, **endorsed**

Two valid extractions from red-sent are: **(Obama; gained; popularity)** and **(Oprah; endorsed him for; the presidency)**.

### 1. Part of Speech Coverage (POSC)

Penalize if some important words do not belong to at least one extraction.

In red-sent: all the words **Obama**, **gained**, **popularity**, **Oprah**, **endorsed**, **presidency** must be covered in the set of extractions.

$$\mathcal{L}_{POSC} = \sum_{\alpha \in [\ell]} IMP^\alpha P_{POSC}(\alpha) \quad (84.37)$$

---

<sup>3</sup>The Sax software uses a different set for  $T_{ex}$  than  $T_{ex} = \{S, R, O, N\}$ . In Sax, we use for  $T_{ex}$  the list **BASE\_EXTAGS** (defined globally in the file **sax\_globals**.) In **BASE\_EXTAGS**, N becomes NONE (or 0) and R becomes REL (or 3). Also note that 2 tranets are trained by Sax, one for extraction (task=ex), and one for splitting (task=cc). For task=cc,  $T_{ex}$  is replaced by  $T_{cc}$ . In Sax, we use for  $T_{cc}$  the list **BASE\_CCTAGS** (defined globally in the file **sax\_globals**.) In **BASE\_CCTAGS**, N becomes NONE (or 0) and R becomes CC (or 3).

$$P_{POSC}(\alpha) = 1 - \max_{\mu \in [M]} \max_{t \in T_{ex} \setminus N} P(\underline{t}^{\mu, \alpha} = t) \quad (84.38)$$

## 2. Head Verb Coverage (HVC)

Penalize if a head verb is not present in the relation (R) of any extraction.

In red-sent: (Obama; gained; popularity), (Obama; gained; presidency) is not a comprehensive set of extractions.

$$\mathcal{L}_{HVC} = \sum_{\alpha \in [\ell]} HV^\alpha P_{HVC}(\alpha) \quad (84.39)$$

$$P_{HVC}(\alpha) = \left| 1 - \sum_{\mu \in [M]} P(\underline{t}^{\mu, \alpha} = R) \right| \quad (84.40)$$

## 3. Head Verb Exclusivity (HVE)

Penalize extractions that contain more than one head verb in their relation (R).

In red-sent: gained popularity after Oprah endorsed is not a good relation as it contains two head verbs

$$\mathcal{L}_{HVE} = \sum_{\mu \in [M]} \left( \sum_{\alpha \in [\ell]} HV^\alpha P(\underline{t}^{\mu, \alpha} = R) - 1 \right)_+ \quad (84.41)$$

## 4. Extraction Count (EC)

Penalize if the total number of extractions with head verbs in the relation (R) is too small; i.e., it is smaller than the number of head verbs in the sentence.

$$\mathcal{L}_{EC} = \left( \sum_{\alpha \in [\ell]} HV^\alpha - \sum_{\mu \in [M]} EC^\mu \right)_+ \quad (84.42)$$

$$EC^\mu = \max_{\alpha \in [\ell]} HV^\alpha P(\underline{t}^{\mu, \alpha} = R) \quad (84.43)$$

# Chapter 85

## Shannon Information Theory

Throughout this book, we often use the definitions of entropy, mutual information, conditional mutual information, cross entropy, etc. All these definitions originated from the seminal work of Claude Shannon. Note that the connection between bnets and Shannon Information Theory (SIT) goes much deeper than that. Most of SIT can be expressed graphically using bnets, as we explain in Ref.[79].

# Chapter 86

## Shapley Explainability

This chapter is based on Refs.[37] and [38], which I highly recommended.

“AI” is an ill-defined term. So is the term “explainability”. So the term “Explainable AI (XAI)” is doubly ill-defined. In 2018, the European Union codified the need for XAI — because of an individual’s “right to explanation” — into a law called the General Data Protection Right (GDPR). This EU law was a strong motivation for Neural Net and boosted decision tree practitioners to come up with a way to enhance their machine learning algorithms so that these comply with that law. Shapley explainability (SX) is one of the most popular methods for doing XAI.

So what does SX do? It ranks, for each individual of a population, the features (for example, race) of a dataset, in the order of how influential those features were in arriving at the decision the classifier made for that individual.

In my opinion, the goal of XAI is accomplished better with bnets than with SX enhanced NNs. SX “explains”, *a posteriori*, the outcome of a model, whereas bnets reveal the *a priori* process whereby that outcome was reached. Thus, SX can tell you that a model is racist, but it can’t suggest how to fix it. On the other hand, if a bnet is acting racist, you don’t have to throw it away. It can be fixed. Another weakness of SX is that it is quite expensive computationally. Bnets have explainability built into them. For bnets, explainability is not an additional, posterior and quite onerous, calculation. That is why I like to call bnets the gold standard of XAI.

Let

$F$  be the feature set. For example,  $F = \{age, gender, job\}$ .

$\mathcal{P}(A) = \{S : S \subset A\}$  be the power set of the set  $A$  (*i.e.*, the set of all subsets of  $A$ , including the empty set  $\emptyset$ ).

$$|\mathcal{P}(A)| = \sum_{k=0}^{|A|} \binom{|A|}{k} = \sum_{k=0}^{|A|} \binom{|A|}{k} 1^k 1^{|A|-k} = (1+1)^{|A|} = 2^{|A|}$$

$\mathcal{P}_f(F) = \{S \in \mathcal{P}(F) : f \in S\}$  for  $f \in F$ , be all sets in  $\mathcal{P}(F)$  containing feature  $f$ . Note that  $\mathcal{P}_f(F) = \mathcal{P}(F) - \mathcal{P}(F - \{f\})$

$\mathcal{P}_{!f}(F) = \{S \in \mathcal{P}(F) : f \notin S\}$  for  $f \in F$ , be all sets in  $\mathcal{P}(F)$  not containing feature  $f$ . Note that  $\mathcal{P}_{!f}(F) = \mathcal{P}(F - \{f\})$

Fig.86.1 shows a graph of  $\mathcal{P}(F)$  for  $F = \{age, gender, job\}$ . Henceforth, we will refer to the generalization of Fig.86.1 to an arbitrary finite set  $F$ , as the **power**

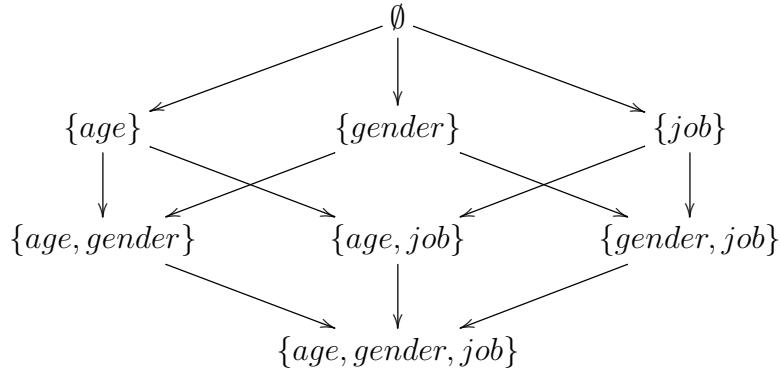


Figure 86.1: Graph of  $\mathcal{P}(F)$  for  $F = \{\text{age}, \text{gender}, \text{job}\}$ . An arrow  $H \leftarrow T$ , where  $H \in \mathcal{P}(F)$  is the head of the arrow and  $T \in \mathcal{P}(F)$  is the tail of the arrow, means  $H \supset T$  and  $|H| = |T| + 1$ .

**set graph of  $F$ .**<sup>1</sup>

For any finite set  $F$ , consider its power set graph. Let  $S \in \mathcal{P}(F)$  be a node of that graph. Let

$$N_{arr/nd}(S) = |S| = \text{number of arrows entering node } S.$$

$$N_{nds}(|S|) = \binom{|F|}{|S|} = \text{number of nodes in level } |S| \text{ (i.e., row } |S|).$$

$N_{arr}(S) = N_{arr/nd}(S)N_{nds}(|S|) = |S|\binom{|F|}{|S|} = \text{number of arrows going from row } |S| - 1 \text{ to row } |S|.$

$$P(S) = \frac{1}{N_{arr}(S)} = \frac{1}{|S|\binom{|F|}{|S|}} = \frac{1}{|F|\binom{|F|-1}{|S|-1}}. \quad (86.1)$$

**Claim 129**

$$\sum_{S \in \mathcal{P}_f(F)} P(S) = 1 \quad (86.2)$$

**proof:**

---

<sup>1</sup>Note that a power set graph is a DAG. We won't define TPMs for its nodes in this chapter, so it's a DAG but not a bnet, in this chapter at least.

$$\sum_{S \in \mathcal{P}_f(F)} P(S) = \sum_{S \in \mathcal{P}_f(F)} \frac{1}{|F| \binom{|F|-1}{|S|-1}} \quad (86.3)$$

$$= \sum_{k=1}^{|F|} \sum_{S \in \mathcal{P}_f(F)} \mathbb{1}(|S|=k) \frac{1}{|F| \binom{|F|-1}{k-1}} \quad (86.4)$$

$$= \sum_{k=1}^{|F|} \frac{1}{|F| \binom{|F|-1}{k-1}} \underbrace{\sum_{S \in \mathcal{P}_f(F)} \mathbb{1}(|S|=k)}_{\binom{|F|-1}{k-1}} \quad (86.5)$$

$$= 1 \quad (86.6)$$

**QED**

Consider any  $S \in \mathcal{P}(F)$ . Henceforth, we will represent a Machine Learning (ML) model  $ML_S$  as follows.  $ML_S$  can be a Linear Regression ( $LR_S$ ) model, a Neural Net model ( $NN_S$ ), or any other type of ML model. We will list a dataset; i.e., a set of tuples indexed by the individuals  $\sigma$  of a population  $\Sigma$  such that  $|\Sigma| = nsam$ . The independent variables of  $ML_S$  (i.e.,  $x_S^\sigma = [x_f^\sigma : f \in S]$ ) will be shown unboxed and the dependent variable (a.k.a. target feature) (i.e.,  $y^\sigma$ ) will be shown inside a box. Then we will show an arrow with the superscript “ML-fit”, followed by the fit function obtained by performing  $ML_S$ .

$$ML_S : \{(\sigma, x_S^\sigma, \boxed{y^\sigma}) : \sigma \in \Sigma\} \xrightarrow{\text{ML-fit}} \hat{y}(x_S) \quad (86.7)$$

For any feature  $f \in F$  and individual  $\sigma \in \Sigma$ , define the **Shapley Value** (SHAP) by

$$SHAP_f^\sigma = \sum_{S \in \mathcal{P}_f(F)} P(S) [\hat{y}(x_S^\sigma) - \hat{y}(x_{S-\{f\}}^\sigma)] \quad (86.8)$$

$$= E_S[\hat{y}(x_S^\sigma) - \hat{y}(x_{S-\{f\}}^\sigma)] \quad (86.9)$$

Hence,

- $SHAP_f^\sigma$  is an average over the ensemble  $\{ML_S : S \in \mathcal{P}_f(F)\}$  for each individual  $\sigma \in \Sigma$ .
- $SHAP_f^\sigma$  averages the change in output  $\hat{y}$  when we change the model from one without feature  $f$  to one with feature  $f$ .
- $SHAP_f^\sigma$  can be negative or positive. Zero  $SHAP_f^\sigma$  for individual  $\sigma$  means feature  $f$  does not influence how the decision  $\hat{y}$  was arrived at for individual  $\sigma$ .

- An exact calculation of  $SHAP_f^\sigma$ , for all  $f$  and for a single  $\sigma$ , requires training a different ML model for each node of the power set graph of  $F$ , so it requires training  $2^{|F|}$  models. Yikes! As  $|F|$  grows, this quickly becomes unfeasible. For large  $|F|$ , one must resort to using sampling and approximations to get an approximation of the SHAP.

### 86.0.1 Numerical examples of SHAP

Next we present 2 numerical examples of SHAP. The figures and numerical values in this section were taken directly from Refs. [37] and [38].

1. Predicting Income from  $F = \{age, gender, job\}$ .

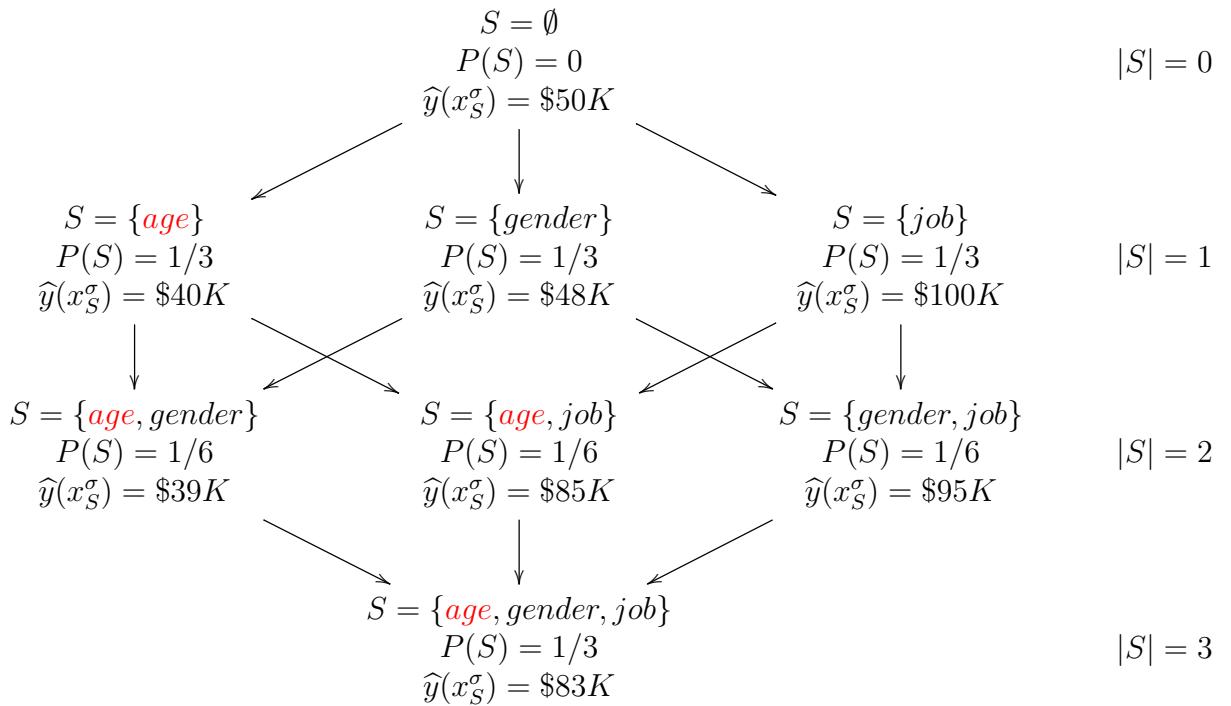


Figure 86.2: Same as Fig.86.1, but with added information for a specific individual  $\sigma$ . This figure contains enough information to evaluate  $SHAP_{age}^\sigma$ .

Consider the problem of predicting the income of a person based on the feature set  $F = \{age, gender, job\}$ . Suppose we are given a dataset for this problem. We can train models  $ML_S$  for each  $S \in \mathcal{P}_{age}(F)$  where  $\hat{y}$  is the income. Then we can calculate the matrix  $SHAP_{age}^\sigma$ . Fig.86.2 gives all the information necessary to calculate  $SHAP_{age}^\sigma$  for a single individual  $\sigma$ .

$$P(S) = \frac{1}{3^{\binom{|S|}{2}}} = \begin{cases} \frac{1}{3^{\binom{2}{0}}} = \frac{1}{3} & \text{if } |S| = 1 \\ \frac{1}{3^{\binom{2}{1}}} = \frac{1}{6} & \text{if } |S| = 2 \\ \frac{1}{3^{\binom{2}{2}}} = \frac{1}{3} & \text{if } |S| = 3 \end{cases} \quad (86.10)$$

$$SHAP_{age}^\sigma = \underbrace{P(age)}_{1/3} [\widehat{y}(x_{age}^\sigma) - \widehat{y}(x_\emptyset^\sigma)] \quad (86.11)$$

$$+ \underbrace{P(age, job)}_{1/6} [\widehat{y}(x_{age, job}^\sigma) - \widehat{y}(x_{job}^\sigma)] \quad (86.12)$$

$$+ \underbrace{P(age, gender)}_{1/6} [\widehat{y}(x_{age, gender}^\sigma) - \widehat{y}(x_{gender}^\sigma)] \quad (86.13)$$

$$+ \underbrace{P(age, gender, job)}_{1/3} [\widehat{y}(x_{age, gender, job}^\sigma) - \widehat{y}(x_{gender, job}^\sigma)] \quad (86.14)$$

$$= -\$11.33K \quad (86.15)$$

## 2. Predicting passenger survival in the Titanic disaster.

	Pclass	Sex	Age	SibSp	Parch	Fare	Embarked
PassengerId							
1	3	male	22.0	1	0	7.2500	S
2	1	female	38.0	1	0	71.2833	C
3	3	female	26.0	0	0	7.9250	S
4	1	female	35.0	1	0	53.1000	S
5	3	male	35.0	0	0	8.0500	S

Figure 86.3: First five rows (passengers) of an abridged version of the Titanic Dataset available at kaggle.com. This figure shows  $(\sigma, x_F^\sigma)$  for  $\sigma = 1, 2, \dots, 5$ . It doesn't show the column  $y^\sigma \in \{died, survived\}$ .

Consider the problem of predicting whether an individual will survive or not based on a Titanic Dataset. We can train models  $ML_S$  for each  $S \in \mathcal{P}(F)$  where  $\widehat{y} \in \{died, survived\}$ . Then we can calculate the matrix  $SHAP_f^\sigma$  for all individuals  $\sigma$  and features  $f$ . Fig.86.0.1 shows the first 5 rows of an abridged<sup>2</sup> version of the Titanic Dataset available at kaggle.com. Fig.86.4 displays  $SHAP_f^\sigma$  in tabular form and Fig.86.5 displays  $SHAP_f^\sigma$  in graphical form (in what is called a beeswarm plot).

---

<sup>2</sup>The Titanic Dataset available at kaggle.com has 891 rows and 15 columns, including columns for passenger ID and for  $y^\sigma = survived? \in \{0, 1\}$ . This abridged version has 8 columns.

	Pclass	Sex	Age	SibSp	Parch	Fare	Embarked
PassengerId							
1	-0.36	-0.76	0.11	0.05	-0.03	-0.3	-0.08
2	1.22	2.18	0.1	0.06	0.1	0.78	0.42
3	-0.75	1.62	0.07	0.1	-0.02	-0.01	-0.13
4	1.15	2.07	0.11	0.05	0.08	0.89	-0.13
5	-0.41	-0.73	-0.06	0.08	-0.03	-0.15	-0.08

Figure 86.4: For the Titanic dataset, this is a table of  $SHAP_f^\sigma$ , where  $\sigma \in \{1, 2, \dots, 5\}$  and  $f \in F$ . Cells with positive SHAP are colored green, and those with negative SHAP are colored red. The colors are not an indication of whether the passenger died or survived. Note that the table of a dataset and the matrix  $SHAP_f^\sigma$  have the same shape ( $|\Sigma|, |F|$ ).

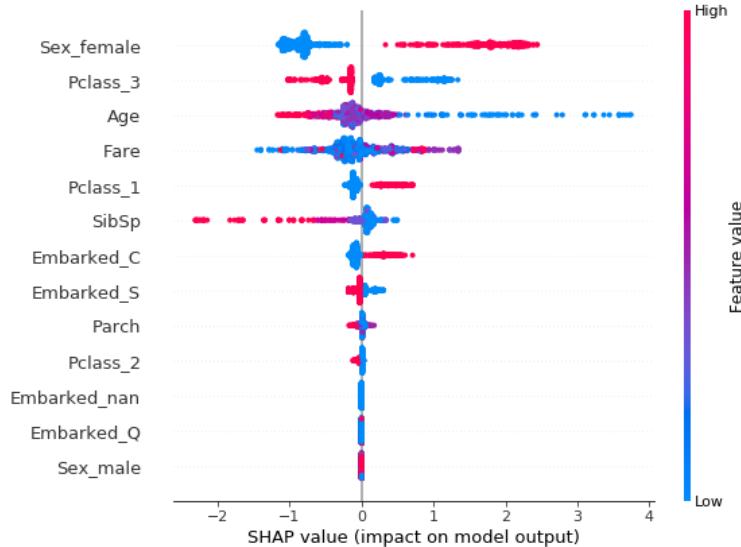


Figure 86.5: For the Titanic Dataset, this is a so called “beeswarm” plot of  $SHAP_f^\sigma$ , where  $\sigma \in \{1, 2, \dots, 891\}$  and  $f \in F$ . In a beeswarm plot, the thickness of each row is proportional to how many individuals of the population have that value of the  $x$  coordinate. This plot comes from Ref.[37], where it was generated using the Titanic Dataset from kaggle.com and the wonderful Python library “SHAP”. The SHAP library can plot Shapley Values in many other styles besides this one.

# Chapter 87

## Simpson's Paradox

This chapter is based on Chapter 6 of "The Book of Why", Ref.[56]. See also Ref.[154] and references therein.

Simpson's paradox is a recurring nightmare for all statisticians overseeing a clinical trial for a medicine. It is possible that if they leave out a certain "confounding" variable from a study, the study's conclusion on whether a medicine is effective or not, might be, without measuring that confounding variable, the opposite of what it would have been had that variable been measured.

Simpson's Paradox is greatly clarified by Judea Pearl's theory of causality. At the end of this chapter, we explain how.

Here is a simple example of Simpson's Paradox.

An equal number of patients of male and female genders are given a heart medicine or a placebo in a double blind study. Some subsequently have a heart attack. Let

$\underline{a}$  = heart attack? No=0, Yes=1

$\underline{t}$  = took medicine? No=0, Yes=1

$\underline{g}$  = gender? Female=F, Male=M

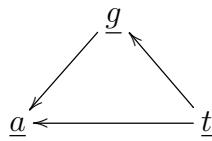


Figure 87.1: bnet for a simple example of Simpson's paradox. Here node  $\underline{g}$  is a chain junction and a mediator.

This situation can be modeled by either bnet Fig.87.1. or bnet Fig.87.2. The two bnets are probabilistically equivalent (i.e., they both represent the same probability distribution  $P(a, t, g)$ ) because

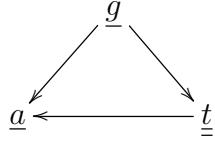


Figure 87.2: bnet that is probabilistically but not physically equivalent to bnet Fig.87.1. Here node  $g$  is a fork junction and a confounder.

$$P(g|t)P(t) = P(g,t) = P(t|g)P(g) . \quad (87.1)$$

For the bnet Fig.87.1, one has

$$P(a,g,t) = P(a|g,t)P(g|t)P(t) . \quad (87.2)$$

Therefore,

$$P(a = 1|t) = \sum_g P(a = 1|t, g)P(g|t) = E_{g|t}P(a = 1|t, g) , \quad (87.3)$$

where  $E_{g|t}$  is a conditional expected value (a kind of weighted average).

Suppose  $q_0, q_1$  are non-negative real numbers. For the vector  $\vec{q} = (q_0, q_1)$ :

Define a negative outcome (or failure or  $q_t$  increasing with  $t$ ) if  $q_0 \leq q_1$ .

Define a positive outcome (or success or  $q_t$  decreasing with  $t$ ) if  $q_0 \geq q_1$ .

Let

$$\vec{q}^g = [P(\underline{a} = 1|t, g)]_{t=0,1} \quad (87.4)$$

for  $g = M, F$ , and

$$\vec{q}^* = [P(\underline{a} = 1|t)]_{t=0,1} . \quad (87.5)$$

It is possible (see Fig.87.3 for a graphical explanation of how) to find perverse cases in which  $P(a = 1|t, g = M)$  and  $P(a = 1|t, g = F)$  increase with  $t$  but  $P(a = 1|t)$  decreases with  $t$ . So it is possible to conclude that the medicine is a failure for each of the two  $g$  populations considered separately, yet the medicine is a success when both populations are “amalgamated”. The lesson is that a “trend reversal” is possible upon amalgamation. Trends are not necessarily preserved when we do a weighted average of type  $E_{g|t}$ .  $E_{g|t}$  is an expected value on the random variable  $g$  conditioned on the root random variable  $t$ .

So far we have assumed  $a \in \{0, 1\}$ . Suppose that instead we assume  $a$  is a continuous variable taking values in the interval  $[0, 1]$ . This could reflect a continuum of possible attacks from none to a deadly one. Likewise, suppose the treatment variable  $t$  takes on values in the interval  $[0, 1]$ . This might reflect a continuum of

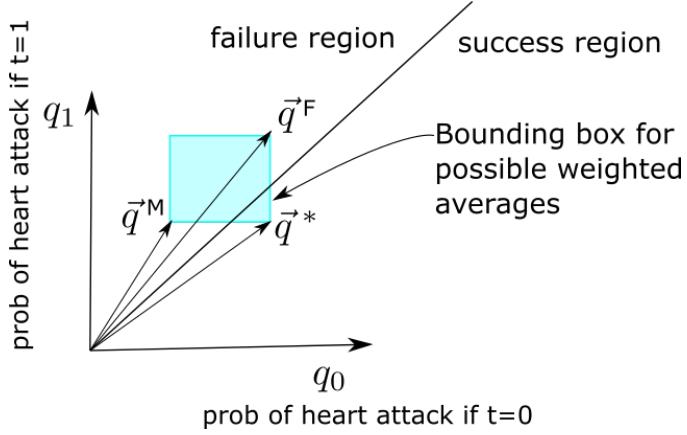


Figure 87.3:  $\vec{q}^M$ ,  $\vec{q}^F$  vectors and bounding box for vector  $\vec{q}^*$ .

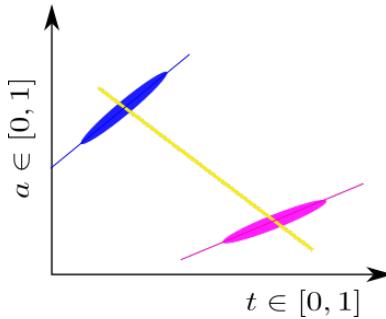


Figure 87.4: Illustrative example of Simpson's paradox, assuming  $t$  and  $a$  are continuous. The pink (for  $g = F$ ) and blue (for  $g = M$ ) elliptical regions are clouds of sample points. The lines are the result of doing linear regression. For  $g = M, F$  separately, increasing treatment increases the probability of attack, but the opposite trend occurs if we amalgamate genders.

possible doses of a medicine. Fig. 87.4 gives an illustrative example of Simpson's paradox for this case of continuous  $a$  and  $t$ .

So far, we have proven that probabilistically, the drug can be a failure for the populations of both sexes considered separately, but a success for the aggregate population.

## 87.1 Pearl Causality

Pearl Causality would add the following two important insights to this problem:

1. bnets Fig.87.1 and Fig.87.2, although they are probabilistically equivalent, do not represent the same physical situation. In fact, only Fig.87.2 occurs in this case.

2. To decide whether the medicine is effective, we must apply a  $do()$  operator to the  $\underline{t}$  variable in Fig.87.2. The effect of that  $do()$  operator is to erase the arrow going from  $g$  to  $\underline{t}$ . This in turn means that the average  $E_{g|\underline{t}}$  in our equation for  $P(a = 1|\underline{t})$  becomes a simpler average  $E_g$  which is independent of  $\underline{t}$ . But for such an average, the bounding box in Fig.87.3 degenerates to its diagonal line that connects the tips of the two vectors  $\vec{q}^M$  and  $\vec{q}^F$ . The vector  $\vec{q}^*$  must now fall on that diagonal line and must therefore also fall in the success region.

In conclusion, as Judea Pearl would say, if we ask the right question to Nature, i.e., what is  $P[a = 1|do(\underline{t} = t)]$  for  $t = 0, 1$ , we get as an answer that the aggregate population preserves rather than reverses the unanimous trend of the two gendered populations.

## 87.2 Numerical Example

$(a, t, g)$	number of patients segregated by gender	number of patients of either gender
0,0,M	19	47
0,0,F	28	
0,1,M	37	49
0,1,F	12	
1,0,M	1	13
1,0,F	12	
1,1,M	3	11
1,1,F	8	

Table 87.1: Data for numerical example of Simpson's Paradox. This fictitious data was taken directly from Table 6.4, page 210 of "The Book of Why", Ref.[56].

$$P(a|t, g) = \begin{array}{c|cccc} & 0,M & 0,F & 1,M & 1,F \\ \hline 0 & 19/20 & 28/40 & 37/40 & 12/20 \\ 1 & 1/20 & 12/40 & 3/40 & 8/20 \end{array} \quad (87.6)$$

$$P(a|t) = \begin{array}{c|cc} & 0 & 1 \\ \hline 0 & 47/60 & 49/60 \\ 1 & 13/60 & 11/60 \end{array} \quad (87.7)$$

$$\frac{P(a=1,t=1,g=M)}{\sum_a P(a,t=1,g=M)} = P(a = 1|t = 1, g = M) = \frac{3}{40} \quad (87.8)$$

$$\frac{P(a=1,t=0,g=M)}{\sum_a P(a,t=0,g=M)} = P(a = 1|t = 0, g = M) = \frac{1}{20} = \frac{2}{40}$$

$$\frac{P(a=1,t=1,g=F)}{\sum_a P(a,t=1,g=F)} = P(a = 1|t = 1, g = F) = \frac{8}{20} = \frac{16}{40} \quad (87.9)$$

$$\frac{P(a=1,t=0,g=F)}{\sum_a P(a,t=0,g=F)} = P(a = 1|t = 0, g = F) = \frac{12}{40}$$

$$\frac{\sum_g P(a=1,t=1,g)}{\sum_g \sum_a P(a,t=1,g)} = P(a = 1|t = 1) = \frac{11}{60} \quad (87.10)$$

$$\frac{\sum_g P(a=1,t=0,g)}{\sum_g \sum_a P(a,t=0,g)} = P(a = 1|t = 0) = \frac{13}{60}$$

Note that the right hand side of Eq.(87.8) is higher for  $t = 1$  than for  $t = 0$ . Same trend occurs in Eqs.87.9 but is reversed in Eqs.87.10.

# Chapter 88

## Structure and Parameter Learning for Bnets

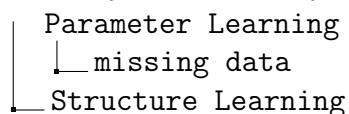
Learning a bnet from data is a computationally intensive NP-complete problem. Therefore, the best one can hope for is for heuristic algorithms that solve this problem approximately. A huge number of such algorithms have been tried and continue to be tried. Luckily, there exists a free open source software library called `bnlearn` that covers many of them. The goal of this chapter is to give a brief overview of the subject of bnet learning, after which we recommend to those readers who want to pursue this subject further, to learn `bnlearn`.

This chapter is based on the `bnlearn` website Ref.[62], and on a 2019 survey paper [63] by Scutari et al. I highly recommend looking at both. Refs. [6] and [35] were also helpful to me in understanding this subject.

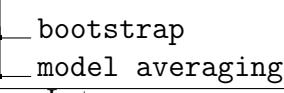
`bnlearn` (Ref.[62]) (free, open source) is very comprehensive and well maintained. It is written mostly in C with an R front-end. It was developed by Marco Scutari and collaborators over a time period of more than 10 years, and is still under active development. How things stand in the field of bnet learning software reminds me of how things stand in the field of linear algebra (LA) software. Perfecting and optimizing LA software takes many years so I would not advise you to write your own LA software library starting from scratch. There is no need to do so. Instead, you can use LAPACK (free, open source), which has been perfected and expanded for decades by world experts. I view `bnlearn` as the LAPACK of bnet learning.

### 88.1 Overview

To give the reader an overview of the subject and of `bnlearn` itself, here is a highly simplified tree, compiled from the `bnlearn` website and documentation, of some of the subjects covered by `bnlearn`.



- tree-like structures given a priori
  - Naive Bayes
  - Chow-Liu tree
  - Tree Augmented Naive Bayes (TAN)
  - ARACNE
- score based
  - algorithms
    - hill climbing (HC)
    - HC with random restarts
    - HC with Tabu list (Tabu)
    - simulated annealing
    - genetic algorithms
  - scoring functions
    - Information Theoretic scores
    - Bayesian Information Criterion (BIC)
    - Bayesian Dirichlet (BD) family
- constraint based
  - algorithms
    - PC family
    - Grow-Shrink (GS)
    - Incremental Association Markov Blanket (IAMB) family
  - conditional independence tests
    - mutual information (parametric, semiparametric and permutation tests)
    - shrinkage-estimate for the mutual information
- hybrid
  - Max-Min Hill Climbing (MMHC)
  - Hybrid HPC (H2PC)
  - General 2-Phase Restricted Maximization (RSMAX2)
- parallel mode structure learning
- node types
  - all-discrete
  - all-continuous
  - mixed
- utility functions
  - model comparison and manipulation
  - random data generation
  - arc orientation testing
  - simple and advanced plots
  - parameter estimation (maximum likelihood and Bayesian)
  - inference, conditional probability queries
  - cross-validation



- 
- Let
- PL=parameters learning (i.e, learning the TPMs)
  - SL= structure learning (i.e., learning the DAG)
  - ML= model (or bnet) learning, SL+PL

PL is easy, once the structure is known. PL assuming no missing data goes as follows. Using the notation of Chapter 82, define

$$\pi_{k|\mu}^i = P(\underline{x}_i = k \mid pa(\underline{x}_i) = \mu) . \quad (88.1)$$

Then  $\pi_{k|\mu}^i$  can be estimated from the data  $N_{k,\mu}^i$  using:

$$\pi_{k|\mu}^i \approx N_{k|\mu}^i = \frac{N_{k,\mu}^i}{N_{+, \mu}^i} . \quad (88.2)$$

PL described by Eq.(88.2) is only for discrete nodes with no missing data. **bnlearn** can also do PL with missing data and continuous (Gaussian linear only) nodes. See Chapter 59 on missing data and Chapter 31 on Gaussian linear nodes. SL actually does PL and SL at the same time.

There are 3 main types of SL: score based, constraint based, and hybrid. **bnlearn** can perform many algorithms of each of these 3 types of SL. It can perform most of them with either all-discrete, or all-continuous or mixed nodes. It can perform many of them in parallel mode. The 2019 survey paper Ref.[63] by Scutari et al compares the performance of many different bnet learning algorithms.

## 88.2 Score based SL algorithms

Score based SL algorithms require scoring bnets (with either all-discrete, all-continuous or mixed nodes). See Chapter 82 for an introduction to scoring bnets. The BIC score explained in that chapter is very popular and works for all-discrete, all-continuous or mixed nodes.

Score-based SL algorithms apply standard optimisation techniques. In the Hill Climbing algorithm, the current best bnet is changed slightly and then given a score that measures how well it fits the data. The bnet with the highest (=best) score so far, as well as that highest score, are stored. (Hence, this is called a greedy search). The process continues until the latest highest score stops changing. The problem with being greedy all the time is that the answer might converge to a local maximum. To mitigate this problem and allow some probability of visiting more than one local maximum, one uses a Tabu Table, random restarts, simulated annealing, genetic algorithms, etc.

### 88.3 Constraint based SL algorithms

To fully understand constraint based SL algorithms, the reader is advised to read Chapters 23 and 67 first.

Constraint based SL algorithms require estimating from the data the conditional independence  $\underline{x} \perp_P \underline{y} | \underline{a}$ . for any 3 disjoint multinodes  $\underline{x}, \underline{y}, \underline{a}$ . This can be done by estimating the conditional mutual information (CMI)  $H(\underline{x} : \underline{y} | \underline{a})$ . `bnlearn` can calculate CMI and other metrics of  $\underline{x} \perp_P \underline{y} | \underline{a}$ . All these metrics are very similar; they all measure how close  $P(x|y, a)$  and  $\bar{P}(x|a)$  are.

The first constraint-based SL algorithm was the Inductive Causation (IC) algorithm proposed by Pearl and Verma in 1991. Incremental improvements have been proposed since then, such as the PC family of algorithms, Grow-Shrink and the Incremental Association Markov Blanket (IAMB) family of algorithms.

## 88.4 Pseudo-code for some bnet learning algorithms

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**Algorithm 4:** Pseudo-code for Hill Climbing algorithm

---

**Input :** Data  $D$ , Vertices  $V$

**Output:** a bnet  $B = (G, T)$ , where  $G = (V, E)$  is a DAG, where  $V$  are its vertices (nodes) and  $E$  are its edges (arrows).  $T$  are all its Transition Probability Matrices (TPMs)  $T = TPMs(G, D)$ .

```

 $E \leftarrow \emptyset$ 
 $T \leftarrow \emptyset$ 
 $B \leftarrow (V, E, T)$ 
 $maxscore \leftarrow -\infty$ 
// DE= all possible directed edges
 $DE = \{\underline{x} \rightarrow \underline{y} \in V \times V : \underline{x} \neq \underline{y}\}$ 
 $again \leftarrow True$ 
while  $again$  do
    for all  $\underline{x} \rightarrow \underline{y} \in DE$  do
        // add arrow
         $E_+ \leftarrow E \cup \{\underline{x} \rightarrow \underline{y}\}$ 
        // delete arrow
         $E_- \leftarrow E - \{\underline{x} \rightarrow \underline{y}\}$ 
        // reverse arrow
         $E_R \leftarrow E_- \cup \{\underline{y} \rightarrow \underline{x}\}$ 
        for  $E' = E_+, E_-, E_R$  do
            if  $E' \neq E$  and  $G' = (V, E')$  is a legal DAG then
                 $T' \leftarrow TPMs(G', D)$ 
                 $B' \leftarrow (G', T')$ 
                 $newscore = \text{BIC-score}(B')$ 
                if  $newscore > maxscore$  then
                     $B \leftarrow B'$ 
                     $maxscore \leftarrow newscore$ 
                else
                     $again \leftarrow False$ 
    return  $B$ 

```

---

---

**Algorithm 5:** Pseudo-code for PC-Stable algorithm

---

**Input :** Data  $D$ , Vertices (nodes)  $V$ , tolerance in CMI  $\epsilon > 0$

**Output:** partially oriented acyclic graph  $G = (V, E, UE)$ , where  $V$  are the vertices (nodes),  $E$  are the oriented edges (arrows) and  $UE$  are the unoriented edges.

```

 $E \leftarrow \emptyset$ 
// initialize  $UE$  to fully-connected undirected graph
 $UE \leftarrow \{\underline{x} - \underline{y} \in V \times V : \underline{x} - \underline{y} = \underline{y} - \underline{x}, \underline{x} \neq \underline{y}\}$ 
// Shrink phase. Deletes edges from  $E$ .
for  $\lambda = 0, 1, 2, \dots, |V| - 2$  do
    for all  $\underline{x} - \underline{y} \in UE$  do
        for all  $S = \{a \in V : \underline{x} - \underline{a} \in UE, \underline{a} \neq \underline{x}, \underline{y}\} \ni |S| = \lambda$  do
            if  $H(\underline{x} : \underline{y}|S) < \epsilon$  then
                /* If there were an arrow between  $\underline{x}$  and  $\underline{y}$ , then
                   conditioning on  $S$  would not be enough to interrupt
                   info transmission  $H(\underline{x} : \underline{y}|S)$  between  $\underline{x}$  and  $\underline{y}$  */
                 $UE \leftarrow UE - \{\underline{x} - \underline{y}\}$ 
                 $S(\underline{x} - \underline{y}) \leftarrow S$ 
            end if
        end for
    end for
end for
// Growth phase. Adds v structures to  $E$ .
for all  $\underline{x}, \underline{y}, \underline{a}$  such that  $\underline{x} - \underline{a} \in UE, \underline{a} - \underline{y} \in UE, \underline{x} - \underline{y} \notin UE, \underline{a} \notin S(\underline{x} - \underline{y})$  do
    /* If there were no collider at  $\underline{a}$ , then there would be info
       transmission between  $\underline{x}$  and  $\underline{y}$  */
     $UE \leftarrow UE - \{\underline{x} - \underline{a}, \underline{a} - \underline{y}\}$ 
     $E \leftarrow E \cup \{\underline{x} \rightarrow \underline{a}, \underline{y} \rightarrow \underline{a}\}$ 
end for
// Orienting edges.
again  $\leftarrow$  True
size  $\leftarrow |UE|$ 
while again do
    for all  $\underline{x} - \underline{y} \in UE$  do
        if  $\underline{x} \rightarrow \underline{y} \in E, \underline{y} - \underline{z} \in UE, \underline{x} - \underline{z} \notin UE, \nexists \underline{w} \ni \underline{w} \rightarrow \underline{y} \in E$  then
            // to avoid introducing new v structure
             $UE \leftarrow UE - \{\underline{y} - \underline{z}\}$ 
             $E \leftarrow E \cup \{\underline{y} \rightarrow \underline{z}\}$ 
        end if
        if  $\underline{x} \rightarrow \underline{y} \in E$  and there is directed path from  $\underline{x}$  to  $\underline{y}$  in  $E$  then
            // to avoid introducing cycles
             $UE \leftarrow UE - \{\underline{x} - \underline{y}\}$ 
             $E \leftarrow E \cup \{\underline{x} \rightarrow \underline{y}\}$ 
        end if
    end for
    newsize  $\leftarrow |UE|$ 
    if size == newsize then
        again  $\leftarrow$  False
    else
        size  $\leftarrow$  newszie
    end if
end while
return  $G = (V, E, UE)$ 

```

---

# Chapter 89

## Support Vector Machines And Kernel Method

This chapter is based on Refs.[128]. [157] and [129].

The Support Vector Machines (SVM) method was first invented with a linear kernel, but was later generalized to arbitrary kernels. We will use the terms SVM method and Kernel Method indistinguishably.

The SVM method is a fairly general method for calculating, via supervised learning, a *binary* classifier. The SVM method finds a continuous surface that separates a space into two disjoint parts.

Let  $\Sigma = [0, 1, 2, \dots, nsam - 1]$  be a list of individuals (samples) in a population. In this chapter, we will use the notation  $A^\sigma = A[\sigma]$  and  $\vec{A} = [A^\sigma : \sigma \in \Sigma]$  for a list (vector, 1-D array) indexed by  $\Sigma$ . We will refer to  $DS = (\vec{x}, \vec{y})$  where  $x^\sigma \in S_{\underline{x}}$ ,  $y^\sigma \in \{-1, 1\}$ , as a dataset. Let  $x^\sigma = (x_0^\sigma, x_1^\sigma, \dots, x_{nf-1}^\sigma) \in S_{\underline{x}_0} \times S_{\underline{x}_1} \times \dots \times S_{\underline{x}_{nf-1}} = S_{\underline{x}}$ . When  $x_j^\sigma \in \mathbb{R}$  for all  $j$ , we will take  $x^\sigma \in \mathbb{R}^{nf}$  to be a column vector.  $x^\sigma$  is the feature vector for individual  $\sigma$ , and its components  $x_i^\sigma$  for  $i = 0, 1, \dots, nf - 1$  are the features.  $y^\sigma \in \{-1, 1\}$  is the binary class to which  $x^\sigma$  belongs.

Let  $\hat{y}(x^{\sigma_0}) \in \{-1, 1\}$  be an estimate of  $y^{\sigma_0} \in \{-1, 1\}$ . The **SVM classifier** is defined as

$$\hat{y}(x^{\sigma_0}) = \text{sign}(Y(x^{\sigma_0})) \quad (89.1)$$

where<sup>1</sup>

$$Y(x^{\sigma_0}) = \sum_{\sigma} \alpha^\sigma y^\sigma K(x^\sigma, x^{\sigma_0}). \quad (89.2)$$

The **binary weight coefficients**  $\alpha^\sigma \in \{0, 1\}$  for all  $\sigma \in \Sigma$  are found by training, via an algorithm to be described below.

The function  $K : S_{\underline{x}} \times S_{\underline{x}} \rightarrow \mathbb{R}$  is called the **Kernel or Similarity function**. We assume that  $K(x^\sigma, x^{\sigma_0})$  grows bigger when its two arguments  $x^\sigma$  and  $x^{\sigma_0}$  become

---

<sup>1</sup>Define  $\text{sign}(0) = 1$ .

more “similar”. We also assume that  $K(x^\sigma, x^{\sigma_0})$  is symmetric in its two arguments.

## 89.1 Learning Algorithm for SVM Classifier

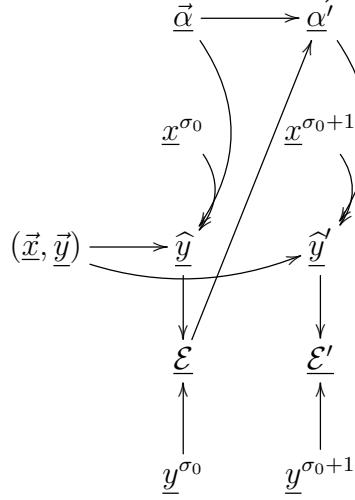


Figure 89.1: Time-slice  $\sigma_0$  of dynamical bnet for learning binary weights  $\vec{\alpha}$  of SVM classifier.

Given a kernel function  $K$  and a dataset  $(\vec{x}, \vec{y})$ , the SVM classifier is fully specified except for its binary weights  $\vec{\alpha}$ . Those weights can be learned via the algorithm represented as a causal diagram in Fig.89.1. That figure shows two time-slices of a dynamical bnet. The TPMs, printed in blue, of bnet Fig.89.1, are as follows:

$$P(\hat{y}|\vec{\alpha}, (\vec{x}, \vec{y}), x^{\sigma_0}) = \mathbb{1}(\hat{y} = \text{ given by Eq.(89.1).}) \quad (89.3)$$

$$P(\mathcal{E}|\hat{y}, y^{\sigma_0}) = \mathbb{1}(\mathcal{E} = \mathbb{1}(\hat{y} \neq y^{\sigma_0})) \quad (89.4)$$

The first (but not the second, third , etc.)  $\vec{\alpha}$  node of Fig.89.1 is a root node. The TPM for that root node should set all components of  $\vec{\alpha}$  to zero:

$$P(\vec{\alpha}) = \prod_{\sigma} \mathbb{1}(\alpha^{\sigma} = 0). \quad (89.5)$$

After that initialization,

$$P(\vec{\alpha}'|\vec{\alpha}, \mathcal{E}) = \mathbb{1}((\alpha')^{\sigma_0} = \alpha^{\sigma_0} + \mathcal{E}) \prod_{\sigma \neq \sigma_0} \mathbb{1}((\alpha')^{\sigma} = \alpha^{\sigma}) \quad (89.6)$$

Why this learning algorithm works.

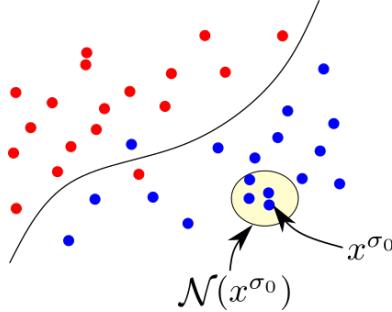


Figure 89.2: Define the neighborhood of  $x^{\sigma_0}$  by  $\mathcal{N}(x^{\sigma_0}) = \{x^\sigma : |K(x^\sigma, x^{\sigma_0})| < \epsilon\}$  for some  $\epsilon > 0$ .

$K(x^\sigma, x^{\sigma_0})$  sets to zero any contribution to  $Y(x^{\sigma_0})$  from points  $x^\sigma$  outside the neighborhood  $\mathcal{N}(x^{\sigma_0})$  of  $x^{\sigma_0}$ . (See Fig.89.2). If  $\hat{y}(x^{\sigma_0}) = y^{\sigma_0}$ , keep  $\alpha^{\sigma_0} = 0$  because the neighbors of  $x^{\sigma_0}$  are giving the correct  $\hat{y}(x^{\sigma_0})$  when they are polled and the majority wins. If, on the other hand,  $\hat{y}(x^{\sigma_0}) \neq y^{\sigma_0}$ , then switch  $\alpha^{\sigma_0}$  from 0 to 1, which means  $x^{\sigma_0}$  gets to vote by adding  $y^{\sigma_0}$  to  $Y(x^{\sigma_0})$ . So we start off with all  $\alpha^\sigma = 0$  and we end with most of them still zero except for a select few. If we were to set all  $\alpha^\sigma$  equal to one, we would get overfitting and a very jagged separation between the two classes. The fact that we end with only a select few  $\alpha^\sigma$  equal to 1, and the rest equal to 0, helps make the demarcation between the two classes less jagged.

## 89.2 Linear (dot-product) Kernel

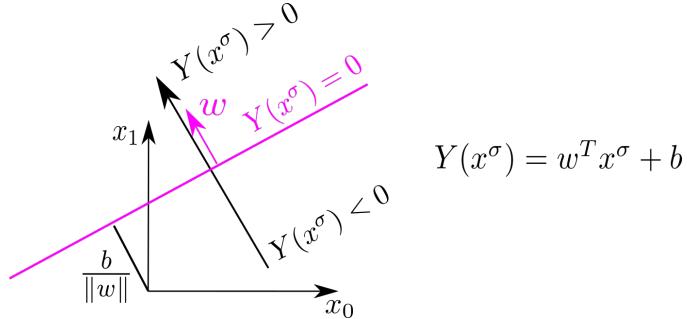


Figure 89.3: Graph of line  $Y(x^\sigma) = 0$  splits plane into regions with  $Y < 0$ ,  $Y = 0$  and  $Y > 0$ .

So far, we have discussed the SVM method for an arbitrary kernel. This section is devoted to the **Linear (a.k.a. dot-product) Kernel**. Said kernel is defined as

$$K(x^\sigma, x^{\sigma_0}) = (x^\sigma)^T x^{\sigma_0} . \quad (89.7)$$

For this kernel, Eq.(89.2) specializes to

$$Y(x^{\sigma_0}) = \sum_{\sigma} \alpha^{\sigma} y^{\sigma} K(x^{\sigma}, x^{\sigma_0}) + b \quad (89.8)$$

$$= w^T x^{\sigma_0} + b \quad (89.9)$$

where

$$w = \sum_{\sigma} \alpha^{\sigma} y^{\sigma} x^{\sigma}. \quad (89.10)$$

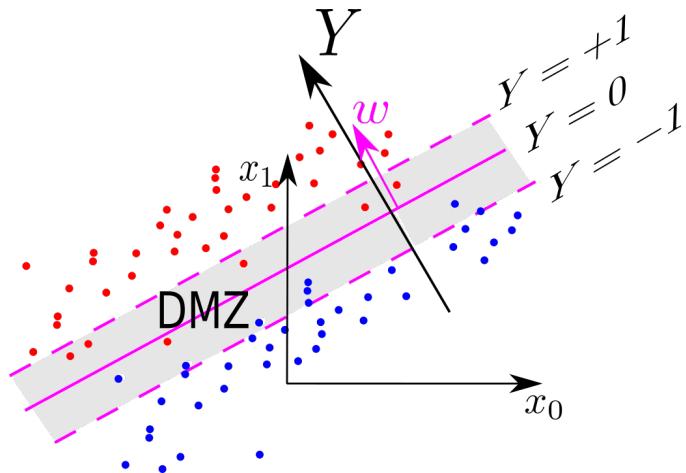


Figure 89.4: We refer to the gray shaded region with  $-1 < Y < 1$ , where  $Y = w^T x + b$ , as the DMZ.

We started this chapter by pulling the SVM classifier out of a hat. We did give reasons why it works, but we did not derive it from a more general minimization principle. Such a derivation is possible, at least in the linear kernel case, and we give it next.

Consider the following 3 straight lines:

$$w^T x^{\sigma} + b = +A \quad (89.11)$$

$$w^T x^{\sigma} + b = 0 \quad (89.12)$$

$$w^T x^{\sigma} + b = -A \quad (89.13)$$

where  $w, x^{\sigma} \in \mathbb{R}^{nf}$ , and  $b, A \in \mathbb{R}$ . We can re-scale the vector  $w$  and scalar  $b$  so as to get rid of the  $A$ . (i.e., replace  $w \rightarrow wA$  and  $b \rightarrow bA$  and divide common factor  $A$  out of equations). This rescaling does not affect the graphs (i.e.,  $x$  loci) of these 3 lines. Now we have:

$$w^T x^\sigma + b = +1 \quad (89.14)$$

$$w^T x^\sigma + b = 0 \quad (89.15)$$

$$w^T x^\sigma + b = -1 \quad (89.16)$$

If  $Y$  stands for

$$Y = w^T x^\sigma + b, \quad (89.17)$$

then we define the **DMZ (demilitarized zone)** to be the region

$$DMZ = \{x^\sigma : |Y(x^\sigma)| < 1\}. \quad (89.18)$$

The lines  $Y = \pm 1$  will be called the **borders (a.k.a. margins)** of the DMZ, and line  $Y = 0$  will be called the **line of demarcation** of the DMZ. The DMZ is illustrated in Fig.89.4.

Let  $D_{DMZ}$  be the **DMZ width** (i.e., the distance from one border of the DMZ to the other.) Position vectors pointing from the origin to either of the two DMZ borders are called **support vectors**. Suppose  $X^+, X^- \in \mathbb{R}^{nf}$  are two support vectors on opposite DMZ borders with  $|X^+ - X^-| = D_{DMZ}$ . Then

$$w^T X^+ + b = 1 \quad (89.19)$$

$$w^T X^- + b = -1 \quad (89.20)$$

so

$$D_{DMZ} = \frac{2}{|w|}. \quad (89.21)$$

For any  $a \in \mathbb{R}$ , let the **positive  $a_+$  and negative  $a_-$  parts of  $a$**  be given by

$$a = \underbrace{a_+}_{a \mathbb{1}(a>0)} + \underbrace{a_-}_{a \mathbb{1}(a \leq 0)}. \quad (89.22)$$

When  $Y = \pm 1$ , an error in  $Y(x^\sigma)$  occurs iff  $y^\sigma Y(x^\sigma) = -1$ . But how should we define errors when  $Y$  is a real number? Define the **Cost of erring for sample  $\sigma$**  to be

$$CE^\sigma(x^\sigma, y^\sigma) = (1 - y^\sigma Y(x^\sigma))_+. \quad (89.23)$$

$CE^\sigma$  is shown in Fig.89.5. As you can see, there is a penalty for living on the incorrect side, and even a penalty for living on the correct side but too close to the DMZ.

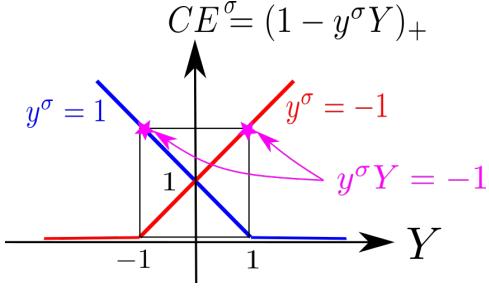


Figure 89.5: Plot of  $CE^\sigma$  versus  $Y$ .

Note that the line of demarcation should have the lowest  $CE^\sigma$  for all possible  $w, b$ . So to find that line, we want to minimize  $CE^\sigma$  with respect to  $w, b$ . But note that  $CE^\sigma \geq 0$ , and it can be zero for an appropriately chosen  $w$ . So we need to add another cost in order to get a non-zero total cost. Define the **DMZ cost** as

$$CZ = \frac{1}{2}|w|^2 = \frac{2}{D_{DMZ}^2} \quad (89.24)$$

Note that  $CZ \rightarrow \infty$  as  $D_{DMZ} \rightarrow 0$ , so  $CZ$  penalizes DMZ's that are too narrow.

Now define a Lagrangian  $\mathcal{L}$  to be the sum of these 2 contributions.

$$\mathcal{L} = CZ + \sum_{\sigma} CE^\sigma \quad (89.25)$$

$$= \frac{1}{2}|w|^2 + \sum_{\sigma} (1 - y^{\sigma}Y(x^{\sigma}))_{+} \quad (89.26)$$

This particular choice of  $CZ$  is not unique, but it isn't totally arbitrary either. We want it to be independent of the sample  $\sigma$ , and to depend on a geometrical aspect of the DMZ, like its width  $D_{DMZ} = 2/|w|$ . Note that  $CE^\sigma$  behaves, when  $|w| \rightarrow \infty$ , linearly in  $|w|$ . We are going to differentiate  $\mathcal{L}$  with respect to  $|w|$  to find an optimum. But straight lines have no optima, so we need  $CZ$  to behave, when  $|w| \rightarrow \infty$ , as  $|w|^p$  for some integer  $p > 1$ .

Setting the variation  $\delta\mathcal{L}$  to zero, we get

$$0 = \delta\mathcal{L} = \delta w_i \left\{ w_i - \sum_{\sigma} \mathbb{1}(y^{\sigma}Y(x^{\sigma}) < 1)y^{\sigma}x_i^{\sigma} \right\} \quad (89.27)$$

so

$$w = \sum_{\sigma} \underbrace{\mathbb{1}(y^{\sigma}Y(x^{\sigma}) < 1)}_{\alpha^{\sigma}} y^{\sigma}x^{\sigma}. \quad (89.28)$$

### 89.3 Alternatives to Linear Kernel

Sometimes it is convenient to replace the dot-product kernel given above by a different kernel. Other popular kernels are:

- **Radial Basis Function (RBF) Kernel.** In this case,  $K$  is a radial function; i.e., a function that depends only on the magnitude (radius, Euclidean distance,  $L^2$  norm) of a vector. An example of an RBF kernel is the **Gaussian Kernel**

$$K(x^\sigma, x^{\sigma_0}) = e^{-\gamma|x^\sigma - x^{\sigma_0}|^2} \quad (89.29)$$

for some free parameter  $\gamma > 0$ .

- **Inhomogeneous Polynomial Kernel**

$$K(x^\sigma, x^{\sigma_0}) = [(x^\sigma)^T x^{\sigma_0} + 1]^d \quad (89.30)$$

for some positive integer  $d$ .

- **Homogeneous Polynomial Kernel**

$$K(x^\sigma, x^{\sigma_0}) = [(x^\sigma)^T x^{\sigma_0}]^d \quad (89.31)$$

for some positive integer  $d$ .

- **"Kernel trick" Kernel.** Consider a map  $\Phi : \mathbb{R}^{nf} \rightarrow \mathbb{R}^N$ . Usually  $N > nf$ .  $\Phi$  can be a rectangular matrix  $A \in \mathbb{R}^{N \times nf}$  so that  $\Phi(x^\sigma) = Ax^\sigma \in \mathbb{R}^N$ . Let

$$K(x^\sigma, x^{\sigma_0}) = [\Phi(x^\sigma)]^T \Phi(x^{\sigma_0}) \quad (89.32)$$

Although the constant surfaces of this kernel are hyperplanes in  $\mathbb{R}^N$ , its constant surfaces in  $\mathbb{R}^{nf}$  can be curved and even closed compact surfaces (e.g. spheres).

### 89.4 Random Forest and Kernel Method

# Chapter 90

## Survival Analysis

This chapter is based on Refs.[169] and [158].

Survival Analysis (SA) is used for curve-fitting, to fit a curve  $S(t)$  to data indicating the number of patients surviving after receiving a treatment for time  $t$ . Alternatively, it can be used with data indicating the number of devices that haven't failed after running for time  $t$ . SA can also be used to compare two such  $S(t)$  curves—for example, one for treated patients, and another for untreated patients. Hence, SA can be used to analyze the data of an RCT.

---

Let

$\sigma \in \Sigma$ , individual (e.g., patient) in population  $\Sigma$ .

$N = |\Sigma|$ , size of  $\Sigma$ , nsam, number of samples

Note: A subset of  $\Sigma$ , (a.k.a, sub-population or stratum) is often called a **cohort** in epidemiology.

$\tau^\sigma \geq 0$ , time to **final event** such as death of an organism, or failure of a device, duration of stay, follow-up time period, time period, lifetime.

$\tau^\sigma = b^\sigma - a^\sigma$  for some absolute times  $a^\sigma, b^\sigma$  satisfying  $a^\sigma < b^\sigma$

$U^\sigma$  = **censoring upper bound**

$L^\sigma$  = **censoring lower bound**

$B^\sigma = \min(b^\sigma, U^\sigma)$ , **right censoring**

$A^\sigma = \max(a^\sigma, L^\sigma)$ , **left censoring**

$T^\sigma = B^\sigma - A^\sigma$ , where  $A^\sigma < B^\sigma$

$d^\sigma = \mathbb{1}(b^\sigma < U^\sigma)$ , equals 1 if death (i.e., no censoring), equals 0 if no death (i.e., censoring)

$e^\sigma = \mathbb{1}(a^\sigma > L^\sigma)$ , equals 1 if death (i.e., no censoring), equals 0 if no death (i.e., censoring)

---

Will only use right censoring in this chapter.

---

For  $t \geq 0$ , define

- **Survival function**  $S(t)$  and **Cumulative hazard function**  $\Lambda(t)$

$$S(t) = P(\tau \geq t) = e^{-\Lambda(t)} \quad (90.1)$$

Note that we define in this chapter  $S(t) = P(\tau \geq t)$  (those present among

survivors (PAS)) instead of  $P(\underline{\tau} > t)$  (not PAS), like other authors do. For continuous functions, these 2 definitions of  $S(t)$  are the same.

Note that, since  $S(t)$  is a probability and  $t, \tau \in [0, \infty]$ ,  $\Lambda(t)$  must be a monotonically increasing function with  $\Lambda(0) = 0$  and  $\Lambda(\infty) = \infty$ .

- **hazard function (a.k.a. instantaneous failure rate)**  $\lambda(t)$

$$\Lambda(t) = \int_0^t du \lambda(u) \quad (90.2)$$

$$\lambda(t) = \Lambda'(t) \quad (90.3)$$

Note that  $\lambda(t) \geq 0$  and its integral over  $[0, \infty]$  must be  $\infty$ .  $\lambda(t)$  is in fact a conditional probability as we show next.

$$\lambda(t) = \frac{P(\underline{\tau} = t)}{S(t)} \quad (\text{shown below}) \quad (90.4)$$

$$= \frac{P(\underline{\tau} = t)}{P(\underline{\tau} \geq t)} \quad (90.5)$$

$$= \frac{P(\underline{\tau} = t, \underline{\tau} \geq t)}{P(\underline{\tau} \geq t)} \quad (\text{because } P(A \wedge B) = P(A) \text{ if } A \text{ implies } B) \quad (90.6)$$

$$= P(\underline{\tau} = t | \underline{\tau} \geq t) \quad (90.7)$$

- **$\underline{\tau}$  density function**  $P_{\underline{\tau}}(t)$

$$P_{\underline{\tau}}(t) = -S'(t) = \lambda(t)e^{-\Lambda(t)} = \lambda(t)S(t) \quad (90.8)$$

- **$\underline{\tau}$  cumulative distribution function**  $\Phi_{\underline{\tau}}(t)$

$$\Phi_{\underline{\tau}}(t) = P(\underline{\tau} < t) = 1 - S(t) \quad (90.9)$$

$$P_{\underline{\tau}}(t) = \Phi'_{\underline{\tau}}(t) \quad (90.10)$$

- **mean survival time**  $\mu$

$$\mu = \int_0^\infty dt tP_{\underline{\tau}}(t) \quad (90.11)$$

- **median survival time**  $\tau_{med}$

$$S(\tau_{med}) = 0.5 \quad (90.12)$$

## 90.1 $S(t)$ estimates

### 90.1.1 No-censoring estimate of $S(t)$

Let

$$r^\sigma(t) = \mathbb{1}(\tau^\sigma \geq t) \quad (90.13)$$

$r^\sigma(t)$  equals 1 iff individual  $\sigma$  at risk (i.e., still alive and not censored, not out) at time  $t$

$$\widehat{S}(t) = \frac{1}{N} \sum_{\sigma} r^\sigma(t) \quad (90.14)$$

$\{\underline{r}^\sigma(t) : \sigma \in \Sigma\}$  are i.i.d.

$\underline{r}^\sigma(t) = \underline{x}$  is a Bernoulli random variable  $Bern(p = S(t))$  (i.e., simple coin flip with  $P(\underline{x} = 1) = p$ ,  $P(\underline{x} = 0) = q$ , mean  $p$  and variance  $pq$ , where  $p = S(t)$ )

$$\widehat{S}(t) \rightarrow \mathcal{N} \left( \mu = S(t), \sigma^2 = \frac{S(t)[1 - S(t)]}{N} \right) \text{ as } N \rightarrow \infty \quad (90.15)$$

(convergence in probability) A sanity check for Eq.(90.15) is to note that

$$\begin{aligned} \langle \widehat{S}(t) \rangle &= \frac{1}{N} \sum_{\sigma} \underbrace{\langle \underline{r}^\sigma(t) \rangle}_{S(t)} \quad (90.16) \\ &= S(t) \end{aligned} \quad (90.17)$$

$$\langle \widehat{S}(t), \widehat{S}(t') \rangle = \frac{1}{N^2} \sum_{\sigma} \sum_{\sigma'} \langle \underline{r}^\sigma(t), \underline{r}^{\sigma'}(t') \rangle \quad (90.18)$$

$$= \frac{1}{N^2} \sum_{\sigma} \langle \underline{r}^\sigma(t), \underline{r}^\sigma(t) \rangle \quad (90.19)$$

$$= \frac{S(t)[1 - S(t)]}{N} \quad (90.20)$$

### 90.1.2 Kaplan-Meier estimate of $S(t)$

Let

---

$[\tau^j]_{j=1,2,\dots,J}$ , times at which there is a final event, all measured from the same time origin, and ordered so that  $\tau^j < \tau^{j+1}$

$n_D^j$  = number of individuals that die at time  $\tau^j$

$n_C^j$  = number of individuals that are censored at time  $\tau^j$

$n_O^j = n_D^j + n_C^j$  number of individuals that drop-Out at time  $\tau^j$ , either because they die or are censored

$n_R^j = \sum_{k \geq j} n_O^k$ , number of individuals that are at risk at or after time  $\tau^j$ (i.e., still alive and not censored, not out, surviving before time  $\tau^j$ )

$d^\sigma \in \{0, 1\}$ , it equals 1 iff individual  $\sigma$  dies at any time.

$d^\sigma(t) \in \{0, 1\}$ , it equals 1 iff individual  $\sigma$  dies at time  $t$ .

$d^\sigma(\tau^j) \in \{0, 1\}$ , it equals 1 iff individual  $\sigma$  dies at time  $\tau^j$ .

$d^\sigma(\tau^j) \rightarrow d(\tau^j)$  since i.i.d.

---

$c^\sigma = 1 - d^\sigma$ , it equals 1 iff individual  $\sigma$  is censored at any time.

$c^\sigma(t) = 1 - d^\sigma(t)$ , it equals 1 iff individual  $\sigma$  is censored at time  $t$ .

$c^\sigma(\tau^j) = 1 - d^\sigma(\tau^j)$ , it equals 1 iff individual  $\sigma$  is censored at time  $\tau^j$ .

$c^\sigma(\tau^j) \rightarrow c(\tau^j)$  since i.i.d.

---

$o^\sigma(t) = \mathbb{1}(\tau^\sigma = t)$ , it equals 1 iff individual  $\sigma$  drops out at time  $t$ .

$o^\sigma(\tau^j) = \mathbb{1}(\tau^\sigma = \tau^j)$ , it equals 1 iff individual  $\sigma$  is drops out at time  $\tau^j$ .

$o^\sigma(\tau^j) \rightarrow o(\tau^j)$  since i.i.d.

---

Note that<sup>1</sup>

$$\underbrace{\bigwedge_{k \leq j} \{o^\sigma(\tau^k) = 0\}}_{\sigma \text{ did not drop out in past or present } \tau^j} = \bigoplus_{k > j} \{o^\sigma(\tau^k) = 1\} \quad (90.21)$$

or, replacing  $o^\sigma$  by  $\underline{o}$ ,

$$\bigwedge_{k \leq j} \{\underline{o}(\tau^k) = 0\} = \bigoplus_{k > j} \{\underline{o}(\tau^k) = 1\} \quad (90.22)$$

<sup>1</sup>notation:  $\wedge_{i=1,2} a_i = (a_1 \wedge a_2) = (a_1 \text{ And } a_2)$ ,  
 $\vee_{i=1,2} a_i = (a_1 \vee a_2) = (a_1 \text{ Or } a_2)$ ,  
 $\oplus_{i=1,2} a_i = (a_1 \oplus a_2) = \text{exclusive or} = \text{modulus 2 addition} = \text{binary addition with } (1 \oplus 1) = 0$ .

Kaplan-Meier (KM) estimate of  $S(t)$  (see<sup>2</sup>)

$$\widehat{S}(\tau^j) = P \left( \bigoplus_{k>j} \{\underline{\varrho}(\tau^k) = 1\} \right) \quad (90.23)$$

$$= P \left( \bigwedge_{k \leq j} \{\underline{\varrho}(\tau^k) = 0\} \right) \quad (90.24)$$

$$= \prod_{k \leq j} P \left( \underline{\varrho}(\tau^k) = 0 \mid \bigwedge_{k' < k} \{\underline{\varrho}(\tau^{k'}) = 0\} \right) \quad (\text{chain rule}) \quad (90.25)$$

$$= \begin{cases} \prod_{k \leq j} P \left( \underline{d}(\tau^k) = 0 \mid \bigwedge_{k' < k} \{\underline{\varrho}(\tau^{k'}) = 0\} \right) \\ + \underbrace{\prod_{k \leq j} P \left( \underline{c}(\tau^k) = 0 \mid \bigwedge_{k' < k} \{\underline{\varrho}(\tau^{k'}) = 0\} \right)}_{=0(\text{see footnote})} \end{cases} \quad (90.26)$$

$$= \prod_{k \leq j} \left[ 1 - P \left( \underline{d}(\tau^k) = 1 \mid \bigwedge_{k' < k} \{\underline{\varrho}(\tau^{k'}) = 0\} \right) \right] \quad (90.27)$$

$$= \prod_{k \leq j} \left[ 1 - \frac{n_D^k}{n_R^k} \right] \quad (90.28)$$

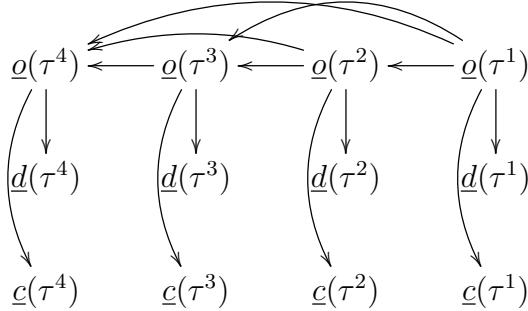


Figure 90.1: Bnet for KM estimate of  $S(t)$  for  $N = 4$ .

Fig.90.1 gives a bnet for the KM estimate of  $S(t)$ . The TPMs, printed in blue, for that bnet, must be as follows:

$$P(\underline{\varrho}(\tau^k) = 1 \mid \bigwedge_{k' < k} \{\underline{\varrho}(\tau^{k'}) = 0\}) = \frac{n_O^k}{n_R^k} \quad (90.29)$$

---

<sup>2</sup>Even though  $S(t)$  has been defined as  $P(\underline{\tau} \geq t)$ , a more precise definition in the presence of censoring is  $P(\underline{\tau} \geq t \mid \text{patient dies rather than being censored})$

$$P(\underline{d}(\tau^k) = 1 \mid \underline{\varrho}(\tau^k) = 1) = \frac{n_D^k}{n_O^k} \quad (90.30)$$

$$P(\underline{c}(\tau^k) = 1 \mid \underline{\varrho}(\tau^k) = 1) = \frac{n_C^k}{n_O^k} \quad (90.31)$$

Intuition: Let

$$\widehat{\lambda}^k = \frac{n_D^k}{n_R^k} \quad (90.32)$$

If  $\widehat{\lambda}^k \ll 1$ , then, since  $e^x \approx 1 + x$  for  $|x| \ll 1$ ,

$$\widehat{S}(\tau^j) \approx \prod_{k \leq j} e^{-\widehat{\lambda}^k} \quad (90.33)$$

$$= \exp\left[-\sum_{k \leq j} \widehat{\lambda}^k\right] \quad (90.34)$$

$$\approx \exp\left[-\int_0^{\tau_j} dt \widehat{\lambda}(t)\right] \quad (90.35)$$

Note that:

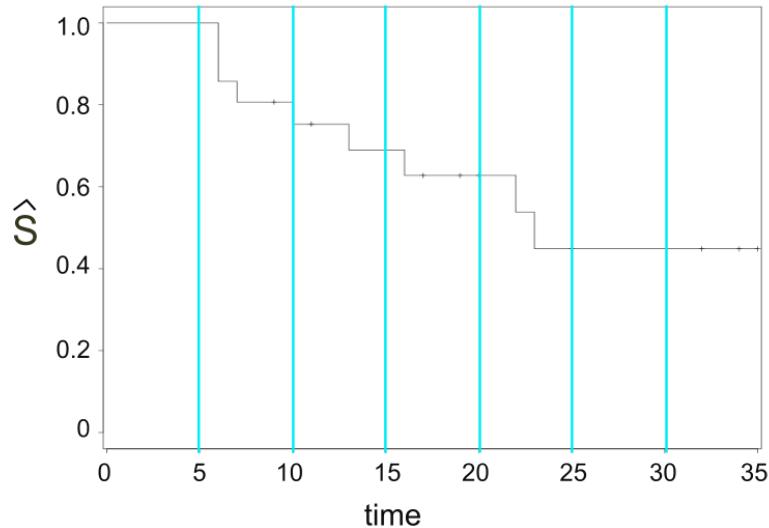
- $\widehat{S}(t)$  only changes when there is a death.
- $\widehat{S}(t) = 1$  before the first death time
- $\widehat{S}(t)$  only goes to 0 if the last observation is a death, so  $n_D^j/n_R^j = 1$ .
- When there is no censoring, the KM estimate equals the no censoring estimate given earlier.

Greenwood's formula for variance of KM estimate of  $S(t)$

$$\left\langle \widehat{S}(t), \widehat{S}(t) \right\rangle = [S(t)]^2 \sum_{k: \tau^{k-1} \leq t} \frac{n_D^k}{n_C^k n_R^k} \quad (90.36)$$

Fig.90.2 and Table 90.1 give a numerical example of the KM estimate.

Fig.90.3 shows relevant parameters for steps  $\tau^{j-1}$  and  $\tau^j$  in a plot of a KM estimate.



6	6	6	6C	7	9C	10
10C	11C	13	16	17C	19C	20C
22	23	25C	32C	32C	34C	35C

Figure 90.2: Plot of KM estimate for  $N = 21$  patients with  $\tau^{\sigma}$  given in table below the plot.  $\tau$ 's with  $C$  are censored.

$j$	$\tau^j$	$n_R^j$	$n_D^j$	$n_C^j$
1	6	21	3	1
2	7	17	1	0
3	9	16	0	1
4	10	15	1	1
5	11	13	0	1

Table 90.1: Parameters  $j, \tau^j, n_R^j, n_D^j, n_C^j$  for first five lifetimes for Fig.90.2.

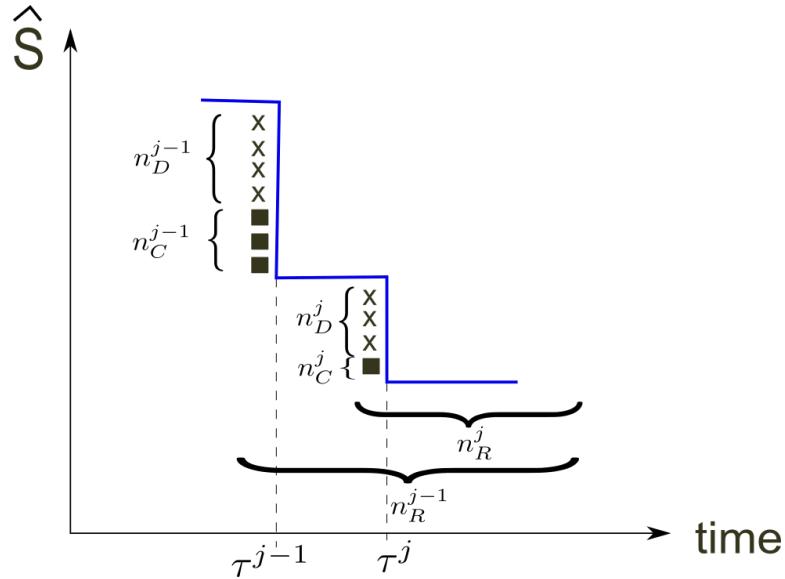


Figure 90.3: Steps  $\tau^{j-1}$  and  $\tau^j$  in a plot of a KM estimate. An **X** indicates a dead individual and **■** a censored one. Note that

$$n_O^j = n_D^j + n_C^j,$$

$$n_R^j = n_R^{j-1} - n_O^j \text{ and}$$

$$n_R^j = \sum_{k \geq j} n_O^k.$$

## 90.2 $\lambda(t)$ models

### 90.2.1 $\lambda(t)$ independent of covariates $Z$

Recall  $t \geq 0$

- $\lambda(t)$  is independent of time

$$\lambda(t) = \lambda \quad (90.37)$$

where  $\lambda \geq 0$ .

$$\Lambda(t) = \lambda t \quad (90.38)$$

$$P_\tau(t) = \lambda e^{-\lambda t} \quad (\text{Exponential distribution}) \quad (90.39)$$

- $\lambda(t)$  is proportional to power of  $t$

$$\lambda(t) = \kappa \lambda t^{\kappa-1} \quad (90.40)$$

where  $\lambda, \kappa \geq 0$ .

$$\Lambda(t) = \lambda t^\kappa \quad (90.41)$$

$$P_{\underline{\tau}}(t) = \kappa \lambda t^{\kappa-1} e^{-\lambda t^\kappa} \quad (\text{Weibull distribution}) \quad (90.42)$$

- $\lambda(t) = a + bt$  for  $a, b \geq 0$
- $\lambda(t)$  is piecewise constant for  $t \in [0, \infty]$
- etc.

Maximum Likelihood Estimate (MLE) of  $\lambda$  for  $\lambda(t) = \lambda$ , allowing censoring: Likelihood function is

$$L(\lambda) = \prod_j [P_{\underline{\tau}}(\tau^j)]^{d(\tau^j)} [S(\tau^j)]^{c(\tau^j)} \quad (90.43)$$

$$= \prod_j [\lambda e^{-\lambda \tau^j}]^{d(\tau^j)} [e^{-\lambda \tau^j}]^{1-d(\tau^j)} \quad (90.44)$$

$$= \prod_j \lambda^{d(\tau^j)} e^{-\lambda \tau^j} \quad (90.45)$$

Hence

$$\ln L(\lambda) = (\ln \lambda) \underbrace{\sum_j d(\tau^j)}_D - \lambda \underbrace{\sum_j \tau^j}_T \quad (90.46)$$

Setting  $\partial_\lambda \ln L = 0$ , we get

$$\hat{\lambda} = \frac{D}{T} \quad (90.47)$$

### 90.2.2 $\lambda(t)$ dependent on covariates $Z$

Suppose  $\beta, Z \in \mathbb{R}^{nind}$  are column vectors, where  $nind$  is number of independent variables (covariates) in a regression.

**Cox Proportional Hazards (PH) model for  $\lambda(t)$**

$$\lambda(t) = \lambda(t|Z) = \lambda_0(t) e^{\beta^T Z} \quad (90.48)$$

where  $\lambda_0(t) \geq 0$ .  $\lambda_0(t)$  is called the **baseline hazard function**. This  $\lambda(t)$  model is called a PH model because  $\lambda(t|Z_1)/\lambda(t|Z_2) = \exp[\beta^T(Z_1 - Z_2)]$  is independent of time. In a **Cox hazards model with time-dependent covariates (TC)**, one assumes that the covariates  $Z(t)$  depend on time.

Note that since exponentials are always positive, the components of  $\beta$  and  $Z$  can range over all real values. If we had chosen  $\lambda(t) = \lambda_0(t)\beta^T Z$  instead, then we would have to constrain  $\beta^T Z \geq 0$ .

If we define

$$\Lambda_0(t) = \int_0^t du \lambda_0(u) \quad (90.49)$$

then

$$P_{\underline{\tau}}(t) = \lambda_0(t)e^{\beta^T Z} \exp[-\Lambda_0(t)e^{\beta^T Z}] \quad (90.50)$$

$P_{\underline{\tau}}(t)$  is called the **Cox PH distribution**. It's a **semi-parametric distribution** because it depends on both, a prior parameter  $\beta$  and a prior function  $\lambda_0(t)$  (a function is like an infinite dimensional parameter). A **parametric distribution** depends only on a prior parameter and a **non-parametric distribution** depends only on a prior function.

Recall that we defined earlier

$n_D^j$  = number of individuals that die at time  $\tau^j$

$n_C^j$  = number of individuals that are censored at time  $\tau^j$

To define the Cox partial likelihood function, we will assume that  $n_D^j + n_C^j = 1$ , i.e., each time  $\tau^j$  has either a single death, or a single censorship, but not both. Since every individual eventually dies or is censored (but, we will assume, not both), there is a 1-1 onto map  $j(\sigma)$  mapping  $\Sigma$  to the set of indices  $j$  of  $\tau^j$ . So we can label the population individuals  $\sigma$  by their index  $j$ , or vice versa.

Let

$$L^j(\beta) = \frac{e^{\beta^T Z^j}}{\sum_{k \geq j} e^{\beta^T Z^k}} \quad (90.51)$$

Then define the **Cox partial likelihood function** by

$$L(\beta) = \prod_j [L^j(\beta)]^{d(\tau^j)} \quad (90.52)$$

Cox's approximate method for finding the best fit for  $\beta$  is to set  $\frac{\partial \ln L(\beta)}{\partial \beta_a} = 0$  for all  $a$ . This does not determine the baseline hazard function, however.

Recall that

$$\lambda(\tau^j | Z^k) = \lambda_0(\tau^j) e^{\beta^T Z^k} = P(\underline{\tau}^k = \tau^j | \underline{\tau}^k \geq \tau^j) \quad (90.53)$$

Therefore

$$L^j(\beta) = \frac{\lambda_0(\tau^j)e^{\beta^T Z^j}}{\sum_{k \geq j} \lambda_0(\tau^j)e^{\beta^T Z^k}} \quad (90.54)$$

$$= \frac{\lambda(\tau^j | Z^j)}{\sum_{k \geq j} \lambda(\tau^j | Z^k)} \quad (90.55)$$

Next, we try to justify Cox's partial likelihood function. We will give two arguments.

### 1. Bayesian argument

Assume that  $Z^k$  is a random variable with a non-informative prior  $P(Z^k) = \mathcal{N}(!k)$ . Then

$$P(Z^k | \tau^j) = f(\tau^j) \underbrace{P(\tau^j | Z^k)}_{\lambda(\tau^j | Z^k)} \quad (90.56)$$

for some function  $f : \mathbb{R} \rightarrow \mathbb{R}$ . Hence

$$L^j(\beta) = \frac{P(Z^j | \tau^j)}{\sum_{k \geq j} P(Z^k | \tau^j)} \quad (90.57)$$

$$= \frac{P(Z^j | \tau^j)}{P(\bigvee_{k \geq j} \{\underline{Z}^k = Z^k\} | \tau^j)} \quad (\text{because the } Z^k \text{ are independent}) \quad (90.58)$$

$$= \frac{P(Z^j, \bigvee_{k \geq j} \{\underline{Z}^k = Z^k\}, \tau^j)}{P(\bigvee_{k \geq j} \{\underline{Z}^k = Z^k\}, \tau^j)} \quad (\text{because } P(A \wedge B) = P(A) \text{ if } A \implies B) \quad (90.59)$$

$$= P(Z^j | \bigvee_{k \geq j} \{\underline{Z}^k = Z^k\}, \tau^j) \quad (90.60)$$

Note that  $L^j(\beta)$  depends on  $\{Z^k : k \geq j\}$  because at time  $j$ , the past  $Z^k$  are fixed already, so the only ones we are allowed to optimize (remember, we are acting as Bayesians here, so we can optimize parameters) are the present and future ones.

### 2. Maximum Likelihood argument

$$L^j(\beta) = \begin{cases} P(\underline{\tau} \geq \tau^j) = S(\tau^j) & \text{if } d(\tau^j) = 0 \text{ (i.e., } c(\tau^j) = 1) \\ P(\underline{\tau} = \tau^j) = \lambda(\tau^j | Z^j)S(\tau^j) & \text{if } d(\tau^j) = 1 \end{cases} \quad (90.61)$$

$$= \lambda(\tau^j | Z^j)^{d(\tau^j)} S(\tau^j) \quad (90.62)$$

$$= \underbrace{\left[ \frac{\lambda(\tau^j | Z^j)}{\sum_{k \geq j} \lambda(\tau^k | Z^j)} \right]^{d(\tau^j)}}_{L_1} \underbrace{\left[ \sum_{k \geq j} \lambda(\tau^k | Z^j) \right]^{d(\tau^j)} S(\tau^j)}_{L_2} \quad (90.63)$$

Cox argued that  $L_2$  varies very slowly with  $\beta$ .

### 90.3 $S_0(t)$ estimates

$$S_Z(t) = e^{-\Lambda(t)} \quad (90.64)$$

$$= e^{-\Lambda_0(t) \exp(\beta^T Z)} \quad (90.65)$$

$$= S_{Z=0}(t)^{\exp(\beta^T Z)} \quad (90.66)$$

**Claim 130** (*Breslow  $S_0(t)$  estimate*)

$$\widehat{S}_0(t) = e^{-\widehat{\Lambda}_0(t)} \quad (90.67)$$

where

$$\widehat{\Lambda}_0(t) = \sum_{j: \tau^j < t} \left[ \frac{n_D^j}{\sum_{k \geq j} e^{\beta^T Z^k}} \right] \quad (90.68)$$

**proof:**

$$\frac{n_D^j}{\Delta t} \approx \sum_{k \geq j} P(\underline{\tau}^k = \tau^j | \underline{\tau}^k \geq \tau^j) \quad (90.69)$$

$$= \sum_{k \geq j} \lambda(\tau^j | Z^k) \quad (90.70)$$

$$= \lambda_0(\tau^j) \sum_{k \geq j} e^{\beta^T Z^k} \quad (90.71)$$

Hence

$$\lambda_0(\tau^j) \Delta t = \frac{n_D^j}{\sum_{k \geq j} e^{\beta^T Z^k}} \quad (90.72)$$

If we now apply  $\sum_{j:\tau^j < t}$  to both sides of the last equation, we get Eq.(90.68).

**QED**

Note that

$$\widehat{S}_0(t) = \prod_{j:\tau^j < t} \exp \left[ \frac{-n_D^j}{\sum_{k \geq j} e^{\beta^T Z^k}} \right] \quad (90.73)$$

$$\approx \prod_{j:\tau^j < t} \left[ 1 - \underbrace{\frac{n_D^j}{\sum_{k \geq j} e^{\beta^T Z^k}}}_{\widehat{\lambda}^j} \right] \text{ (because } e^x \approx 1 + x \text{ for } |x| \ll 1) \quad (90.74)$$

# Chapter 91

## Synthetic Controls

This chapter is based on Refs.[14] and [12].

This chapter assumes that the reader has read Chapter 18 on the Difference-in-Differences (DID) method.

The Synthetic Controls (SC) method is a simple enhancement of the DID method. SC enhances DID in two simple yet powerful ways:

1. **Better time resolution.** DID considers just 2 time-snapshots (i.e., a time-series with only 2 times) whereas SC considers arbitrarily many time-snapshots (i.e., a time-series with more than 2 times).
2. **Weighted average of controls.** DID divides the population of individuals into just 2 kinds: the treated and the untreated (a.k.a. controls). SC divides the total population into treated and controls just like DID does, but it goes further and divides the control population into multiple subpopulations, and calculates a weighted average, called a “synthetic control”, of those subpopulations. The weights of the synthetic control are chosen so that it mimics as closely as possible the behavior of the treated population for all times measured before the treatment was applied.

Let us describe these two enhancements more precisely.

- **timing:** Let  $t_k$  for  $k = 0, 1, \dots, n_{pre} - 1$  be the pre-treatment times at which a measurement occurs. Let  $t_k$  for  $k = n_{pre}, n_{pre} + 1, \dots, n_t - 1$  be the post-treatment times at which a measurement occurs. Note that  $n_{pre} + n_{post} = n_t$ . Note that  $t_* = t_{n_{pre}+1}$  is the first measurement time after the treatment is applied,  $t_0$  is the first measurement time, and  $t_{fin} = t_{n_t-1}$  is the last one.
- **subpopulations:** Let  $S_1 = \{\sigma_1\}$  be the set of treated units (just one). Let  $S_0 = \{\sigma : \sigma \neq \sigma_1\}$  be the set of untreated units (i.e., controls). Let  $nsam$  = number of all units  $\sigma$ ,  $n_1 = |S_1| = 1$ , and  $n_0 = |S_0| = nsam - 1$ .
- **weights:**

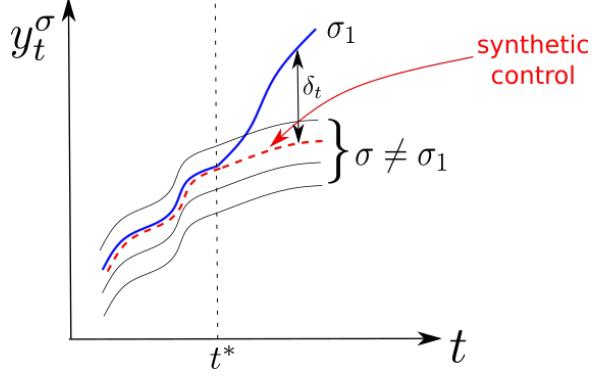


Figure 91.1: Pictorial representation of the Synthetic Controls (SC) method. The outcome  $y$  of the synthetic control unit is colored red and that of the treated unit is colored blue. They roughly agree for  $t < t_*$ .

We want to define a time-independent weight  $w^\sigma$  for each unit  $\sigma$  in such a way that the output  $y_t^\sigma$  for the synthetic control unit behaves like the output for the treated unit  $\sigma_1$  for  $t < t_*$ .

Let

$$w^{\sigma_1} = 0 \quad (91.1)$$

and

$$w^{n_0} = \{w^\sigma\}_{\sigma \neq \sigma_1}. \quad (91.2)$$

Define a cost function  $\mathcal{C}$ :

$$\mathcal{C}(w^{n_0}) = \sum_{t < t_*} \left( y_t^{\sigma_1} - \sum_{\sigma \neq \sigma_1} w^\sigma y_t^\sigma \right)^2 \quad (91.3)$$

Then calculate  $w^{n_0}$  by minimizing the cost function, subject to the constraint that  $w^{n_0}$  be a probability distribution:

$$w^{n_0} = \underset{W^{n_0}}{\operatorname{argmin}} \left\{ \mathcal{C}(W^{n_0}) : W^\sigma \geq 0, \sum_{\sigma \neq \sigma_1} W^\sigma = 1 \right\}. \quad (91.4)$$

---

Now that we have defined a weight  $w^\sigma$  for every unit  $\sigma$ , we can define for  $c \in \{0, 1\}$ ,

$$y_t^{\sigma_1}(c) = \begin{cases} y_t^{\sigma_1} & \text{if } c = 1 \\ \sum_{\sigma \neq \sigma_1} w^\sigma y_t^\sigma & \text{if } c = 0 \end{cases} \quad (91.5)$$

$$\mathcal{Y}_c(t) = E_\sigma[y_t^\sigma(c)] \quad (91.6)$$

and

$$\delta_t = \mathcal{Y}_1(t) - \mathcal{Y}_0(t) \quad (91.7)$$

$\delta_t$  is illustrated in Fig.91.1. It approximates  $ATE(t)$ .

## 91.1 PO analysis

In this section, we show how to analyze the SC method using the formalism of PO theory.

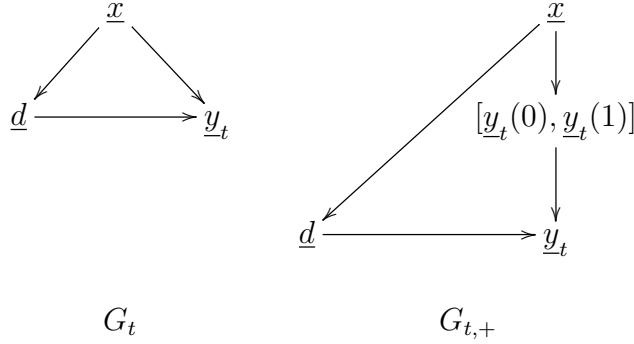


Figure 91.2:  $t \in \{t_0, t_1, \dots, t_{fin}\}$ . Bnet  $G_{t,+}$  is obtained by adding two new nodes  $y_t(0)$  and  $y_t(1)$  to bnet  $G_t$ .

As usual for PO theory, we will consider expected values of  $y_t^\sigma$ :

$$E_{\sigma|d,x}[y_t^\sigma(c)] = E_{y_t(c)|d,x}[y_t(c)] = \mathcal{Y}_{c|d,x}(t) \quad (91.8)$$

To calculate these expected values, we need a “model” with probability distributions. In this case, the needed model and probability distributions are provided by the bnets depicted in Fig.91.2. The TPMs, printed in blue, for the bnet  $G_{t,+}$  in Fig.91.2, are as follows. Note that the TPMs for the bnet  $G_{t,+}$  are defined in terms of the TPMs for the bnet  $G_t$ .

$$P(x) = P_{\underline{x}}(x) \quad (91.9)$$

$$P(d|x) = P_{d|\underline{x}}(d|x) \quad (91.10)$$

$$P(y_t|y_t(0), y_t(1), d) = \mathbb{1}(y_t = y_t(d)) \quad (91.11)$$

$$P(y_t(c)|x) = P(y_t(c)|d, x) = \text{given} \quad (91.12)$$

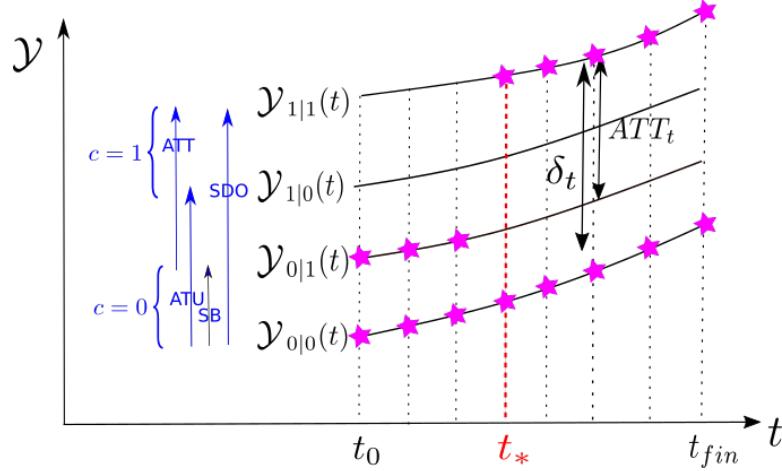


Figure 91.3: Four different time-dependent expected values  $\mathcal{Y}_{c|d}(t)$  of  $y_t^\sigma$  for bnet  $G_{t,+}$ . The  $2 * nt$  magenta stars represents the  $2 * nt$  SC measurements.

Fig.91.3 depicts the four functions  $\mathcal{Y}_{c|d}(t)$  for  $t$  in the interval  $[t_0, t_{fin}]$  and for  $c, d \in \{0, 1\}$ . The  $\mathcal{Y}$  coordinates of the  $2 * nt$  magenta stars in Fig.91.3 can be calculated using bnet  $G_t$ . Note that in Fig.91.3, we display a large gap between the curves  $\mathcal{Y}_{0|d}(t)$  for  $d \in \{0, 1\}$ . In reality,  $P(y_t(0)|d)$  has been constructed so as to make that gap as small as possible. Thus, to a good(?) approximation,

$$\delta_t \approx ATE_t \quad (91.13)$$

Unlike in the DID method, in the SC method, to a good(?) approximation, we don't have to worry about parallel trends.

# Chapter 92

## Targeted Estimator

This chapter is based on Refs.[5] and [25].

Targeted Estimator (TE) theory addresses the following concerns. Suppose  $\Psi[P]$  is an estimator that depends on the full probability distribution  $P$  of a fixed bayesian network.  $\Psi[P]$  is a functional (i.e., a function of a function) of  $P$ . If  $P$  is perturbed by a small amount  $\delta P$ , we get  $\Psi[P + \delta P]$ .  $\Psi[P + \delta P]$  can be expanded in powers of  $\delta P$ . The term linear in  $\delta P$  defines the "influence function"; it also defines the "functional derivative" of  $\Psi$  with respect to  $P$ . *Why are influence functions useful?* The influence function measures, to first order in  $\delta P$ , how the estimator  $\Psi$  responds to a perturbation  $\delta P$  in  $P$ . In general,  $\Psi$  does not have to be a counterfactual estimator, but it might be one, like an estimator of ATE, or PNS or whatever. *So what is this good for?* It is a way of generating linear "targeted" estimators that are less noisy and converge more quickly. It measures the sensitivity of an estimator to perturbations in  $P$ . It does not, however, measure sensitivity to changes in the DAG (the DAG is fixed throughout). And it does not generate new estimands.

The goal of TE and the strategy one uses to achieve it, is explained more precisely in the next section.

### 92.1 Goal, Strategy, and Rationale of TE theory

Let  $\underline{b} = (\underline{b}_1, \underline{b}_2, \dots, \underline{b}_n)$  denote the  $n$  nodes of a Bayesian Network, and let  $P_{\underline{b}}(b)$  for  $b \in S_{\underline{b}}$  denote the full probability distribution of the bnet.

Consider a population  $\Sigma$  of individuals  $\sigma \in \Sigma$  with  $N = |\Sigma|$ . The **empirical probability distribution**  $P_N : S_{\underline{b}} \rightarrow [0, 1]$  for this bnet is defined by

$$P_N(b) = \frac{1}{N} \sum_{\sigma} \delta(b, b_{\sigma}) \quad (92.1)$$

$$\sum_b P_N(b) f(b) = \frac{1}{N} \sum_{\sigma} f(b_{\sigma}) \quad (92.2)$$

As  $N \rightarrow \infty$ ,  $P_N(b)$  tends to the probability distribution  $P_{\underline{b}}(b)$  of the bnet.

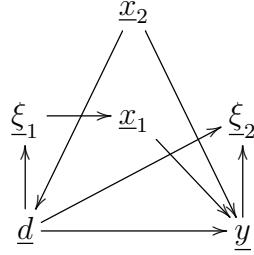


Figure 92.1: Example of bnet considered in TE theory.

Let  $\underline{b} = (\underline{X}, \underline{\xi})$  and  $\underline{X} = (\underline{d}, \underline{x}, \underline{y})$ , where node  $\underline{d} \in \{0, 1\}$  denotes a decision to treat a patient, node  $\underline{y} \in \{0, 1\}$  denotes the treatment outcome, multi-node  $\underline{x}$  denotes the covariates that are good controls, and multi-node  $\underline{\xi}$  denotes the covariates that we don't want to control. See Fig.92.1 for an example of a bnet that fits this description.

The curve-fit  $\hat{y}$  of  $y$  is a function  $\hat{y} : S_{\underline{d}} \times S_{\underline{x}} \rightarrow \mathbb{R}$  that minimizes the **loss** (a.k.a. **loss functional**)  $\mathcal{L}$  given by

$$\mathcal{L}[P, \hat{y}] = \sum_X P(X) \hat{\mathcal{L}}[y, \hat{y}(d, x)]^2, \quad (92.3)$$

where  $\hat{\mathcal{L}}(a, b)$ , the **loss curve-fit**, is a non-negative function that vanishes when  $a = b$ . The function  $\hat{\mathcal{L}}$  is designed to minimize a particular kind of error. In this chapter, the  $\hat{\mathcal{L}}$  is designed to reduce ATE error.

The estimate  $\Psi[P, \hat{y}]$  for the curve-fit  $\hat{y}$  is defined by

$$\Psi[P, \hat{y}] = \sum_X P(X) \hat{y}(d, x) \quad (92.4)$$

Unfortunately, the words "estimator" and "estimate" are often used interchangeably. See Section C.22. In this chapter, we use  $(\hat{y}, \Psi)$  for our (estimator, estimate) pair, and refer to estimators as curve-fits.

Let

$$\delta P(X) = P(X) - P_{in}(X) \quad (92.5)$$

where  $P, P_{in} : S_{\underline{X}} \rightarrow [0, 1]$  are probability distributions.

Define  $\delta\hat{y}(X)$  by

$$\delta\hat{y}(X) = \frac{\hat{y}(d, x)\delta P(X)}{P(X)} \quad (92.6)$$

Hence

$$P(X)\delta\hat{y}(X) = \hat{y}(d, x)\delta P(X) \quad (92.7)$$

Since  $\Psi[P, \hat{y}]$  is linear in  $P$  and  $\hat{y}$ , it follows that

$$\Psi[P, \hat{y} + \delta\hat{y}] = \Psi[P + \delta P, \hat{y}] \quad (92.8)$$

Suppose  $P_{in++}$  satisfies

$$P_{in++} = \underset{P_{in}}{\operatorname{argmin}} \mathcal{L}[P_{in}, \hat{y}] \quad (92.9)$$

and

$$\lim_{N \rightarrow \infty} \Psi[P_N, \hat{y} + \delta\hat{y}] = \lim_{N \rightarrow \infty} \Psi[\underbrace{P_N + \delta P}_{P_{in++}}, \hat{y}] = \lim_{N \rightarrow \infty} \Psi[P_N, \hat{y}] . \quad (92.10)$$

Eq.(92.10) is illustrated in Fig.92.2.

The goal of TE theory is to find, given a curve-fit  $\hat{y}$ , a new curve-fit  $\hat{y} + \delta\hat{y}$  so that the estimate  $\Psi[P_N, \hat{y} + \delta\hat{y}]$  has better behavior as  $N \rightarrow \infty$  than  $\Psi[P_N, \hat{y}]$  (i.e., converges faster, has smaller bias and variance).

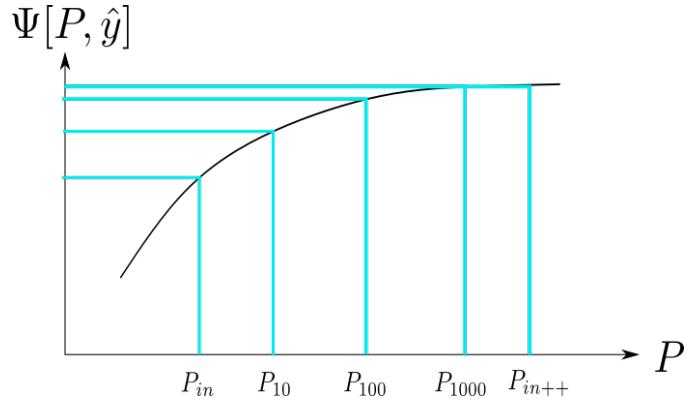


Figure 92.2: Plot of  $\Psi[P, \hat{y}] \in \mathbb{R}$  versus  $P$  at fixed  $\hat{y}$ . In reality, the  $P$  are not real numbers but functions.

## 92.2 Functional Calculus

Define the Hilbert space of square integrable functions over  $\underline{X} \in S_{\underline{X}}$  by

$$\mathcal{H}_{\underline{X}} = \{h : (h : S_{\underline{X}} \rightarrow \mathbb{R}) \text{ and } \sum_{X \in S_{\underline{X}}} [h(X)]^2 < \infty\} \quad (92.11)$$

For any  $f, g \in \mathcal{H}_{\underline{X}}$ , define the dot product (a.k.a. inner product) of  $f$  and  $g$  by

$$f \cdot g = \sum_X f(X)g(X) \quad (92.12)$$

and the norm

$$\| f \|_P = \sqrt{\sum_X [f(X)]^2}. \quad (92.13)$$

Suppose  $P : S_{\underline{X}} \rightarrow [0, 1]$  is a probability distribution. Note that  $P \in \mathcal{H}_{\underline{X}}$ . For any  $f, g \in \mathcal{H}_{\underline{X}}$ , define the  $P$  expected value by

$$\langle f \rangle_P = P \cdot f \quad (92.14)$$

and the  $P$  covariance by

$$\langle f, g \rangle_P = \langle fg \rangle_P - \langle f \rangle_P \langle g \rangle_P \quad (92.15)$$

Suppose  $\Psi[\eta] \in \mathbb{R}$  is a real valued function that depends on a function  $\eta \in \mathcal{H}_{\underline{X}}$ .  $\Psi[\eta]$  is said to be a **functional** of  $\eta$ . Define the **functional derivative or gradient**<sup>1</sup> of  $\Psi[\eta]$  with respect to  $\eta$ , as follows

$$\frac{\delta \Psi[\eta]}{\delta \eta(a)} = \lim_{\epsilon \rightarrow 0} \frac{\Psi[\eta(x) + \epsilon \frac{\delta(x,a)}{\Delta x}] - \Psi[\eta(x)]}{\epsilon} \quad (92.16)$$

where  $\delta(x, a)$  is the Kronecker delta function. For example,

$$\frac{\delta}{\delta \eta(a)} \sum_x \Delta x \eta(x) h(x) = \sum_x \Delta x \frac{\delta(x, a)}{\Delta x} h(x) = h(a) \quad (92.17)$$

Let  $\delta(x - a)$  denote the Dirac delta function. If we replace  $\frac{\delta(x,a)}{\Delta x} \rightarrow \delta(x - a)$  and  $\sum_x \Delta x \rightarrow \int dx$ , we go from the discrete to the continuous version of the functional derivative.

$$\sum_x \Delta x \frac{\delta(x, a)}{\Delta x} \rightarrow \int dx \delta(x - a) \quad (92.18)$$

In this chapter, we will use only the discrete version. The  $\Delta x$  in the numerator and the one in the denominator, always cancel each other when we go from discrete to continuous, so we can set  $\Delta x = 1$  with impunity.

We will also use the notation

$$\nabla \Psi[\eta](a) = \frac{\delta \Psi[\eta]}{\delta \eta(a)}. \quad (92.19)$$

Suppose  $\eta, \eta_0 \in \mathcal{H}_{\underline{X}}$ . Define the **functional Taylor expansion** of  $\Psi[\eta]$  at  $\eta_0$ , as follows:

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<sup>1</sup>Functional derivatives are commonly used in Physics especially in Quantum Field Theory. See Ref.[113] for more information about them.

$$\Psi[\eta] = \Psi[\eta_0] + \sum_x \left[ \frac{\delta \Psi[\eta]}{\delta \eta(x)} \right]_{\eta=\eta_0} \delta \eta(x) + \frac{1}{2!} \sum_{x,x'} \left[ \frac{\delta^2 \Psi[\eta]}{\delta \eta(x) \delta \eta(x')} \right]_{\eta=\eta_0} \delta \eta(x) \delta \eta(x') + \dots \quad (92.20)$$

where we abbreviate  $\eta = \eta(x)$ ,  $\eta_0 = \eta_0(x)$  and  $\delta \eta(x) = \eta(x) - \eta_0(x)$ .

Define the **functional directional derivative of  $\Psi[\eta]$  in the  $h \in \mathcal{H}_X$  direction** by  $h \cdot \frac{\delta \Psi[\eta]}{\delta \eta}$ . If one compares functional calculus with vector calculus, we see that  $\frac{\delta \Psi[\eta]}{\delta \eta}$  corresponds to a gradient  $\nabla f(\vec{x})$  and  $h \cdot \frac{\delta \Psi[\eta]}{\delta \eta}$  corresponds to a directional derivative  $\vec{d} \cdot \nabla f(\vec{x})$ . For  $|\vec{d}| \ll 1$ ,  $\vec{d} \cdot \nabla f(\vec{x})$  approximates the change in  $f(\vec{x})$  when  $\vec{x}$  moves from  $\vec{x}$  to  $\vec{x} + \vec{d}$

### 92.3 Linear Approximation of $\Psi[P_N]$

Consider probability distributions  $P, P_{in} : S_X \rightarrow [0, 1]$ . The **linear approximation (a.k.a. one-step-approximation)** to the Taylor expansion of  $\Psi[P]$  at  $P_{in}$  is given by

$$\underbrace{\Psi[P] - \Psi[P_{in}]}_{\delta \Psi[P, P_{in}]} = \sum_X \underbrace{\left[ \frac{\delta \Psi[P]}{\delta P(X)} \right]_{P=P_{in}}}_{\nabla \Psi[P_{in}](X)} \underbrace{\delta P(X)}_{P(X) - P_{in}(X)} + \mathcal{R}[P, P_{in}] \quad (92.21)$$

If we set

$$\nabla \Psi_{in} = \langle \nabla \Psi[P_{in}] \rangle_{P_{in}}, \quad (92.22)$$

then Eq.(92.21) becomes

$$\delta \Psi[P, P_{in}] = \sum_X P(X) \underbrace{\{\nabla \Psi[P_{in}](X) - \nabla \Psi_{in}\}}_{\lambda(X)} + \mathcal{R}[P, P_{in}] \quad (92.23)$$

$\lambda(X)$  is called the **efficient influence curve (EIF)**.

Recall the Cauchy-Schwartz (CS) inequality for  $\vec{a}, \vec{b} \in \mathbb{R}^n$ :

$$\vec{a} \cdot \vec{b} = |\vec{a}| |\vec{b}| \cos \theta \leq |\vec{a}| |\vec{b}| \quad (92.24)$$

Note that

$$\langle \lambda \rangle_P = \sum_X \lambda(X) \sqrt{P(X)} \sqrt{P(X)} \quad (92.25)$$

$$= (\sqrt{P} \lambda) \cdot \sqrt{P} \quad (92.26)$$

$$\leq \sqrt{\sqrt{P} \lambda \cdot \sqrt{P} \lambda} \underbrace{\sqrt{\sqrt{P} \cdot \sqrt{P}}}_{=1} \quad (\text{by CS inequality}) \quad (92.27)$$

$$\leq \sqrt{\langle \lambda^2 \rangle_P} \quad (92.28)$$

When  $P = P_N$ ,

$$\Psi[P_N] \approx \Psi[P_{in}] + \frac{1}{N} \sum_{\sigma} \lambda(X_{\sigma}) \quad (92.29)$$

If the random variables  $\{\underline{X}_{\sigma}\}_{\sigma \in \Sigma}$  are i.i.d. with probability distribution  $P_{\underline{X}}(X)$ , then, as  $N \rightarrow \infty$ ,  $\Psi[P_N]$  tends to a normally distributed random variable with mean

$$\langle \Psi[P_N] \rangle_{P_{\underline{X}}} = \Psi[P_{in}] + \frac{1}{N} \sum_{\sigma} \langle \lambda(X_{\sigma}) \rangle_{P_{\underline{X}}} \quad (92.30)$$

$$= \Psi[P_{in}] + \langle \lambda \rangle_{P_{\underline{X}}} \quad (92.31)$$

and variance

$$\langle \Psi[P_N], \Psi[P_N] \rangle_{P_{\underline{X}}} = \frac{1}{N^2} \sum_{\sigma} \sum_{\sigma'} \left\langle \lambda(X_{\sigma}), \lambda(X^{\sigma'}) \right\rangle_{P_{\underline{X}}} \quad (92.32)$$

$$= \frac{1}{N} \underbrace{\langle \lambda, \lambda \rangle_{P_{\underline{X}}}}_{\langle \lambda^2 \rangle_{P_{\underline{X}}} - \langle \lambda \rangle_{P_{\underline{X}}}^2} \quad (92.33)$$

Later on, we will discuss the so called TMLE estimate, for which  $P_{in}$  takes a special value  $P_{in++}$  that makes  $\langle \lambda \rangle_{P_{\underline{X}}} = 0$ , so  $\Psi[P_N]$  tends to a normally distributed random variable with mean  $\Psi[P_{in++}]$  and variance  $\frac{1}{N} \langle \lambda^2 \rangle_{P_{\underline{X}}}$ .

## 92.4 ATE estimand

If we set

$$\mathcal{Y}_{|d,x}[P] = \sum_y y P(y|d, x) = P(\underline{y} = 1|d, x) \quad (92.34)$$

and

$$\mathcal{Y}_{|d}[P] = \sum_x \mathcal{Y}_{|d,x}[P] P(x), \quad (92.35)$$

then the **Average Treatment Effect (ATE)** is defined as follows

$$ATE = \mathcal{Y}_{|1}[P_N] - \mathcal{Y}_{|0}[P_N] \quad (92.36)$$

The rest of this chapter is devoted to discussing ATE estimates.

In discussing ATE, it is convenient to define the **propensity**  $g[P]$ :

$$g[P](y) = P(\underline{d} = 1|y) \quad (92.37)$$

and the Kronecker difference function  $\Delta(d)$  for  $d \in \{0, 1\}$ :

$$\Delta(d) = \delta(d, 1) - \delta(d, 0) \quad (92.38)$$

$$= (2d - 1)\mathbb{1}(d \in \{0, 1\}). \quad (92.39)$$

**Claim 131**

$$\left\langle y \frac{\delta(d', d)}{P(d|x)} \right\rangle_P = \mathcal{Y}_{|d'}[P] \quad (92.40)$$

**proof:**

$$\left\langle y \frac{\delta(d', d)}{P(d|x)} \right\rangle_P = \sum_d \sum_y \sum_x P(y|d, x) \cancel{P(d|x)} P(x) y \frac{\delta(d', d)}{\cancel{P(d|x)}} \quad (92.41)$$

$$= \sum_y \sum_x P(y|\underline{d} = d', x) P(x) y \quad (92.42)$$

$$= \mathcal{Y}_{|\underline{d}=d'}[P] \quad (92.43)$$

QED

## 92.5 ATE estimates

### 92.5.1 $\Psi^E$

Empirical (E) estimate  $\Psi^E$ .

$$P_N(y, d, x) = \frac{1}{N} \sum_{\sigma} \delta(y, y_{\sigma}) \delta(d, d_{\sigma}) \delta(x, x_{\sigma}) \quad (92.44)$$

$$P_N(d, x) = \frac{1}{N} \sum_{\sigma} \delta(d, d_{\sigma}) \delta(x, x_{\sigma}) \quad (92.45)$$

$$P_N(x) = \frac{1}{N} \sum_{\sigma} \delta(x, x_{\sigma}) \quad (92.46)$$

$$P_N(y|d, x) = \frac{P_N(y, d, x)}{P_N(d, x)} \quad (92.47)$$

$$\Psi^E = \sum_x P_N(x) \sum_y y \sum_d P_N(y|d, x) \Delta(d) \quad (92.48)$$

### 92.5.2 $\Psi^G$

**G estimate**  $\Psi^G$  (a.k.a. g-computing or g-formula estimate).

Use Generalized Linear Modeling (GLM)<sup>2</sup> to approximate  $y_{\sigma}$ :

$$y_{\sigma} \approx E_{\underline{y}|d_{\sigma}, x_{\sigma}; \hat{\beta}}[\underline{y}] , \quad (92.49)$$

where  $\hat{\beta}$  are the best curve fit parameters.

$$\Psi^G = \sum_x P_N(x) \{ E_{\underline{y}|d=1, x; \hat{\beta}}[\underline{y}] - E_{\underline{y}|d=0, x; \hat{\beta}}[\underline{y}] \} \quad (92.50)$$

### 92.5.3 $\Psi^{IPW}$

**Inverse Propensity Weighted (IPW) estimate**  $\Psi^{IPW}$  (a.k.a. Inverse Probability of Treatment Weighted (IPTW) estimate).

Assume propensity  $P(\underline{d} = 1|x)$  is known.

Define

$$\Psi^{IPW}[P] = \left\langle y \frac{\Delta(d)}{P(d|x)} \right\rangle_P \quad (92.51)$$

$$\Psi^{IPW} = \Psi^{IPW}[P_N] = \left\langle y \frac{\Delta(d)}{P(d|x)} \right\rangle_{P_N} = \frac{1}{N} \sum_{\sigma} y_{\sigma} \frac{\Delta(d_{\sigma})}{P(d_{\sigma}|x_{\sigma})} \quad (92.52)$$

### 92.5.4 $\Psi^{LIPW}$

**Linearized IPW (LIPW) estimate**  $\Psi^{LIPW}$ .

$\Psi^{LIPW}$  is the linear approximation of  $\Psi^{IPW}[P_N]$  at point  $P_{in}$ :

$$\Psi^{LIPW} = \Psi^{IPW}[P_{in}] + \left\langle \nabla \Psi^{IPW}[P_{in}] \right\rangle_{P_N} - \nabla \Psi^{IPW}_{in} \quad (92.53)$$

---

<sup>2</sup>GLM is discussed in Chapter 32.

**Claim 132**

$$\nabla \Psi^{IPW}[P](X) = \mathcal{Y}_{|1,x}[P] - \mathcal{Y}_{|0,x}[P] + \frac{\Delta(d)}{P(d|x)}(y - \mathcal{Y}_{|d,x}[P]) \quad (92.54)$$

**proof:**

$$\frac{\delta \Psi^{IPW}[P]}{\delta P(X)} = \sum_{X'} y' \Delta(d') \frac{\delta}{\delta P(X)} \frac{P(X')}{P(d'|x')} \quad (92.55)$$

$$\frac{\delta}{\delta P(X)} \frac{P(X')}{P(d'|x')} = \frac{\delta(X, X')}{P(d'|x')} - \frac{P(X')}{[P(d'|x')]^2} \frac{\delta P(d'|x')}{\delta P(X)} \quad (92.56)$$

$$= \frac{\delta(X, X')}{P(d'|x')} - \frac{P(X')}{P(d'|x')} \frac{\delta \ln P(d'|x')}{\delta P(X)} \quad (92.57)$$

$$= \underbrace{\frac{\delta(X, X')}{P(d'|x')}}_{\delta^3/P(d'|x')} - P(y'|d', x') P(x') \frac{\delta \ln P(d'|x')}{\delta P(X)} \quad (92.58)$$

$$\frac{\delta \ln P(d', x')}{\delta P(X)} = \frac{1}{P(d', x')} \sum_{y'} \frac{\delta P(X')}{\delta P(X)} \quad (92.59)$$

$$= \underbrace{\frac{\delta(d, d') \delta(x, x')}{P(d', x')}}_{\delta^2/P(d', x')} \quad (92.60)$$

$$\frac{\delta \ln P(x')}{\delta P(X)} = \underbrace{\frac{\delta(x, x')}{P(x')}}_{\delta^1/P(x')} \quad (92.61)$$

$$\frac{\delta \ln P(d'|x')}{\delta P(X)} = \frac{\delta^2}{P(d', x')} - \frac{\delta^1}{P(x')} \quad (92.62)$$

$$\frac{\delta}{\delta P(X)} \frac{P(X')}{P(d'|x')} = \frac{\delta^3}{P(d'|x')} - P(y'|d', x') P(x') \left[ \frac{\delta^2}{P(d', x')} - \frac{\delta^1}{P(x')} \right] \quad (92.63)$$

$$\sum_{X'} y' \Delta(d') \left[ \frac{\delta^3}{P(d'|x')} \right] = \boxed{\frac{\Delta(d)}{P(d|x)} y} \quad (92.64)$$

$$\sum_{X'} y' \Delta(d') \left[ \frac{-P(y'|d', x')\delta^2}{P(d'|x')} \right] = - \sum_{y'} y' \Delta(d) \frac{P(y'|d, x)}{P(d|x)} \quad (92.65)$$

$$= \boxed{\frac{\Delta(d)}{P(d|x)} (-\mathcal{Y}_{|d,x}[P])} \quad (92.66)$$

$$\sum_{X'} y' \Delta(d') [P(y'|d', x')\delta^1] = \sum_{y'} \sum_{d'} y' \Delta(d') P(y'|d', x) \quad (92.67)$$

$$= \boxed{\mathcal{Y}_{|1,x}[P] - \mathcal{Y}_{|0,x}[P]} \quad (92.68)$$

QED

**Claim 133**

$$\langle \nabla \Psi^{IPW}[P] \rangle_P = \Psi^{IPW}[P] \quad (92.69)$$

Hence,

$$\nabla \Psi_{in}^{IPW} = \langle \nabla \Psi^{IPW}[P_{in}] \rangle_{P_{in}} = \Psi^{IPW}[P_{in}] \quad (92.70)$$

**proof:**

$$\nabla \Psi^{IPW}[P](X) = \mathcal{Y}_{|1,x}[P] - \mathcal{Y}_{|0,x}[P] + \frac{\Delta(d)}{P(d|x)} (y - \mathcal{Y}_{|d,x}[P]) \quad (92.71)$$

$$\langle \mathcal{Y}_{|1,x}[P] - \mathcal{Y}_{|0,x}[P] \rangle_P = \sum_x P(x) (\mathcal{Y}_{|1,x}[P] - \mathcal{Y}_{|0,x}[P]) \quad (92.72)$$

$$= \Psi^{IPW}[P] \quad (92.73)$$

$$\left\langle \frac{\Delta(d)}{P(d|x)} y \right\rangle_P = \Psi^{IPW}[P] \quad (92.74)$$

$$\left\langle \frac{\Delta(d)}{P(d|x)} \mathcal{Y}_{|d,x}[P] \right\rangle_P = \sum_y \sum_x \sum_d P(y|d, x) P(x) \Delta(d) \mathcal{Y}_{|d,x}[P] \quad (92.75)$$

$$= \sum_x \sum_d P(x) \Delta(d) \mathcal{Y}_{|d,x}[P] \quad (92.76)$$

$$= \Psi^{IPW}[P] \quad (92.77)$$

**QED**

Note the following cancellation:

$$\Psi^{IPW}[P] = \Psi^{IPW}[P_{in}] + \langle \nabla \Psi^{IPW}[P_{in}] \rangle_P - \nabla \Psi_{in}^{IPW} + \mathcal{R}^{IPW}[P, P_{in}] \quad (92.78)$$

$$= \cancel{\Psi^{IPW}[P_{in}]} + \langle \nabla \Psi^{IPW}[P_{in}] \rangle_P - \cancel{\Psi^{IPW}[P_{in}]} + \mathcal{R}^{IPW}[P, P_{in}] \quad (92.79)$$

$$= \langle \nabla \Psi^{IPW}[P_{in}] \rangle_P + \mathcal{R}^{IPW}[P, P_{in}] \quad (92.80)$$

**Claim 134**

$$\mathcal{R}^{IPW}[P, P_{in}] = - \sum_x P(x) \sum_d \Delta(d) (P(d|x) - P_{in}(d|x)) \left( \frac{\mathcal{Y}_{|d,x}[P] - \mathcal{Y}_{|d,x}[P_{in}]}{P_{in}(d|x)} \right) \quad (92.81)$$

**proof:**

$$\mathcal{R}^{IPW}[P, P_{in}] = \Psi^{IPW}[P] - \langle \nabla \Psi^{IPW}[P_{in}] \rangle_P \quad (92.82)$$

$$= \left\langle y \frac{\Delta(d)}{P(d|x)} - \left( \mathcal{Y}_{|1,x}[P_{in}] - \mathcal{Y}_{|0,x}[P_{in}] + \frac{\Delta(d)}{P_{in}(d|x)} (y - \mathcal{Y}_{|d,x}[P_{in}]) \right) \right\rangle_P \quad (92.83)$$

$$= \begin{cases} \sum_x P(x) (-\mathcal{Y}_{|1,x}[P_{in}] + \mathcal{Y}_{|0,x}[P_{in}]) \\ + \sum_{d,x} P(d, x) \left( \frac{\Delta(d)}{P_{in}(d|x)} \mathcal{Y}_{|d,x}[P_{in}] \right) \\ + \sum_{y,d,x} P(y, d, x) \left( \frac{1}{P(d|x)} - \frac{1}{P_{in}(d|x)} \right) y \Delta(d) \end{cases} \quad (92.84)$$

$$= \sum_x P(x) \sum_d \Delta(d) \begin{cases} \left( \frac{P(d|x)}{P_{in}(d|x)} - 1 \right) \mathcal{Y}_{|d,x}[P_{in}] \\ + \sum_y P(y|d, x) \left( \frac{P_{in}(d|x) - P(d|x)}{P_{in}(d|x)} \right) y \end{cases} \quad (92.85)$$

$$= \sum_x P(x) \sum_d \Delta(d) \left( \frac{P(d|x) - P_{in}(d|x)}{P_{in}(d|x)} \right) (\mathcal{Y}_{|d,x}[P_{in}] - \mathcal{Y}_{|d,x}[P]) \quad (92.86)$$

**QED**

Claim 134 allows us to put a bound on the absolute value of the remainder  $\mathcal{R}^{IPW}$ :

$$|\mathcal{R}^{IPW}[P, P_{in}]| \leq \sum_d \sum_x \underbrace{\sqrt{P(x)} |P(d|x) - P_{in}(d|x)|}_{A(d,x)} \underbrace{\sqrt{P(x)} \left| \frac{\mathcal{Y}_{|d,x}[P] - \mathcal{Y}_{|d,x}[P_{in}]}{P_{in}(d|x)} \right|}_{B(d,x)} \\ (\text{because } |\Delta(d)| = 1, \text{ and } \left| \sum_i a_i \right| \leq \sum_i |a_i| ) \quad (92.87)$$

$$\leq \sum_d \underbrace{\sqrt{\sum_x A^2(d,x)}}_{A_P(d)} \underbrace{\sqrt{\sum_x B^2(d,x)}}_{B_P(d)} \quad (\text{by CS inequality}) . \quad (92.88)$$

Define

$$A_P(d') = \sqrt{\sum_x P(x) (P(d'|x) - P_{in}(d'|x))^2} \quad (92.89)$$

$$= \sqrt{\langle (P(d'|x) - P_{in}(d'|x))^2 \rangle_P} \quad (92.90)$$

and

$$B_P(d') = \sqrt{\sum_x P(x) \left( \frac{\mathcal{Y}_{|d',x}[P] - \mathcal{Y}_{|d',x}[P_{in}]}{P_{in}(d'|x)} \right)^2} \quad (92.91)$$

$$= \sqrt{\left\langle \left( \frac{\mathcal{Y}_{|d',x}[P] - \mathcal{Y}_{|d',x}[P_{in}]}{P_{in}(d'|x)} \right)^2 \right\rangle_P} . \quad (92.92)$$

Then

$$|\mathcal{R}^{LIPW}[P_N, P_{in}]| \leq \sum_{d'=0}^1 A_{P_N}(d') B_{P_N}(d') \quad (92.93)$$

If either  $A_{P_N}(1) = A_{P_N}(0) = 0$  (i.e., zero error in the propensities) or  $B_{P_N}(0) = B_{P_N}(1) = 0$  (i.e., zero bias), then  $\mathcal{R}^{LIPW}[P_N, P_{in}] = 0$ . This property of  $\Psi^{LIPW}$  is referred to as **double robustness**.

### 92.5.5 $\Psi^{LIPW++}$ (a.k.a. $\Psi^{TMLE}$ )

**LIPW++ estimate**  $\Psi^{LIPW++}$  (a.k.a, targeted minimum loss estimate (TMLE)) .

$\Psi^{LIPW++}$  is the linear approximation of  $\Psi^{IPW}[P_N]$  at the point  $P_{in++}$ , where the linear term of its Taylor expansion vanishes:

$$\Psi^{LIPW++} = \Psi^{TMLE} = \Psi^{IPW}[P_{in++}] + \underbrace{\langle \nabla \Psi^{IPW}[P_{in++}] \rangle_{P_N} - \nabla \Psi_{in++}^{IPW}}_{=0} \quad (92.94)$$

This property of  $\Psi^{TMLE}$  that the linear term in its Taylor expansion at  $P_{in++}$  vanishes is referred to as **substitution invariance**, and  $\Psi^{TMLE}$  is said to be a **substitution estimate**. A substitution estimate is very desirable because its absolute value is bounded, unlike the value of  $\Psi^{LIPW}$ .

$\Psi^{TMLE}$  is both a doubly robust estimate and a substitution estimate.

Claim 132 allows us express more explicitly the constraint that defines  $P_{in++}$ :

$$0 = P_N \cdot \nabla \Psi^{IPW}[P_{in++}] - \nabla \Psi_{in++}^{IPW} \quad (92.95)$$

$$= -\nabla \Psi_{in++}^{IPW} + \left\{ \overbrace{\frac{1}{N} \sum_{\sigma} (\mathcal{Y}_{|1,x_{\sigma}}[P_{in++}] - \mathcal{Y}_{|0,x_{\sigma}}[P_{in++}])}^{\approx \nabla \Psi^{IPW}[P_{in++}]} + \frac{1}{N} \sum_{\sigma} \frac{\Delta(d_{\sigma})}{P_{in++}(d_{\sigma}|x_{\sigma})} (y_{\sigma} - \mathcal{Y}_{|d_{\sigma},x_{\sigma}}[P_{in++}]) \right\} \quad (92.96)$$

$$= \frac{1}{N} \sum_{\sigma} \underbrace{\frac{\Delta(d_{\sigma})}{P_{in++}(d_{\sigma}|x_{\sigma})} (y_{\sigma} - \mathcal{Y}_{|d_{\sigma},x_{\sigma}}[P_{in++}])}_{\lambda(X_{\sigma})} \quad (92.97)$$

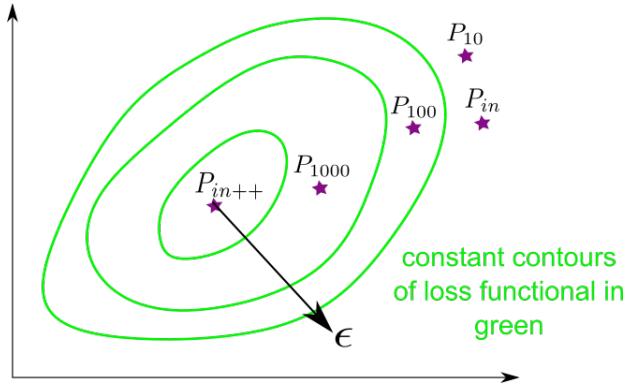


Figure 92.3: This figure portrays the space of functions  $\mathcal{H}_X$  as if it were the real plane  $\mathbb{R}^2$ , and the functional  $\mathcal{L}[P, \hat{y} = \text{fixed}] : \mathcal{H}_X \rightarrow \mathbb{R}$  as if it were a real valued function on  $\mathbb{R}^2$ . It shows the constant contours of the loss functional  $\mathcal{L}[P, \hat{y}]$  at fixed  $\hat{y}$  in green.  $P_N$  for  $N = 10, 100, 1000$  represent empirical distributions. The loss is non-negative and it equals zero when  $\epsilon = 0$  and  $P = P_{in++}$ .

Note that function  $\lambda(X_\sigma)$  defined in Eq.(92.97) can be positive or negative. Hence, it can't be defined as the loss curve-fit, because a loss curve-fit must be non-negative. However, it can be defined as the derivative of a loss curve-fit. Suppose we define an  $\epsilon \in \mathbb{R}$  parameterized family of probability distributions  $P_\epsilon : S_{\underline{X}} \rightarrow [0, 1]$ , and we expand the loss  $\mathcal{L}[P_\epsilon, \hat{y}]$  in powers of  $\epsilon$ :

$$\mathcal{L}[P_\epsilon, \hat{y}] = \mathcal{L}[P_0, \hat{y}] + \epsilon \{\partial_\epsilon \mathcal{L}[P_\epsilon, \hat{y}]\}_{\epsilon=0} + \mathcal{O}(\epsilon^2) \quad (92.98)$$

The parameter  $\epsilon$  is called the **fluctuation parameter**. The function  $\mathcal{L}[P_\epsilon, \hat{y}]$  is obviously not unique because all we know about it is the value of its  $\epsilon$  derivative in the vicinity of  $\epsilon = 0$ . Next we will pick a convenient  $\mathcal{L}[P_\epsilon, \hat{y}]$  that satisfies

$$\mathcal{L}[P_\epsilon, \hat{y}] \geq 0, \quad \mathcal{L}[P_0, \hat{y}] = 0, \quad \partial_\epsilon \{\mathcal{L}[P_\epsilon, \hat{y}]\}_{\epsilon=0} = 0 \quad (92.99)$$

Use as loss curve-fit  $\hat{\mathcal{L}}$  the Cross Entropy  $CE(p \parallel q)$  for  $p, q \in [0, 1]$

$$\hat{\mathcal{L}} = CE(p \parallel q) = -[p \ln q + (1-p) \ln(1-q)] \quad (92.100)$$

$\hat{\mathcal{L}} \geq 0$  and attains its minimum when  $p = q$ . When  $p = q$ , it equals the entropy of  $p$ , i.e., when  $p = q$ ,  $\hat{\mathcal{L}} = -\sum_{x \in \{0,1\}} P(x) \ln P(x) = H(P)$ , where  $P(0) = p, P(1) = 1-p$ .

For some  $y \in \{0, 1\}$  and  $\epsilon \in \mathbb{R}$ , make the following substitutions in the loss curve-fit  $\hat{\mathcal{L}}$  and call it  $\hat{\mathcal{L}} = \hat{\mathcal{L}}(\beta, y, \hat{y}, \epsilon)$ .<sup>3</sup>

$$p = y, \quad q = \text{expit}[\text{logit}(\hat{y}) + \epsilon\beta] \quad (92.101)$$

Note that since  $p = y$  is binary, the minimum of this loss curve-fit is zero.

Recall that in Section C.21, we proved that the derivative of  $\text{expit}(x)$  satisfies

$$\text{expit}'(x) = \text{expit}(x)[1 - \text{expit}(x)]. \quad (92.102)$$

Hence,

$$\lim_{\epsilon \rightarrow 0} \partial_\epsilon \hat{\mathcal{L}}(\beta, y, \hat{y}, \epsilon) = \lim_{\epsilon \rightarrow 0} \left[ -\frac{p}{q} + \frac{1-p}{1-q} \right] \partial_\epsilon q \quad (92.103)$$

$$= \left[ -\frac{y}{\hat{y}} + \frac{1-y}{1-\hat{y}} \right] \lim_{\epsilon \rightarrow 0} \left\{ \begin{array}{l} \text{expit}[\text{logit}(\hat{y}) + \epsilon\beta] \\ * \{1 - \text{expit}[\text{logit}(\hat{y}) + \epsilon\beta]\} \end{array} \right\} \beta \quad (92.104)$$

$$= \left[ -\frac{y}{\hat{y}} + \frac{1-y}{1-\hat{y}} \right] \hat{y}(1-\hat{y})\beta \quad (92.105)$$

$$= \beta[\hat{y} - y] \quad (92.106)$$

If we define  $\hat{\mathcal{L}}(X)$  by

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<sup>3</sup>To agree with the TE literature, we are using  $\text{expit}(x)$  (resp.,  $\text{logit}(p)$ ) to denote the sigmoid function (resp., log-odds function) which we normally denote in this book by  $\text{smoid}(x)$  (resp.,  $\text{lodds}(p)$ ).

$$\widehat{\mathcal{L}}(X) = \widehat{\mathcal{L}} \left( \begin{array}{l} \beta = \frac{\Delta(d)}{P_{in++}(d|x)}, \\ y = y, \\ \widehat{y} = \mathcal{Y}_{|d,x}[P_{in++}], \\ \epsilon = \epsilon \end{array} \right), \quad (92.107)$$

and  $\mathcal{L}$  by

$$\mathcal{L} = \frac{1}{N} \sum_{\sigma} \widehat{\mathcal{L}}(X_{\sigma}) = P_N \cdot \widehat{\mathcal{L}}, \quad (92.108)$$

then

$$\left\{ \begin{array}{l} \mathcal{L} = P_N \cdot \widehat{\mathcal{L}} \geq 0 \\ \mathcal{L}_{\epsilon=0} = P_N \cdot \widehat{\mathcal{L}}_{\epsilon=0} = 0 \\ \{\partial_{\epsilon}\mathcal{L}\}_{\epsilon=0} = P_N \cdot \{\partial_{\epsilon}\widehat{\mathcal{L}}\}_{\epsilon=0} = 0 \end{array} \right. \quad (92.109)$$

## 92.6 $\Psi^{TMLE}$ in practice

This section is based on Ref.[25].

In practice, one can calculate  $\Psi^{TMLE}$  by performing the following steps.

Below, "ML-fit" denotes a curve fitting obtained using any valid machine learning method, such as linear regression, a Neural Net, a decision tree, etc. The TE software often uses a "Super-Learner", a program that merges the results of multiple fits obtained via various ML methods and also does cross validation.

Below,  $\{(\sigma, d_{\sigma}, x_{\sigma}, \boxed{y_{\sigma}}) : \sigma \in \Sigma\}$  represents a dataset. The dependent variable  $y_{\sigma}$  is boxed, the independent ones  $d_{\sigma}, x_{\sigma}$  (a.k.a. covariates) aren't.

1. Find curve-fit  $\widehat{y}(d, x) = \mathcal{Y}_{|d,x}$  of outcome  $y$

$$\{(\sigma, d_{\sigma}, x_{\sigma}, \boxed{y_{\sigma}}) : \sigma \in \Sigma\} \xrightarrow{\text{ML-fit}} \widehat{y}(d, x) \quad (92.110)$$

2. Estimate propensity  $g(x)$

$$g(x) = P(\underline{d} = 1|x) \approx \frac{\sum_{\sigma} \delta(d_{\sigma}, 1)\delta(x_{\sigma}, x)}{\sum_{\sigma} \delta(x_{\sigma}, x)} \quad (92.111)$$

$$P(d|x) = dg(x) + (1 - d)[1 - g(x)] \quad (92.112)$$

$$\beta(d, x) = \frac{\Delta(d)}{P(d|x)} \quad (92.113)$$

3. Estimate fluctuation parameter  $\epsilon$

$$\eta(d, x) = \underbrace{\text{logit}[\hat{y}(d, x)]}_{\lambda(d, x)} + \epsilon \beta(d, x) \quad (92.114)$$

$$\{(\sigma, \lambda(d_\sigma, x_\sigma), \beta(d_\sigma, x_\sigma), \boxed{\eta(d_\sigma, x_\sigma)} : \sigma \in \Sigma\} \xrightarrow{\text{ML-fit}} \widehat{\eta}(d, x) \quad (92.115)$$

4. Estimate ATE

$$ATE = \frac{1}{N} \sum_{\sigma} \{\text{expit}[\widehat{\eta}(d = 1, x_\sigma)] - \text{expit}[\widehat{\eta}(d = 0, x_\sigma)]\} \quad (92.116)$$

# Chapter 93

## Time Series Analysis: ARMA and VAR

This chapter is based mostly on the book Ref.[20] on time series analysis by Hamilton, and on the lectures Ref. [31] by Chung-Ming Kuan. In writing this chapter, we also profited greatly from numerous Wikipedia entries on time series analysis, such as the entries on time series (Ref.[159]), ARMA time series (Ref.[89]), AR time series (Ref.[88]), MA time series (Ref.[140]), and VAR time series (Ref.[164]).

We cover only a small fraction of the treasures covered in those sources, and only cover stationary time-series. Non-stationary time series we don't even touch. But we hope to have covered enough to pique our readers's interest in time series analysis, and make him/her appreciate how bnets make time series much more intuitive and fun. The time-series considered in this chapter can be represented by one of the simplest types of bnets, namely, the LDEN bnets introduced in Chapter 48.

As usual, for  $t, t_a, t_b \in \mathbb{Z}$ , let  $\mathbb{Z}_{<t} = \{t-1, t-2, t-3, \dots\}$ ,  $\mathbb{Z}_{[t_a, t_b]} = \{t_a, t_a+1, \dots, t_b\}$ , etc.

Let  $\underline{x}_t \in \mathbb{R}$ . A **time series (t-series)**, denoted variously by  $\{\underline{x}_1, \underline{x}_2, \dots, \underline{x}_{nt}\} = \{\underline{x}_t\}_{t=1}^{nt} = \{\underline{x}_t\}_{t \in \mathbb{Z}}$ , is a set of real numbers index by a discrete set of times  $\mathbb{Z}_{[0, nt]}$ .

For  $t_a < t_b$ , let  $\underline{x}_{[t_a, t_b]} = (\underline{x}_{t_a}, \underline{x}_{t_a+1}, \dots, \underline{x}_{t_b})$ . Let  $x_{<t} = (\dots, x_{t-2}, \underline{x}_{t-1})$ .

### 93.1 White noise

By **white noise**  $\{\underline{n}_t\}_{\forall t} \sim WN(0, \sigma^2)$  we mean a t-series  $\{\underline{n}_t\}_{\forall t}$  that satisfies

$$E[\underline{n}_t] = 0 \tag{93.1}$$

and

$$\langle \underline{n}_t, \underline{n}_{t'} \rangle = \sigma^2 \delta(t, t') . \tag{93.2}$$

**Gaussian white noise**  $\{\underline{n}_t\}_{\forall t} \sim WN(0, \sigma^2)_{\mathcal{N}}$  is white noise such that also  $\underline{n}_t \sim \mathcal{N}(0, \sigma^2)$ .

## 93.2 Backshift operator

$\mathcal{B}$  is the backshift (a.k.a. lag) operator. For any t-series  $\{\underline{x}_t\}_{\forall t}$ ,  $\{\underline{y}_t\}_{\forall t}$  and scalars  $a, b \in \mathbb{R}$ ,

$$\mathcal{B}\underline{x}_t = \underline{x}_{t-1} \quad (93.3)$$

$$\mathcal{B}(a\underline{x}_t + b\underline{y}_t) = a\mathcal{B}(\underline{x}_t) + b\mathcal{B}(\underline{y}_t) \quad (93.4)$$

A  $\mathcal{B}$  Polynomial with coefficients  $\alpha_{[0,p]}$ :

$$\alpha(\mathcal{B}) = \alpha_0 + \alpha_1\mathcal{B} + \alpha_2\mathcal{B}^2 + \dots + \alpha_p\mathcal{B}^p \quad (93.5)$$

$\mathcal{B}^{-1}$  is the inverse of the backshift operator (a.k.a. frontshift operator)

$$\mathcal{B}^{-1}\underline{x}_t = \underline{x}_{t+1} \quad (93.6)$$

The following two Taylor expansions prove useful in finding the inverse of backshift operator polynomials:

- $$\frac{1}{1-z} = 1 + z + z^2 + \dots \quad (93.7)$$

converges for  $z \in \mathbb{C}$  with  $|z| < 1$ . We will use this expansion with  $z$  replaced by  $\alpha\mathcal{B}$ , where  $\alpha \in \mathbb{R}$ .

- $$\frac{1}{1-z} = (-z^{-1}) \left[ \frac{1}{1-z^{-1}} \right] = (-z^{-1}) [1 + z^{-1} + z^{-2} + \dots] \quad (93.8)$$

converges for  $z \in \mathbb{C}$  with  $|z| > 1$ . We will use this expansion with  $z^{-1}$  replaced by  $(\alpha\mathcal{B})^{-1}$ , where  $\alpha \in \mathbb{R}$ .

## 93.3 Metrics

Consider a t-series  $\{\underline{x}_t\}_{\forall t}$ .

In general, if we have a metric like Auto-covariance (ACov) that is defined for  $\tau = 1, 2, 3, \dots$ , it is conventional in time series analysis to refer to the plot of that metric for all values of  $\tau$  as the Auto-covariance *Function* (ACovF).

- Expected value and Variance

$$E[\underline{x}_t] \quad (93.9)$$

$$Var[\underline{x}_t] = \langle \underline{x}_t, \underline{x}_t \rangle \quad (93.10)$$

- **Auto-covariance (ACov)**

$$\gamma_{t,t+\tau} = \langle \underline{x}_t, \underline{x}_{t+\tau} \rangle \quad (93.11)$$

- **Auto-correlation (ACorr)** (assumes w-stationarity)

$$\rho(\tau) = \frac{\gamma(\tau)}{\gamma(0)} \quad (93.12)$$

- **Generating function of auto-covariance** (assumes w-stationarity)

$$\tilde{\gamma}(z) = \sum_{\tau=-\infty}^{\infty} \gamma(\tau) z^{\tau} \quad (93.13)$$

Note that this transform is double sided. Fourier Transform if  $z = e^{-i\omega\tau}$ .

- **Expected value and variance conditioned on all past information**

For  $\tau = 1, 2, 3, \dots$ ,

$$E_{|x_{\leq t}}[\underline{x}_{t+\tau}] \quad (93.14)$$

$$Var_{|x_{\leq t}}[\underline{x}_{t+\tau}] = \langle \underline{x}_{t+\tau}, \underline{x}_{t+\tau} \rangle_{|x_{\leq t}} \quad (93.15)$$

- **Partial auto-covariance (PACov)**

Assume w-stationarity. For  $\tau = 1, 2, 3, \dots$

$$\gamma^{part}(\tau) = \langle \underline{x}_t, \underline{x}_{t+\tau} \rangle_{|x_{\leq t}, \underline{x}_{t+\tau}} \quad (93.16)$$

The idea is that we set to zero the nodes  $\underline{x}_{(t,t+\tau)} = \{\underline{x}_{t+1}, \underline{x}_{t+2}, \dots, \underline{x}_{t+\tau-1}\}$  that lie between (but not including)  $\underline{x}_t$  and  $\underline{x}_{t+\tau}$ .

- **Partial auto-correlation (PACorr)**

$$\rho^{part}(\tau) = \frac{\gamma^{part}(\tau)}{\gamma^{part}(0)} \quad (93.17)$$

---

**weak stationarity (w-stationarity)** means that  $E[\underline{x}_t] = \mu$  and  $\gamma_{t,t+\tau} = \gamma(\tau)$  are both independent of  $t$ . If we have w-stationarity, then

$$\gamma(-\tau) = \langle \underline{x}_t, \underline{x}_{t-\tau} \rangle \quad (93.18)$$

$$= \langle \underline{x}_{t-\tau}, \underline{x}_t \rangle \quad (93.19)$$

$$= \gamma(\tau) \quad (93.20)$$

We will often abbreviate  $\gamma(\tau)$  by  $\gamma_\tau$ .

Example of various metrics. If  $\{\underline{n}_t\}_{\forall t} \sim WN(0, \sigma^2)$  then

$$E[\underline{n}_t] = 0 \quad (93.21a)$$

$$\gamma(\tau) = \sigma^2 \delta(\tau, 0) \quad (93.21b)$$

$$\gamma(0) = \sigma^2 \quad (93.21c)$$

$$\tilde{\gamma}(z) = \gamma(0) \quad (93.21d)$$

For  $\tau > 0$ ,

$$E_{|\underline{n}_{\leq t}}[\underline{n}_{t+\tau}] = E[\underline{n}_{t+\tau}] = 0 \quad (93.21e)$$

$$\langle \underline{n}_{t+\tau}, \underline{n}_{t+\tau} \rangle_{|\underline{n}_{\leq t}} = E[\underline{n}_{t+\tau}^2] = \sigma^2 \quad (93.21f)$$

### 93.4 Definition of ARMA( $p, q$ ), AR( $p$ ) and MA( $q$ ).

Suppose  $\{\underline{y}_t\}_{\forall t}$  is a zero mean t-series. Hence  $\underline{y}_t = \underline{Y}_t - \mu$ ,  $E[\underline{Y}_t] = \mu$ ,  $E[\underline{y}_t] = 0$ .  $\underline{y}_t$  is said to be the **demeaned** version of  $\underline{Y}_t$ .

Suppose also that  $\{\underline{n}_t\}_{\forall t} \sim WN(0, \sigma^2)$ .

Then we define the **Auto-Regressive Moving-Average t-series ARMA( $p, q$ )** by

$$\underline{y}_t = \underbrace{\sum_{j=1}^p \alpha_j \underline{y}_{t-j}}_{\mathcal{Y}_t^{AR(p)}} + \underline{n}_t + \underbrace{\sum_{j=1}^q \nu_j \underline{n}_{t-j}}_{\mathcal{Y}_t^{MA(q)}} \quad (93.22)$$

( $\alpha$  stands for the first letter of “auto-regressive”.  $\nu$  stands for first letter of “noise”.)

Special cases

#### 1. Auto-Regressive t-series AR( $p$ )

$$\underline{y}_t = \mathcal{Y}_t^{AR(p)} + \underline{n}_t \quad (93.23)$$

#### 2. Moving-Average t-series MA( $q$ )

$$\underline{y}_t = \underline{n}_t + \mathcal{Y}_t^{MA(q)} \quad (93.24)$$

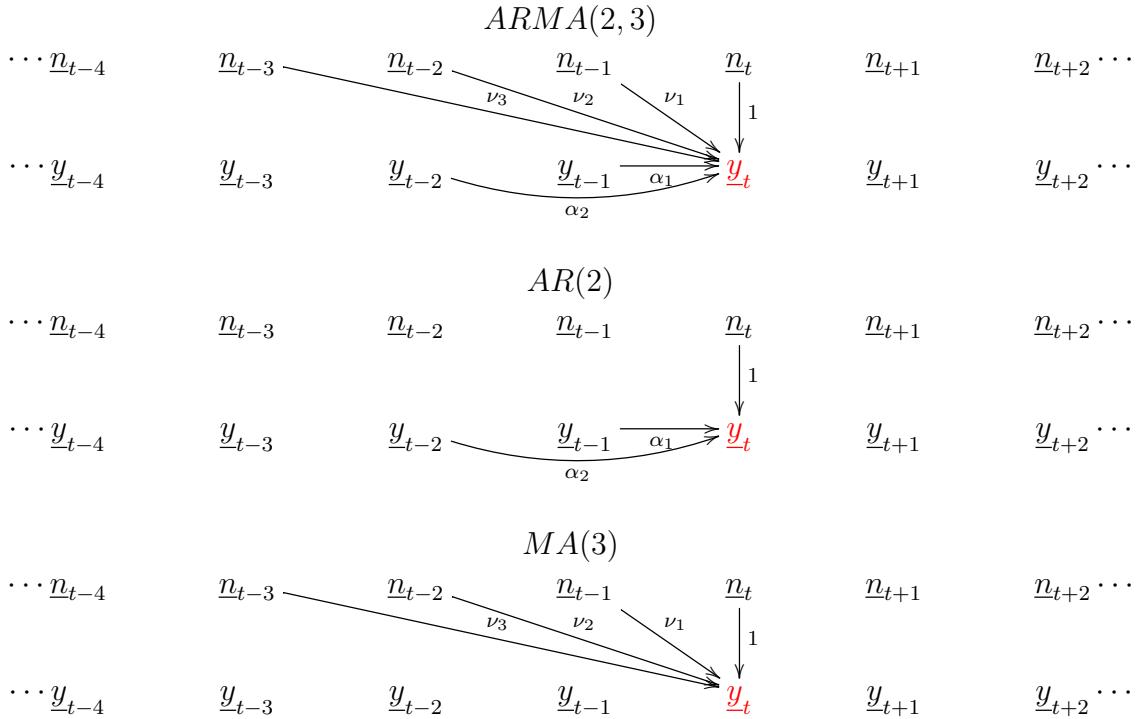


Figure 93.1:  $ARMA(2,3)$ ,  $AR(2)$  and  $MA(3)$  bnets. For clarity, we show only the arrows entering node  $y_t$ . The full bnet has the same structural pattern of incoming arrows (including the weights  $\alpha_j, \nu_j$ ) for each node  $y_{t'}$  for all  $t'$ .

Fig.93.1 shows the bnets for  $ARMA(2,3)$ ,  $AR(2)$  and  $MA(3)$ . The TPM, printed in blue, for node  $y_t$  in those bnets, is as follows:

For  $ARMA(p,q)$ ,

$$P(y_t | y_{[t-p,t-1]}, n_{[t-q,t]}) = \mathbb{1}(y_t = \text{see Eq.93.22})) \quad (93.25)$$

For  $AR(p)$ ,

$$P(y_t | y_{[t-p,t-1]}, n_t) = \mathbb{1}(y_t = \text{see Eq.93.23})) \quad (93.26)$$

For  $MA(q)$ ,

$$P(y_t | n_{[t-q,t]}) = \mathbb{1}(y_t = \text{see Eq.93.24})) \quad (93.27)$$

The  $n_t$  variable is variously referred to as the **external noise**, **impulse**, **shock**, **innovation** at time  $t$ .

### 93.5 Solving $AR(p)$

Suppose  $\{\underline{y}_t\}_{\forall t}$  is an  $AR(p)$  t-series. Hence

$$\underline{y}_t = \sum_{j=1}^p \alpha_j \underline{y}_{t-j} + \underline{n}_t \quad (93.28)$$

$AR(0)$  satisfies:

$$\underline{y}_t = \underline{n}_t \quad (93.29)$$

See Fig.93.2. This is just white noise.

$AR(1)$  satisfies:

$$\underline{y}_t = \alpha_1 \underline{y}_{t-1} + \underline{n}_t \quad (93.30)$$

See Fig.93.2. This is a Markov chain with external i.i.d. noise injected to each node.  $AR(1)$  is the discrete form of the so called **Ornstein-Uhlenbeck t-series** (a.k.a. as the **Langevin Equation**). When  $\alpha_1 = 1$ , it is called a **random walk**.

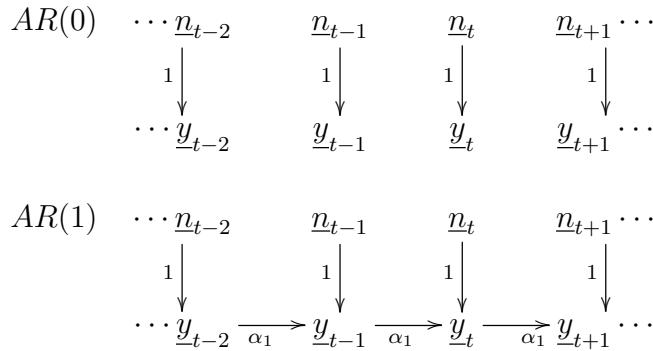


Figure 93.2: BNets for  $AR(0)$  and  $AR(1)$ .

Note that

$$\alpha^-(\mathcal{B}) \underline{y}_t = \underline{n}_t \quad (93.31)$$

where

$$\alpha^-(\mathcal{B}) = 1 - \sum_{j=1}^p \alpha_j \mathcal{B}^j \quad (93.32)$$

Note that we can get  $AR(p)$  from  $AR(\infty)$  by setting  $\alpha_{>p} = 0$ .

If  $\alpha^-(\beta)$  is invertible, then, using the Taylor expansion Eq.(93.7), we get

$$\underline{y}_t = \alpha'(\mathcal{B})\underline{n}_t \quad (93.33)$$

where

$$\alpha'(\mathcal{B}) = \frac{1}{\alpha^-(\mathcal{B})} = 1 + \sum_{k=1}^{\infty} \left[ \sum_{j=1}^p \alpha_j \mathcal{B}^j \right]^k = \sum_{j=0}^{\infty} \alpha'_j \mathcal{B}^j \quad (93.34)$$

where  $\alpha'_0 = 1$ .

## 93.6 Solving $MA(q)$

Suppose  $\{\underline{y}_t\}_{\forall t}$  is an  $MA(q)$  t-series. Hence,

$$\underline{y}_t = \underline{n}_t + \sum_{j=1}^q \nu_j \underline{n}_{t-j} = \sum_{j=0}^q \nu_j \underline{n}_{t-j} \quad (93.35)$$

where  $\nu_0 = 1$ . Thus,

$$\underline{y}_t = \nu(\mathcal{B})\underline{n}_t \quad (93.36)$$

where

$$\nu(\mathcal{B}) = 1 + \sum_{j=1}^q \nu_j \mathcal{B}^j = \sum_{j=0}^q \nu_j \mathcal{B}^j . \quad (93.37)$$

Note that we can get  $MA(q)$  from  $MA(\infty)$  by setting  $\nu_{>q} = 0$ .

**Claim 135** *If  $\{\underline{y}_t\}_{\forall t}$  is an  $MA(q)$  t-series, then*

$$E[\underline{y}_t] = 0 \quad (93.38a)$$

For  $\tau \geq 0$ ,

$$\gamma(\tau) = \mathbb{1}(\tau \leq q) \sigma^2 \sum_{j=0}^{q-\tau} \nu_j \nu_{\tau+j} \quad (93.38b)$$

$$\gamma(0) = \sigma^2 \sum_{j=0}^q \nu_j^2 \quad (93.38c)$$

**proof:**

$$\gamma(\tau) = \left\langle \underline{y}_t, \underline{y}_{t+\tau} \right\rangle \quad (93.39)$$

$$= \left\langle \sum_{j=0}^q \nu_j \underline{n}_{t-j}, \sum_{k=0}^q \nu_k \underline{n}_{t+\tau-k} \right\rangle \quad (93.40)$$

$$= \sigma^2 \sum_{j=0}^q \sum_{k=0}^q \nu_j \nu_k \delta(t-j, t+\tau-k) \quad (93.41)$$

$$= \sigma^2 \sum_{j=0}^q \sum_{k=0}^q \nu_j \nu_k \delta(k, \tau+j) \quad (93.42)$$

$$= \mathbb{1}(\tau \leq q) \sigma^2 \sum_{j=0}^{q-\tau} \nu_j \nu_{\tau+j} \quad (93.43)$$

QED

### 93.7 Solving $ARMA(p, q)$

Suppose  $\{\underline{y}_t\}_{\forall t}$  is an  $ARMA(p, q)$  t-series. Hence, using Eqs.(93.31) and (93.36),  $\underline{y}_t$  satisfies

$$\alpha^-(\mathcal{B}) \underline{y}_t = \nu(\mathcal{B}) \underline{n}_t \quad (93.44)$$

If  $\alpha^-(\beta)$  is invertible, then, using the Taylor expansion Eq.(93.7), we get

$$\underline{y}_t = \frac{\nu(\mathcal{B})}{\alpha^-(\mathcal{B})} \underline{n}_t = \nu(\mathcal{B}) \alpha'(\mathcal{B}) \underline{n}_t \quad (93.45)$$

We see that, if the  $\alpha^-(\mathcal{B})$  operator is invertible, an  $AR(p)$  or an  $ARMA(p, q)$  t-series can be represented as an  $MA(\infty)$  t-series.  $MA(\infty)$  is often called **Wold's Decomposition**. Furthermore, if the  $\nu(\mathcal{B})$  operator is invertible, an  $MA(q)$  or an  $ARMA(p, q)$  t-series can be represented as an  $AR(\infty)$  t-series.

The polynomials  $\alpha^-(z)$  and  $\nu(z)$  can be expressed in factored form  $\alpha^-(z) = \prod_{j=1}^p (z - z_j^\alpha)$  and  $\nu(z) = \prod_{j=1}^q (z - z_j^\nu)$ . If these two polynomials have a root  $z_0$  in common, both polynomials should be divided by  $(z - z_0)$ . This reduces an  $ARMA(p, q)$  t-series to an  $ARMA(p-1, q-1)$  t-series. The bnet for  $ARMA(p-1, q-1)$  has one less  $\alpha_j$  arrow and one less  $\nu_j$  arrow than the bnet for  $AR(p, q)$ .

### 93.8 Auto-correlation and partial auto-correlation

Note from Eq.(93.38b) that if  $\{\underline{y}_t\}_{\forall t}$  is a  $MA(q)$  t-series, then  $\gamma(\tau) = 0$  for all  $\tau > q$ . Fig.93.3 gives a graphical proof, using bnets and the d-separation theorem, that for

a  $MA(2)$  t-series,  $\gamma(\tau) = 0$  for  $\tau > 2$ . As a consequence of this, a plot of  $\gamma(\tau)$  versus  $\tau$  for a typical  $MA(2)$  t-series looks like Fig.93.4.

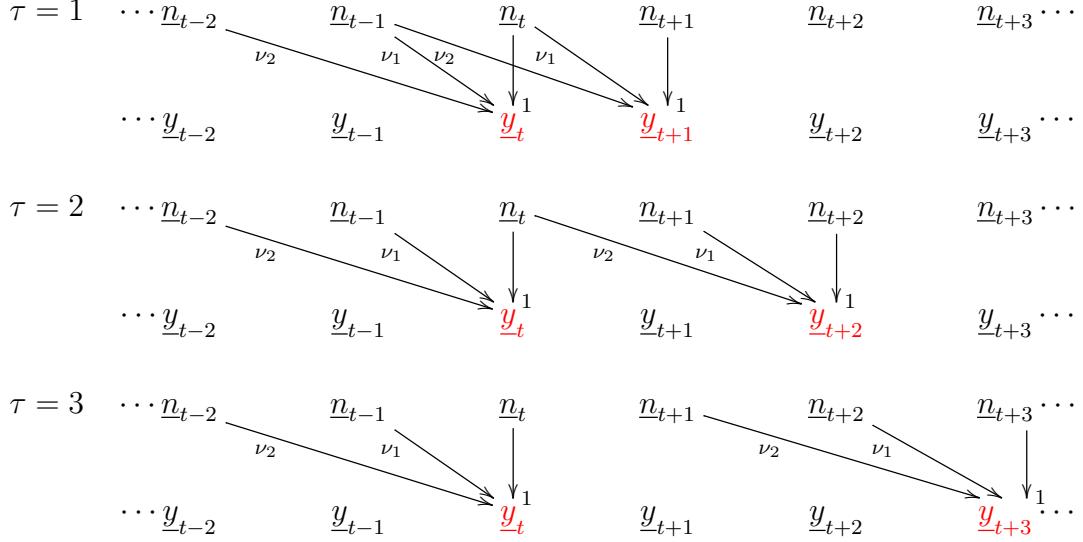


Figure 93.3:  $MA(2)$  bnet. For clarity, we show only arrows entering nodes  $\underline{y}_t$  and  $\underline{y}_{t+\tau}$  for  $\tau = 1, 2, 3$ . For  $\tau = 1, 2$ , there is a path through which information can flow from node  $\underline{y}_t$  to node  $\underline{y}_{t+\tau}$ . For  $\tau = 2$ , there is no such path.

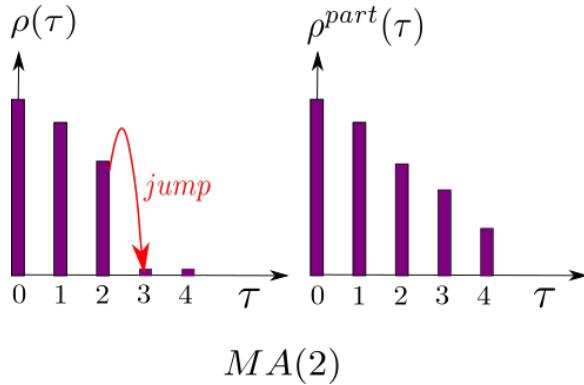


Figure 93.4: Plot of auto-correlation function (ACorrF)  $\rho(\tau)$  and partial auto-correlation function (PACorrF)  $\rho^{part}(\tau)$  for an instance of  $MA(2)$ . Note that  $\rho(\tau)$  vanishes for  $\tau > 2$ .

**Claim 136** If  $\{\underline{y}_t\}_{\forall t}$  is an  $AR(p)$  t-series, then  $\gamma^{part}(\tau) = 0$  for all  $\tau > p$ .

**proof:**

Let

$$\underline{\xi} = \underline{y}_{\leq t}, \underline{y}_{t+\tau} \quad (93.46)$$

Recall that

$$\gamma^{part}(\tau) = \left\langle \underline{y}_t, \underline{y}_{t+\tau} \right\rangle_{|\xi} \quad (93.47)$$

$$= \left\langle \underline{y}_t \underline{y}_{t+\tau} \right\rangle_{|\xi} - \left\langle \underline{y}_t \right\rangle_{|\xi} \left\langle \underline{y}_{t+\tau} \right\rangle_{|\xi} \quad (93.48)$$

$$= \left\langle \underline{y}_t \underline{y}_{t+\tau} \right\rangle_{|\xi} \quad (93.49)$$

Define

$$Z_{(t,t+\tau)} = \mathbb{1}(\underline{y}_{(t,t+\tau)} = 0) \quad (93.50)$$

Hence, the operator  $Z_{(t,t+\tau)}$  sets all  $\underline{y}_{t'}$  with  $t' < t + \tau$  equal to zero. Note that we can express the PACov as

$$\gamma^{part}(\tau) = \left\langle Z_{(t,t+\tau)} (\underline{y}_t \underline{y}_{t+\tau}) \right\rangle. \quad (93.51)$$

Since

$$\underline{y}_{t+\tau} = \sum_{j=1}^p \alpha_j \underline{y}_{t+\tau-j} + \underline{n}_{t+\tau} \quad (93.52)$$

$$= \alpha_p \underline{y}_{t+\tau-p} + \dots + \alpha_2 \underline{y}_{t+\tau-2} + \alpha_1 \underline{y}_{t+\tau-1} + \underline{n}_{t+\tau}, \quad (93.53)$$

we get

$$Z_{(t,t+\tau)} \underline{y}_{t+\tau} = \underline{n}_{t+\tau} \quad \text{if } \tau > p. \quad (93.54)$$

Hence, for  $\tau > p$ ,

$$\gamma^{part}(\tau) = \left\langle \underline{y}_t \underline{n}_{t+\tau} \right\rangle = 0 \quad (93.55)$$

**QED**

Fig.93.5 gives a graphical proof, using bnets and the d-separation theorem, that for an AR(2) t-series,  $\gamma^{part}(\tau) = 0$  for  $\tau > 2$ . As a consequence of this, a plot of  $\gamma^{part}(\tau)$  versus  $\tau$  for a typical AR(2) t-series looks like Fig.93.6.

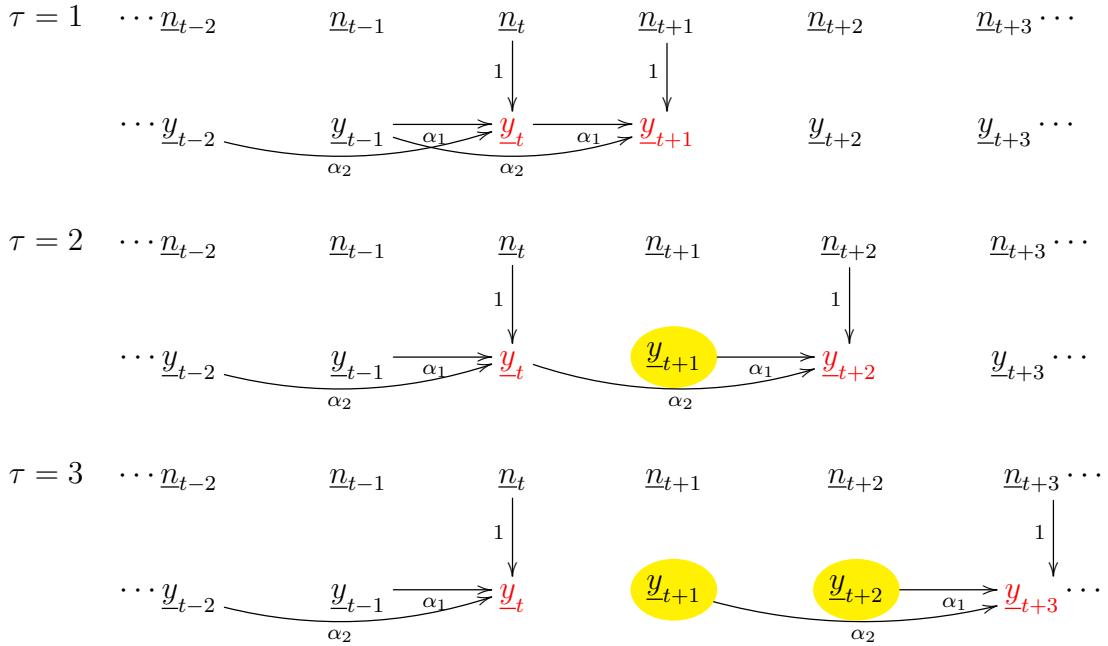


Figure 93.5:  $AR(2)$  bnet. For clarity, we show only arrows entering nodes  $\underline{y}_t$  and  $\underline{y}_{t+\tau}$  for  $\tau = 1, 2, 3$ . Yellow nodes are in set  $\underline{y}_{(t,t+\tau)}$ . They are conditioned on, so information can't flow through them to node  $\underline{y}_{t+\tau}$  by the d-separation theorem.

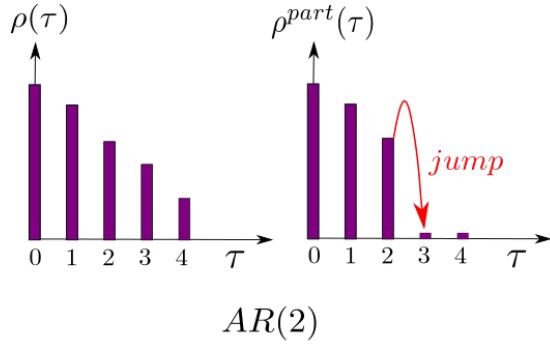


Figure 93.6: Plot of auto-correlation function (ACorrF)  $\rho(\tau)$  and partial auto-correlation function (PACorrF)  $\rho^{part}(\tau)$  for an instance of  $AR(2)$ . Note that  $\rho^{part}(\tau)$  vanishes for  $\tau > 2$ .

	ACorr	PACorr
$AR(p)$	tapers off	jumps to zero for $\tau > p$
$MA(q)$	jumps to zero for $\tau > q$	tapers off

Table 93.1: Detecting  $AR(p)$  and  $MA(q)$  using auto-correlation and partial auto-correlation.

### 93.9 Generating function of auto-correlation

**Claim 137** *If*

$$\alpha(z) = \sum_{\tau=-\infty}^{\infty} \alpha_{\tau} z^{\tau} \quad (93.56)$$

*then*

$$\alpha(z)\alpha(z^{-1}) = \sum_{\tau=-\infty}^{\infty} z^{\tau} \sum_{j=-\infty}^{\infty} \alpha_j \alpha_{j+\tau} \quad (93.57)$$

**proof:**

$$\alpha(z)\alpha(z^{-1}) = \sum_{j'=-\infty}^{\infty} z^{j'} \alpha_{j'} \sum_{j=-\infty}^{\infty} z^{-j} \alpha_j \quad (93.58)$$

$$= \sum_{\tau=-\infty}^{\infty} \sum_{j'=-\infty}^{\infty} \sum_{j=-\infty}^{\infty} z^{\tau} \alpha_{j'} \alpha_j \delta(j' - j, \tau) \quad (93.59)$$

$$= \sum_{\tau=-\infty}^{\infty} z^{\tau} \sum_{j=-\infty}^{\infty} \alpha_j \alpha_{j+\tau} \quad (93.60)$$

**QED**

As an example of this claim, note that

$$(\alpha_0 + \alpha_1 z)(\alpha_0 + \alpha_1 z^{-1}) = \alpha_0 \alpha_1 z^{-1} + (\alpha_0^2 + \alpha_1^2) + \alpha_0 \alpha_1 z \quad (93.61)$$

**Claim 138** *If  $\{\underline{y}_t\}_{t \in \mathbb{N}}$  is an  $AR(p)$  t-series, then*

$$\tilde{\gamma}(z) = \alpha'(z) \sigma^2 \alpha'(z^{-1}) \quad (93.62)$$

**proof:** Left to reader. See Claim 137.

**QED**

**Claim 139** *If  $\{\underline{y}_t\}_{t \in \mathbb{N}}$  is an  $MA(q)$  t-series, then*

$$\tilde{\gamma}(z) = \nu(z) \sigma^2 \nu(z^{-1}) \quad (93.63)$$

**proof:**

$$\underline{y}_t = \sum_{j=-\infty}^{\infty} \nu_j \underline{n}_{t-j} \quad (93.64)$$

$$\tilde{\gamma}(z) = \sum_{\tau=-\infty}^{\infty} \langle \underline{y}_0, \underline{y}_{\tau} \rangle z^{\tau} \quad (93.65)$$

$$= \sum_{\tau=-\infty}^{\infty} z^{\tau} \sum_{j=-\infty}^{\infty} \sum_{j'=-\infty}^{\infty} \nu_j \nu_{j'} \underbrace{\langle \underline{n}_{-j}, \underline{n}_{\tau-j'} \rangle}_{\sigma^2 \delta(j', \tau+j)} \quad (93.66)$$

$$= \sigma^2 \sum_{\tau=-\infty}^{\infty} z^{\tau} \sum_{j=-\infty}^{\infty} \nu_j \nu_{j+\tau} \quad (93.67)$$

Now use Claim 137.

**QED**

**Claim 140** *If  $\{\underline{y}_t\}_{\forall t}$  is an ARMA( $p, q$ ) t-series, then*

$$\tilde{\gamma}(z) = \alpha'(z) \nu(z) \sigma^2 \nu(z^{-1}) \alpha'(z^{-1}) \quad (93.68)$$

**proof:** Left to reader. See Claim 137.

**QED**

## 93.10 Impulse Response

The derivatives

$$IR_{\tau} = \frac{\partial y_{t+\tau}}{\partial n_t} \quad (93.69)$$

are called **impulse responses** or **dynamical multipliers**. Note that this derivative depends on  $\tau$  but not  $t$  by w-stationarity. A plot of  $IR_{\tau}$  versus  $\tau$  is called the **Impulse Response Function (IRF)**. Examples:

- **Claim 141** *For MA( $q$ ),*

$$\frac{\partial y_{t+\tau}}{\partial n_t} = \nu_{\tau} \mathbb{1}(0 \leq \tau \leq q) \quad (93.70)$$

where  $\nu_0 = 1$ . (See Fig.93.7)

**proof:**

$$\underline{y}_{t+\tau} = \sum_{j=0}^q \nu_j \underline{n}_{t+\tau-j} \quad (93.71)$$

so Eq.(93.70) follows.

**QED**

- **Claim 142** *For AR(1),*

$$\frac{\partial \underline{y}_{t+\tau}}{\partial n_t} = (\alpha_1)^\tau \mathbb{1}(\tau \geq 0). \quad (93.72)$$

(See Fig.93.8)

**proof:**

$$(1 - \alpha_1 \mathcal{B}) \underline{y}_{t+\tau} = \underline{n}_{t+\tau} \quad (93.73)$$

Therefore, using the Taylor expansion Eq.(93.7),

$$\underline{y}_{t+\tau} = 1 + \sum_{j=1}^{\infty} \alpha_1^j \mathcal{B}^j \underline{n}_{t+\tau} \quad (93.74)$$

$$= 1 + \sum_{j=1}^{\infty} \alpha_1^j \underline{n}_{t+\tau-j} \quad (93.75)$$

so Eq.(93.72) follows.

**QED**

In general,  $IR_\tau$  equals a sum over paths from  $\underline{n}_t$  to  $\underline{y}_{t+\tau}$ . Each path contributes the product of the weights of all the arrows in the path.

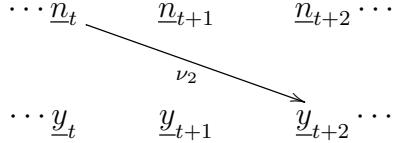


Figure 93.7: Pictorial representation of impulse response  $IR_2 = \nu_2$  for a  $MA(q)$  t-series with  $q \geq 2$ .

### 93.11 $AR(p)$ and Yule-Walker equations

**Claim 143** (*Yule-Walker equations*) *If  $\{\underline{y}_t\}_{\forall t}$  is an  $AR(p)$  t-series,*

$$\gamma_\tau = \sum_{j=1}^p \gamma_{\tau-j} \alpha_j + \sigma^2 \delta(\tau, 0) \quad (93.76)$$

*for all  $\tau \in \mathbb{Z}$ , where we are abbreviating  $\gamma(j) = \gamma_j$  for all  $j$ .*

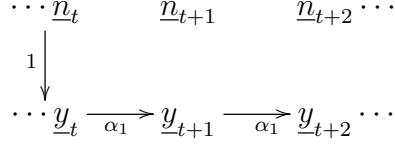


Figure 93.8: Pictorial representation of impulse response  $IR_2 = \alpha_1^2$  for an  $AR(1)$  t-series.

**proof:**

Recall that

$$\underline{y}_\tau = \sum_{j=1}^p \underline{y}_{\tau-j} \alpha_j + \underline{n}_\tau \quad (93.77)$$

Therefore

$$\underbrace{\langle \underline{y}_0, \underline{y}_\tau \rangle}_{\gamma_\tau} = \sum_{j=1}^p \underbrace{\langle \underline{y}_0, \underline{y}_{\tau-j} \rangle}_{\gamma_{\tau-j}} \alpha_j + \underbrace{\langle \underline{y}_0, \underline{n}_\tau \rangle}_{\sigma^2 \delta(\tau, 0)} \quad (93.78)$$

QED

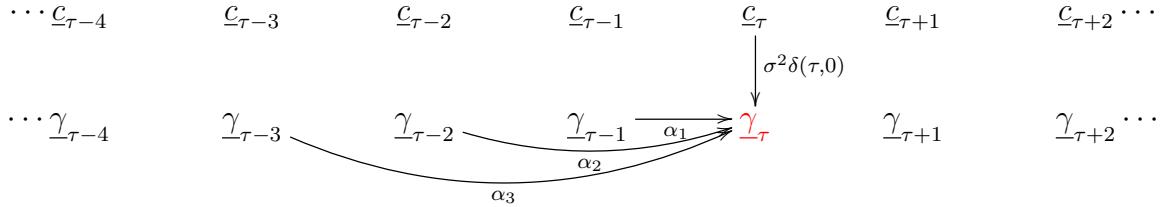


Figure 93.9: Bnet representing Yule-Walker (Christmas Walker) Eqs.(93.76) with  $p = 3$ . For clarity, we show only arrows entering node  $\gamma_\tau$ . The full bnet has the same structural pattern of incoming arrows (including the  $\alpha_j$ ) for each node  $\gamma_{\tau'}$ .

Fig.93.9 shows a bnet for the Yule-Walker Eqs.(93.76). The TPMs, printed in blue, for the  $\tau$  time-slice of that bnet, are as follows:

$$P(\gamma_\tau) = \mathbb{1}(\gamma_\tau = \text{ See Eq.(93.76)}) \quad (93.79)$$

$$P(c_\tau) = \mathbb{1}(c_\tau = \sigma^2 \delta(\tau, 0)) \quad (93.80)$$

The Yule-Walker Eqs.(93.76) imply that

$$\underbrace{\begin{bmatrix} \gamma_1 \\ \gamma_2 \\ \vdots \\ \gamma_p \end{bmatrix}}_{\gamma^p} = \underbrace{\begin{bmatrix} \gamma_0 & \gamma_{-1} & \gamma_{-2} & \cdots & \gamma_{1-p} \\ \gamma_1 & \gamma_0 & \gamma_{-1} & \cdots & \gamma_{2-p} \\ \vdots & & & & \\ \gamma_{p-1} & \gamma_{p-2} & \gamma_{p-3} & \cdots & \gamma_0 \end{bmatrix}}_{\Gamma} \underbrace{\begin{bmatrix} \alpha_1 \\ \alpha_2 \\ \vdots \\ \alpha_p \end{bmatrix}}_{\alpha^p} \quad (93.81)$$

Hence

$$\gamma^p = \Gamma \alpha^p . \quad (93.82)$$

If  $\Gamma$  is invertible,

$$\alpha^p = \Gamma^{-1} \gamma^p . \quad (93.83)$$

Once we know  $\alpha^p$ , we can solve for  $\sigma^2$

$$\gamma_0 = \sum_{j=1}^p \gamma_{-j} \alpha_j + \sigma^2 , \quad (93.84)$$

i.e., Eq.(93.76) for  $\tau = 0$ .

## 93.12 Forecasting

Before submerging the reader in the messy details of t-series forecasting, and running the risk of quickly losing him/her, let me explain to the reader that what we are about to do in this section, is, in the final analysis, quite trivial, and boils down to solving simple systems of linear equations. That is all there is to it!! How hard can that be? In reading this section, don't lose sight of that fact and you'll be okay.

Suppose  $\{\underline{y}_t\}_{\forall t}$  is an  $AR(\infty)$  t-series. For  $\tau > 0$ , the "orthogonal projection"  $\underline{y}_{t+\tau} | \underline{y}_{\leq t}$  is defined as the linear combination of  $\underline{y}_{\leq t}$  obtained by doing Linear Regression with x-variables  $\underline{y}_{\leq t}$  and y-variable  $\underline{y}_{t+\tau}$ . Thus

$$E \left[ \underline{y}_{t+\tau} | \underline{y}_{\leq t} \right] = E_{|\underline{y}_{\leq t}} [\underline{y}_{t+\tau}] \quad (93.85)$$

and

$$Var \left[ \underline{y}_{t+\tau} | \underline{y}_{\leq t} \right] = E \left[ \left( \underline{y}_{t+\tau} | \underline{y}_{\leq t} - E[\underline{y}_{t+\tau} | \underline{y}_{\leq t}] \right)^2 \right] \quad (93.86)$$

$$= Var_{|\underline{y}_{\leq t}} [\underline{y}_{t+\tau}] . \quad (93.87)$$

For example, for  $\tau = 1$ ,

$$\underline{y}_{t+1} = \sum_{j=1}^p \alpha_j \underline{y}_{t+1-j} + \underline{n}_{t+1} \quad (93.88)$$

$$\underline{y}_{t+1} | \underline{y}_{\leq t} = \sum_{j=1}^p \alpha_j \underline{y}_{t+1-j} \quad (93.89)$$

$$\underline{y}_{t+1} - \underline{y}_{t+1 | \underline{y}_{\leq t}} = \underline{n}_{t+1} \quad (93.90)$$

$$E \left[ \underline{y}_{t+1} | \underline{y}_{\leq t} \right] = E_{|\underline{y}_{\leq t}} [\underline{y}_{t+1}] \quad (93.91)$$

$$= 0 \quad (93.92)$$

$$Var \left[ \underline{y}_{t+1} | \underline{y}_{\leq t} \right] = Var_{|\underline{y}_{\leq t}} [\underline{y}_{t+1}] \quad (93.93)$$

$$= \sigma^2 \quad (93.94)$$

If  $\{\underline{y}_t\}_{\forall t}$  is an  $AR(\infty)$  t-series and  $\tau > 0$ , by **forecasting**  $\underline{y}_{t+\tau} | \underline{y}_{\leq t}$ , we will mean finding  $\underline{y}_{t+\tau} | \underline{y}_{\leq t}$ , given  $\underline{y}_{\leq t}$  as input data or some other input data from which  $\underline{y}_{\leq t}$  can be derived. Fig.93.10 illustrates 3 types of input data that we will consider next.

Note that if  $\{\underline{y}_t\}_{\forall t}$  is an  $AR(\infty)$  t-series, then  $\alpha^-(\mathcal{B})\underline{y}_t = \underline{n}_t$ . Thus,  $\underline{n}_{\leq t}$  can be expressed in terms of  $\underline{y}_{\leq t}$ , yielding a function  $\underline{n}_{\leq t}(\underline{y}_{\leq t})$ . If the operator  $\alpha^-(\mathcal{B})$  is invertible, the opposite is also true:  $\underline{y}_{\leq t}$  can be expressed in terms of  $\underline{n}_{\leq t}$ , yielding a function  $\underline{y}_{\leq t}(\underline{n}_{\leq t})$ . Thus,

$$\underline{y}_{t+\tau} | \underline{y}_{\leq t} = \underline{y}_{t+\tau} | \underline{y}_{\leq t}(\underline{n}_{\leq t}) = \underline{y}_{t+\tau} | \underline{n}_{\leq t} \quad (93.95)$$

We've seen that if we assume invertibility of  $\alpha^-(\mathcal{B})$ , then, in order to forecast  $\underline{y}_{t+\tau} | \underline{y}_{\leq t}$ , we have the option of considering  $\{\underline{y}_t\}_{\forall t}$  to be either an  $AR(\infty)$  or an  $MA(\infty)$  t-series. We will assume the latter, because this simplifies the algebra necessary to calculate both  $\underline{y}_{t+\tau} | \underline{y}_{\leq t}$  and its variance.

(a) **find**  $\underline{y}_{t+\tau} | \underline{y}_{\leq t}$  **given**  $\underline{y}_{\leq t}$

Suppose  $\{\underline{y}_t\}_{\forall t}$  is an  $MA(\infty)$  t-series. Then

$$\underline{y}_{t+\tau} = \sum_{j=0}^{\infty} \nu_j \underline{n}_{t+\tau-j} \quad (93.96)$$

$$= \underbrace{\sum_{j=0}^{\tau-1} \nu_j \underline{n}_{t+\tau-j}}_{\underline{y}_{t+\tau} - \underline{y}_{t+\tau} | \underline{y}_{\leq t}} + \underbrace{\sum_{j=\tau}^{\infty} \nu_j \underline{n}_{t+\tau-j}}_{\underline{y}_{t+\tau} | \underline{y}_{\leq t}} \quad (93.97)$$

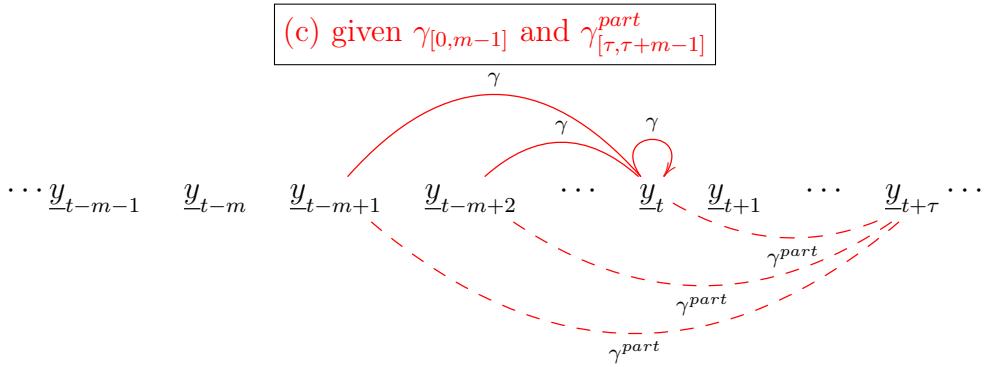
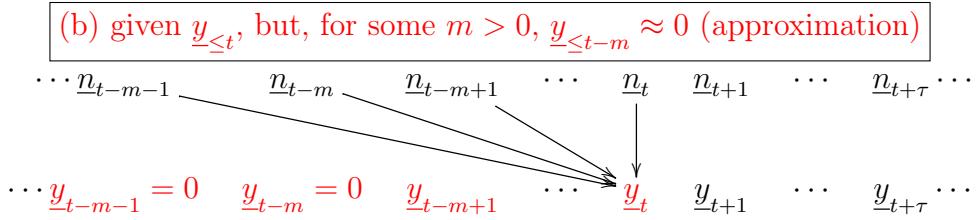
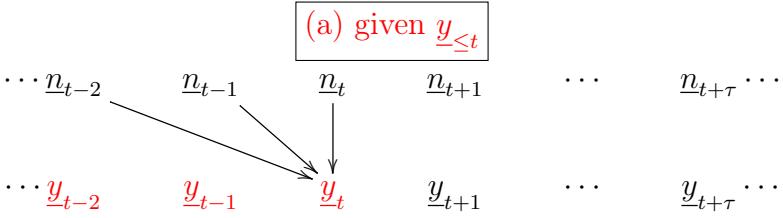


Figure 93.10: Bnet for  $MA(\infty)$  for forecasting  $\underline{y}_{t+\tau} | \underline{y}_{\leq t}$ . Input data in red. For clarity, we show only the arrows entering node  $\underline{y}_t$ .

$$\underline{y}_{t+\tau} | \underline{y}_{\leq t} = \sum_{j=\tau}^{\infty} \nu_j \underline{n}_{t+\tau-j} \quad (93.98)$$

$$E_{|\underline{y}_{\leq t}}[\underline{y}_{t+\tau}] = E[\underline{y}_{t+\tau} | \underline{y}_{\leq t}] = 0^1 \quad (93.99)$$

---

<sup>1</sup>Remember that  $\underline{y}_t$  has zero mean by definition.  $Y_t = y_t + \mu$  for some time independent constant  $\mu$ .

$$\left\langle \underline{y}_{t+\tau} \underline{y}_{t+\tau} \right\rangle_{|y_{\leq t}} = \left\langle \underline{y}_{t+\tau} - \underline{y}_{t+\tau} | y_{\leq t}, \underline{y}_{t+\tau} - \underline{y}_{t+\tau} | y_{\leq t} \right\rangle \quad (93.100)$$

$$= \sum_{j=0}^{\tau-1} \nu_j^2 \quad (93.101)$$

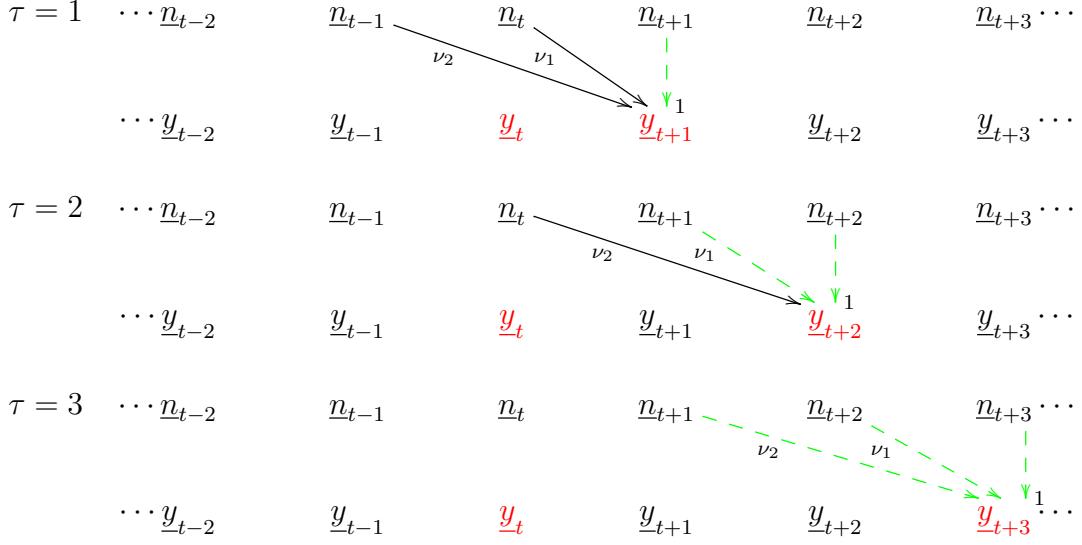


Figure 93.11:  $MA(2)$  bnet. For clarity, we show only arrows entering node  $\underline{y}_{t+\tau}$  for  $\tau = 1, 2, 3$ . Green arrows originate at a time after time  $t$ .

For  $MA(q)$ , because  $\nu_j = 0$  for  $j > q$ , this reduces to

$$\underline{y}_{t+\tau} | y_{\leq t} = \mathbb{1}(\tau \leq q) \sum_{j=\tau}^q \nu_j \underline{n}_{t+\tau-j} \quad (93.102)$$

$$E_{|y_{\leq t}} [\underline{y}_{t+\tau}] = E[\underline{y}_{t+\tau} | y_{\leq t}] = 0 \quad (93.103)$$

$$\left\langle \underline{y}_{t+\tau}, \underline{y}_{t+\tau} \right\rangle_{|y_{\leq t}} = \sum_{j=0}^{\min(\tau-1, q)} \nu_j^2 \quad (93.104)$$

Eq.(93.104) is motivated by Fig.93.11). Only the green arrows entering  $\underline{y}_{t+\tau}$  and originating in a node  $\underline{n}_{t'}$  with  $t' > t$  contribute to the right hand side of Eq.(93.104).

Thus, the mean of  $\underline{y}_{t+\tau}$  can be predicted to remain zero for all  $\tau > 0$  (forever). The error in that prediction increases with  $\tau$  until  $\tau$  reaches  $q$ . After that, the error remains constant.

Note that

$$\underline{y}_{t+\tau} | y_{\leq t} = \sum_{j=\tau}^{\infty} \nu_j \underline{n}_{t+\tau-j} \quad (93.105)$$

$$= \sum_{j=\tau}^{\infty} \nu_j \mathcal{B}^{j-\tau} \underline{n}_t \quad (93.106)$$

$$= \left[ \sum_{j=0}^{\infty} \nu_j \mathcal{B}^{j-\tau} \right]_{\mathcal{B}^{\geq 0}} \underline{n}_t \quad (93.107)$$

$$= [\mathcal{B}^{-\tau} \nu(\mathcal{B})]_{\mathcal{B}^{\geq 0}} \underline{n}_t \quad (93.108)$$

$\mathcal{B}^{\geq 0}$  means only the non-negative powers of  $\mathcal{B}$  are kept. Eq.(93.108) is just Eq.(93.98) in fancy notation.

In  $MA(\infty)$ , if  $\nu(\mathcal{B})$  is invertible, then

$$\underline{n}_t = \nu(\mathcal{B})^{-1} \underline{y}_t \quad (93.109)$$

so

$$\boxed{\underline{y}_{t+\tau} | y_{\leq t} = \mathcal{L}_{WK} \underline{y}_t} \quad (93.110)$$

where

$$\mathcal{L}_{WK} = [\mathcal{B}^{-\tau} \nu(\mathcal{B})]_{\mathcal{B}^{\geq 0}} \nu(\mathcal{B})^{-1} \quad (93.111)$$

Eq.(93.110) is called the **Wiener-Kolgomorov prediction formula (WKPF)**. Next, we apply WKPF to  $AR(1)$  and  $MA(1)$  as examples of its usage.

- $AR(1)$

$$\underbrace{(1 - \alpha_1 \mathcal{B})}_{\nu(\mathcal{B})^{-1}} \underline{y}_t = \underline{n}_t \quad (93.112)$$

$$\underline{y}_t = \underbrace{\left[ \sum_{j=0}^{\infty} (\alpha_1 \mathcal{B})^j \right]}_{\nu(\mathcal{B})} \underline{n}_t \quad (93.113)$$

$$\nu_j = (\alpha_1)^j \quad (93.114)$$

$$[\mathcal{B}^{-\tau} \nu(\mathcal{B})]_{\mathcal{B} \geq 0} = (\alpha_1)^\tau \nu(\mathcal{B}) \quad (93.115)$$

$$\underline{y}_{t+\tau} | y_{\leq t} = (\alpha_1)^\tau \underline{y}_t \quad (93.116)$$

Hence,  $\underline{y}_{t+\tau} | y_{\leq t}$  decreases geometrically as  $\tau$  grows.

- $MA(1)$

$$\underline{y}_t = \underbrace{(1 + \nu_1 \mathcal{B})}_{\nu(\mathcal{B})} \underline{n}_t \quad (93.117)$$

$$[\mathcal{B}^{-\tau} \nu(\mathcal{B})]_{\mathcal{B} \geq 0} = \delta(\tau, 1) \nu_1 \quad (93.118)$$

$$\begin{aligned} \underline{y}_{t+\tau} | y_{\leq t} &= \delta(\tau, 1) \nu_1 \underbrace{\left[ \sum_{j=0}^{\infty} (-\nu_1 \mathcal{B})^j \right]}_{\nu(\mathcal{B})^{-1}} \underline{y}_t \\ &= \delta(\tau, 1) \nu_1 \underline{n}_t \end{aligned} \quad (93.119) \quad (93.120)$$

(b) **find  $\underline{y}_{t+\tau} | y_{\leq t}$  given  $\underline{y}_{\leq t}$ , but, for some  $m > 0$ ,  $\underline{y}_{\leq t-m} \approx 0$  (approximation)**

$$\underline{y}_{t+\tau} | y_{\leq \tau} \approx [\mathcal{L}_{WK}]_{\mathcal{B}^{<m}} \underline{y}_t \quad (93.121)$$

(c) **find  $\underline{y}_{t+\tau} | y_{\leq t}$  given  $\gamma_{[0, m-1]}$  and  $\gamma_{[\tau, \tau+m-1]}^{part}$**

$$\underline{y}_{t+\tau} | y_{\leq t} = \sum_{j=0}^{m-1} \underline{y}_{t-j} \beta_j \quad (93.122)$$

Suppose that  $k \in \mathbb{Z}_{[0, m-1]}$ .

Note that

$$\underline{y}_{t-k} | y_{\leq t} = \underline{y}_{t-k} . \quad (93.123)$$

$$\underbrace{\left\langle \underline{y}_{t-k} | y_{\leq t} , \underline{y}_{t+\tau} | y_{\leq t} \right\rangle}_{\gamma_{\tau+k}^{part}} = \sum_{j=0}^{m-1} \underbrace{\left\langle \underline{y}_{t-k} , \underline{y}_{t-j} \right\rangle}_{\gamma_{k-j}} \beta_j \quad (93.124)$$

$$\begin{bmatrix} \gamma_{\tau}^{part} \\ \gamma_{\tau+1}^{part} \\ \vdots \\ \gamma_{\tau+m-1}^{part} \end{bmatrix} = \underbrace{\begin{bmatrix} \gamma_0 & \gamma_{-1} & \gamma_{-2} & \cdots & \gamma_{1-m} \\ \gamma_1 & \gamma_0 & \gamma_{-1} & \cdots & \gamma_{2-m} \\ \vdots & & & & \\ \gamma_{m-1} & \gamma_{m-2} & \gamma_{m-3} & \cdots & \gamma_0 \end{bmatrix}}_{\Gamma} \underbrace{\begin{bmatrix} \beta_0 \\ \beta_1 \\ \vdots \\ \beta_{m-1} \end{bmatrix}}_{\beta^m} \quad (93.125)$$

Solve Eq.(93.125) for  $\beta^m$  and plug  $\beta^m$  into Eq.(93.122).

## 93.13 Model Learning

### Box-Jenkins Method

#### 1. Filtering Data (FD)

Removing trends and periodicity (seasonality) via differencing, so as to achieve a w-stationary t-series. We deal with FD in Section 93.14.

#### 2. Model Selection

Finding best possible  $p, q$  for  $ARMA(p, q)$  using various statistical tests and metrics.

#### 3. Parameter Learning (PL)

Finding best possible coefficients  $\alpha_j$  and  $\nu_j$ . We deal with PL in Section 93.15.

#### 4. Testing

Measuring the goodness of fit.

## 93.14 Differencing and $ARIMA(p, d, q)$

Let  $\alpha \in (0, 1)$ . We say that  $\{\underline{s}_t\}_{\forall t}$  is a **Simple Exponential Smoothing (SES) t-series** if it satisfies

$$s_t = (1 - \alpha)s_{t-1} + \alpha x_t \quad (93.126)$$

A SES t-series can be represented by the bnet of Fig.93.12. The TPM, printed in blue, for node  $\underline{s}_t$ , is as follows

$$P(s_t) = \mathbb{1}(s_t = \text{ see Eq.(93.126)}) \quad (93.127)$$

One has

$$(1 - (1 - \alpha)\mathcal{B})\underline{s}_t = \alpha\underline{x}_t \quad (93.128)$$

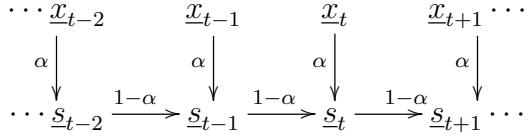


Figure 93.12: Bnet for Simple Exponential Smoothing t-series.  $\alpha \in (0, 1)$

so

$$\underline{s}_t = \frac{\alpha}{1 - (1 - \alpha)\mathcal{B}} \underline{x}_t \quad (93.129)$$

$$= \alpha \sum_{j=0}^{\infty} (1 - \alpha)^j \mathcal{B}^j \underline{x}_t \quad (\text{by Eq.(93.7)}) \quad (93.130)$$

Note from Fig.93.12 and Eq.(93.130) that each shock  $\underline{x}_{t-j}$  with  $j > 0$  contributes to  $\underline{s}_t$  proportionally to the product  $\alpha(1 - \alpha)^j$  of arrow weights in the path from  $\underline{x}_{t-j}$  to  $\underline{s}_t$ . For example,  $\underline{x}_{t-2}$  contributes to  $\underline{s}_t$  in the proportion  $\alpha(1 - \alpha)^2$ . The contributions of  $\underline{x}_{t-j}$  to  $\underline{s}_t$  decrease geometrically as the lag  $j$  increases.

Henceforth, we will abbreviate “differencing” by “diff”.

- First order diff operator

$$\Delta x_t = x_t - x_{t-1} = (1 - \mathcal{B})x_t \quad (93.131)$$

Seasonal first order diff:

$$\Delta_{sea} x_t = x_t - x_{t-ts} \quad (93.132)$$

where  $ts$  is length of season.

- Second order diff operator

$$\Delta^2 x_t = \Delta x_t - \Delta x_{t-1} \quad (93.133)$$

$$= x_t - 2x_{t-1} + x_{t-2} \quad (93.134)$$

$$= (1 - 2\mathcal{B} + \mathcal{B}^2)x_t \quad (93.135)$$

$$= (1 - \mathcal{B})^2 x_t \quad (93.136)$$

- $d$ -th order diff operator

$$\Delta^d \underline{x}_t = (1 - \mathcal{B})^d \underline{x}_t \quad (93.137)$$

Recall that if  $\{\underline{y}_t\}_{\forall t}$  is an  $ARMA(p+d, q)$  t-series,

$$\left(1 - \sum_{j=1}^{p+d} \alpha_j \mathcal{B}^j\right) \underline{y}_t = \left(1 + \sum_{k=1}^q \nu_k \mathcal{B}^k\right) \underline{n}_t \quad (93.138)$$

We will say that  $\{\underline{y}_t\}_{\forall t}$  is an **Autoregressive Integrated Moving Average  $ARIMA(p, d, q)$  t-series** if

$$\left(1 - \sum_{j=1}^p \alpha_j \mathcal{B}^j\right) \underbrace{\Delta^d \underline{y}_t}_{(1-\mathcal{B})^d \underline{y}_t} = \left(1 + \sum_{k=1}^q \nu_k \mathcal{B}^k\right) \underline{n}_t \quad (93.139)$$

So an  $ARIMA(p, d, q)$  t-series is a special case of an  $ARMA(p+d, q)$  t-series.

Define  $\mathcal{O}_{BEF}$  and  $\mathcal{O}_{AFT}$  by

$$\mathcal{O}_{BEF} = 1 - \alpha_1 \mathcal{B} - \alpha_2 \mathcal{B}^2 - \alpha_3 \mathcal{B}^3 \quad (93.140)$$

$$\mathcal{O}_{AFT} = \mathcal{O}_{BEF}(1 - \mathcal{B}) \quad (93.141)$$

$$= \begin{cases} 1 & -\alpha_1 \mathcal{B} & -\alpha_2 \mathcal{B}^2 & -\alpha_3 \mathcal{B}^3 \\ & -\mathcal{B} & +\alpha_1 \mathcal{B}^2 & +\alpha_2 \mathcal{B}^3 & +\alpha_3 \mathcal{B}^4 \end{cases} \quad (93.142)$$

$$= 1 - \underbrace{(\alpha_1 + 1)}_{\alpha'_1} \mathcal{B} - \underbrace{(\alpha_2 - \alpha_1)}_{\alpha'_2} \mathcal{B}^2 - \underbrace{(\alpha_3 - \alpha_2)}_{\alpha'_3} \mathcal{B}^3 - \underbrace{(0 - \alpha_3)}_{\alpha'_4} \mathcal{B}^4 \quad (93.143)$$

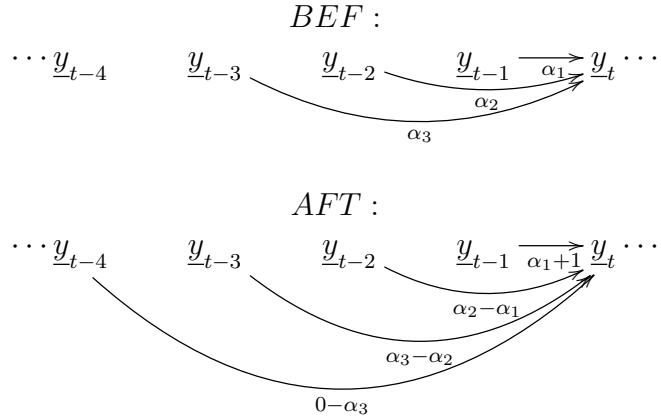


Figure 93.13: Effect on  $\underline{y}_t$  of going from before (BEF) with a t-series  $ARIMA(3,0,0)$  to after (AFT) with a t-series  $ARIMA(3,1,0)$ .

$\mathcal{O}_{BEF}\underline{y}_t$  and  $\mathcal{O}_{AFT}\underline{y}_t$  are illustrated in Fig.93.13. Note that in going from BEF to AFT, a new arrow is introduced with weight  $\alpha'_4 = -\alpha_3$ . The intermediate length

arrows  $\underline{y}_{t-3} \rightarrow \underline{y}_t$  and  $\underline{y}_{t-2} \rightarrow \underline{y}_t$  have weights  $\alpha'_3 = \alpha_3 - \alpha_2$  and  $\alpha'_2 = \alpha_2 - \alpha_1$  so if  $\alpha_j \approx \alpha_{j-1}$ , then those 2 arrows have negligible weights. Only the the longest arrow  $\underline{y}_{t-4} \rightarrow \underline{y}_t$  and the shortest arrow  $\underline{y}_{t-1} \rightarrow \underline{y}_t$  have non-negligible weights.

Suppose

$$\underline{y}_t \approx a + bt + ct^2 + dt^3 \quad (93.144)$$

This smooth, low-order polynomial-fit to the t-series is called its **trend**.

$$\Delta \underline{y}_t \approx \Delta t \frac{d}{dt} \underline{y}_t = b + 2ct + 3dt^2 \quad (93.145)$$

$$\Delta^2 \underline{y}_t \approx (\Delta t)^2 \frac{d^2}{dt^2} \underline{y}_t = 2c + 6dt \quad (93.146)$$

$$\Delta^3 \underline{y}_t \approx (\Delta t)^3 \frac{d^3}{dt^3} \underline{y}_t = 6d \quad (93.147)$$

Note that the mean  $6d$  in  $\Delta^3 \underline{y}_t$  can be adjusted to zero (demeaning). From this example, we see that every time we apply a diff operator to a time series, we reduce the order of its polynomial trend by one.

Note that if  $\{\underline{y}_t\}_{\forall t}$  is an *ARIMA*(0, 1, 1) t-series,

$$\Delta \underline{y}_t = (1 + \nu_1 \mathcal{B}) \underline{n}_t \quad (93.148)$$

$$\underline{y}_t = \underline{y}_{t-1} + \underline{n}_t + \nu_1 \underline{n}_{t-1} \quad (93.149)$$

**Claim 144** *ARIMA*(0, 1, 1) is equivalent to a simple exponential smoothing t-series.

**proof:** Setting

$$\underline{n}_t = \underline{y}_t - \widehat{\underline{y}}_t \quad (93.150)$$

in Eq.(93.148), we get

$$(1 - \mathcal{B}) \underline{y}_t = (1 - \nu_1 \mathcal{B}) (\underline{y}_t - \widehat{\underline{y}}_t) \quad (93.151)$$

$$(1 - \nu_1 \mathcal{B}) \widehat{\underline{y}}_t = (1 - \nu_1) \mathcal{B} \underline{y}_t \quad (93.152)$$

$$\widehat{\underline{y}}_t = \nu_1 \widehat{\underline{y}}_{t-1} + (1 - \nu_1) \underline{y}_{t-1} \quad (93.153)$$

Now replace  $\widehat{\underline{y}}_t \rightarrow \underline{s}_t$ ,  $\underline{y}_{t-1} \rightarrow \underline{n}_t$  and  $\nu_1 \rightarrow 1 - \alpha$ .

Note that this proof has established the equivalence of two different bnets. Those two bnets are pictured in Fig.93.14.

**QED**

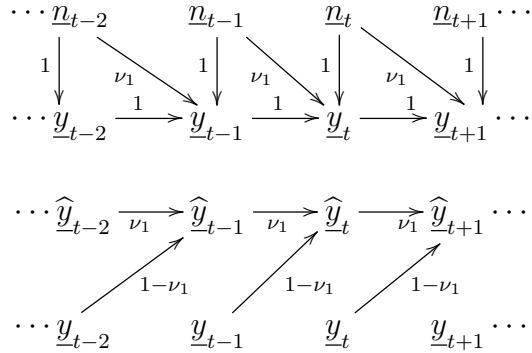


Figure 93.14: Bnets for two t-series that were proven equivalent in Claim 144. Note that the 2 bnets have NO arrows in common!

## 93.15 Parameter Learning

In this section, we will show how to find an estimate  $\hat{\theta}$  for the parameters  $\theta = (\{\alpha_j\}_{\forall j}, \{\nu_j\}_{\forall j}, \sigma^2)$  used in  $ARMA(p, q)$ . We do this **parameter learning (PL)** by postulating a “quasi” log likelihood function  $LL(\theta)$ , and maximizing that over  $\theta$ . The estimate  $\hat{\theta}$  that we obtain is called the **Quasi-Maximum Likelihood Estimate (QMLE)**. The reason for using the prefix “quasi” is that the likelihood probability involved doesn’t really satisfy the i.i.d assumption.

### 93.15.1 PL of $AR(p)$

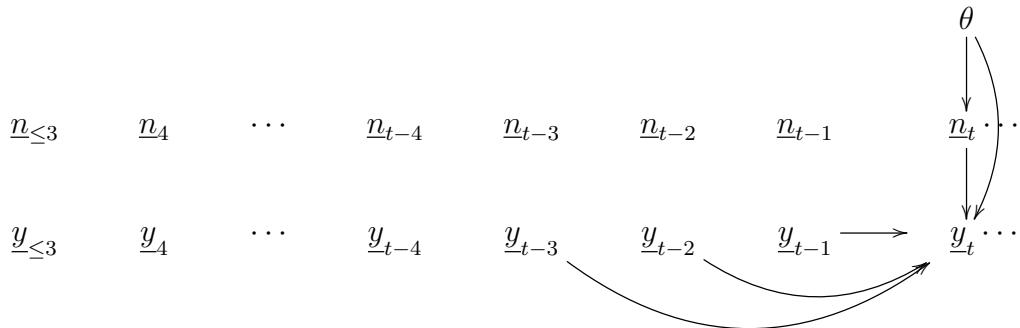


Figure 93.15: Bnet for PL of  $AR(3)$ . For clarity, we show only the arrows entering nodes  $y_t$  and  $n_t$ .

Recall that if  $\{y_t\}_{\forall t}$  is an  $AR(p)$  t-series,

$$y_t = \sum_{j=1}^p \alpha_j y_{t-j} + n_t \quad (93.154)$$

Let  $\theta = (\sigma^2, \alpha_{[1,p]})$ . We want to learn the parameters  $\theta$  of the  $AR(p)$  bnet Fig.93.15, assuming the TPMs, printed in blue, are as follows.

For  $t \geq p+1$

$$P(y_t|y_{<t}, n_t, \theta) = \mathbb{1}(y_t = \text{see Eq.(93.154)}) \quad (93.155)$$

$$P(n_t|\theta) = \frac{1}{\sigma\sqrt{2\pi}} \exp\left[\frac{-(n_t)^2}{2\sigma^2}\right] \quad (93.156)$$

Note that

$$P(y_{\leq t}|\theta) = \sum_{n_{[p+1,t]}} \left\{ \prod_{\tau \in [p+1,t]} P(y_\tau|y_{[\tau-p,\tau-1]}, n_\tau) P(n_\tau|\theta) \right\} P(y_{\leq p}|\theta) \quad (93.157)$$

$$= \prod_{\tau \in [p+1,t]} \left\{ \frac{1}{\sqrt{2\pi}\sigma^2} \exp\left[\frac{-\left(y_\tau - \sum_{j=1}^p \alpha_j y_{\tau-j}\right)^2}{2\sigma^2}\right] \right\} P(y_{\leq p}|\theta) \quad (93.158)$$

The log likelihood function  $LL_t(\theta)$  for this bnet is defined by

$$LL_t(\theta) = \frac{1}{t} \ln P(y_{\leq t}|\theta). \quad (93.159)$$

Hence,

$$LL_t(\theta) = \underbrace{\frac{1}{t} \ln P(y_{\leq p}|\theta)}_{LL_t^{prior}(\theta)} + LL'_t(\theta) \quad (93.160a)$$

where

$$LL'_t(\theta) = \frac{-(t-p)}{t} \ln \sqrt{2\pi\sigma^2} - \frac{1}{2t\sigma^2} \sum_{\tau=p+1}^t \left( y_\tau - \sum_{j=1}^p \alpha_j y_{\tau-j} \right)^2. \quad (93.160b)$$

Henceforth, we will assume that  $y_{[1,t]}$  is known.

We start by assuming that the prior log likelihood  $LL_t^{prior}(\theta)$  is zero. This means that we have uniform (uninformative) priors. Later on, we will consider instead a Gaussian prior that uses the info that  $y_{\leq p}$  is known a priori.

If we assume that  $y_{[1,t]}$  is known, then we can plug this info into  $LL'_t(\theta)$  and use a non-linear optimization method to maximize  $LL'_t(\theta)$  and find the optimum  $\theta$ .

Alternatively, one can use LR. Define the strange looking dataset

$$\mathcal{D} = \{(t, y_{[t-p,t-1]}, \boxed{y_t}) : t\} \quad (93.161)$$

This dataset is strange because it replaces sampling from a population with sampling in time. (i.e., a “stochastic” average by an “ergodic” average.) The datasets that we use to do LR usually satisfy the i.i.d. assumption, but that assumption does not necessarily hold for this one. Luckily, that assumption is not necessary for doing LR with x-variables  $y_{[t-p,t-1]}$ , y-variable  $y_t$ , and regression coefficients  $\alpha_{[1,p]}$ . The LR software gives estimates  $\hat{\alpha}_{[1,p]}$  that we can use to calculate residuals

$$\epsilon_\tau = y_\tau - \sum_{j=1}^p \hat{\alpha}_j y_{\tau-j} \quad (93.162)$$

One can estimate  $\sigma^2$  from those residuals using

$$\hat{\sigma}^2 = \frac{1}{t-p} \sum_{\tau=p+1}^t \epsilon_\tau^2. \quad (93.163)$$

So far, we have assumed an uninformative prior. Alternatively, one can assume the Gaussian prior

$$P(y_{\leq p} | \theta) = \frac{1}{(2\pi\sigma^2)^{\frac{p}{2}}} \exp \left[ -y_{\leq p}^T \frac{\Gamma^{-1}}{2} y_{\leq p} \right] \quad (93.164)$$

where

$$\Gamma_{i,j} = \left\langle \underline{y}_i, \underline{y}_j \right\rangle = \gamma_{j-i} \quad (93.165)$$

for  $i, j \in \mathbb{Z}_{[1,p]}$ . We are assuming that all  $\underline{y}_\tau$  have been demeaned; i.e., the mean

$$\hat{\mu} = \frac{1}{t} \sum_{\tau=1}^t y_\tau \quad (93.166)$$

has been subtracted from each  $y_\tau$  for  $\tau \in \mathbb{Z}_{[1,t]}$ .

### 93.15.2 PL of $MA(q)$

Recall that if  $\{\underline{y}_t\}_{\forall t}$  is an  $MA(q)$  t-series,

$$y_t = \sum_{j=1}^q \nu_j n_{t-j} + n_t \quad (93.167)$$

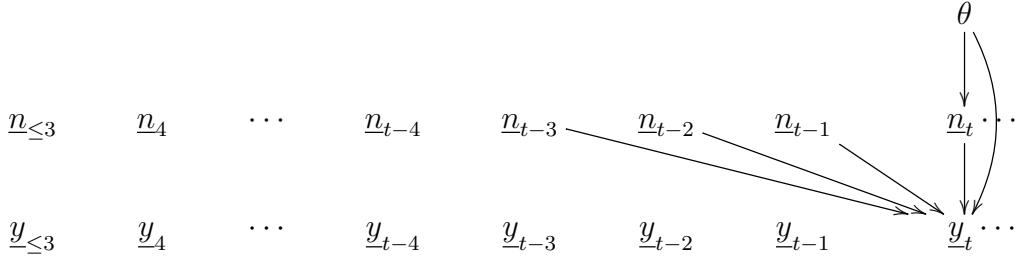


Figure 93.16: Bnet for PL of  $MA(3)$ . For clarity, we show only the arrows entering nodes  $y_t$  and  $n_t$ .

Let  $\theta = (\sigma^2, \nu_{[1,q]})$ . We want to learn the parameters  $\theta$  of the  $MA(q)$  bnet Fig.93.16, assuming the TPMs, printed in blue, are as follows.

For  $t \geq q + 1$ , let

$$P(y_t | n_{\leq t}, \theta) = \mathbb{1}(y_t = \text{see Eq.(93.167)}) \quad (93.168)$$

$$P(n_t | \theta) = \frac{1}{\sigma \sqrt{2\pi}} \exp \left[ \frac{-(n_t)^2}{2\sigma^2} \right] \quad (93.169)$$

Note that

$$P(y_{\leq t} | \theta) = \sum_{n_{[q+1,t]}} \left\{ \prod_{\tau \in [q+1,t]} P(y_\tau | n_{[\tau-q,\tau-1]}, n_\tau) P(n_\tau | \theta) \right\} P(n_{\leq q} | \theta) \quad (93.170)$$

$$= \prod_{\tau \in [q+1,t]} \left\{ \frac{1}{\sqrt{2\pi}\sigma^2} \exp \left[ \frac{-\left(y_\tau - \sum_{j=1}^q \nu_j n_{\tau-j}\right)^2}{2\sigma^2} \right] \right\} P(n_{\leq q} | \theta) \quad (93.171)$$

The log likelihood function  $LL_t(\theta)$  for this bnet is defined by

$$LL_t(\theta) = \frac{1}{t} \ln P(y_{\leq t} | \theta) \quad (93.172)$$

$$LL_t(\theta) = \underbrace{\frac{1}{t} \ln P(y_{\leq q} | \theta)}_{LL_t^{prior}(\theta)} + LL'_t(\theta) \quad (93.173a)$$

where

$$LL'_t(\theta) = \frac{-(t-q)}{t} \ln \sqrt{2\pi\sigma^2} - \frac{1}{2t\sigma^2} \sum_{\tau=q+1}^t \left( y_\tau - \sum_{j=1}^q \nu_j n_{\tau-j} \right)^2 \quad (93.173b)$$

Henceforth, we will assume that  $n_{\leq q} = 0$ . By Eq.(93.167), this implies that  $y_{\leq q} = 0$ , so the prior log likelihood  $LL_t^{prior}(\theta)$  is independent of  $\theta$ .

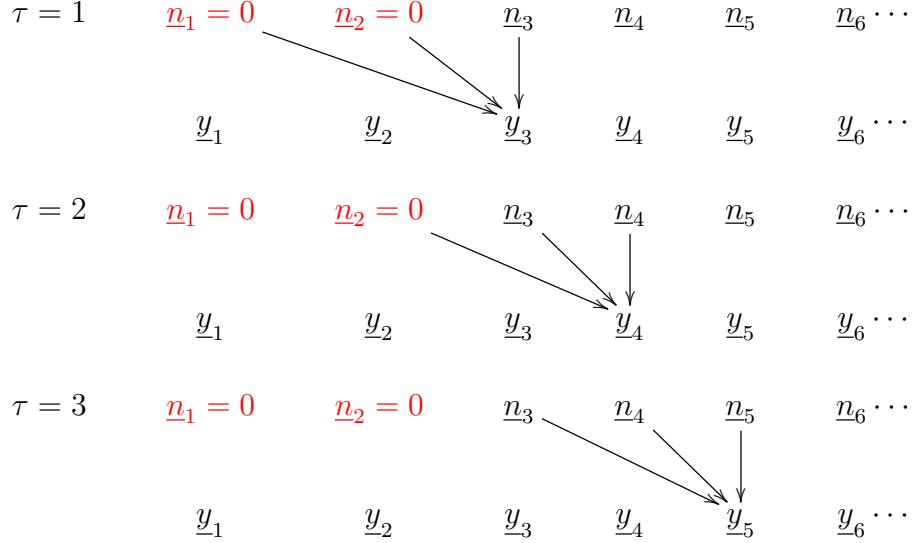


Figure 93.17: Bnet for PL of  $MA(2)$ . We assume  $\underline{n}_1 = \underline{n}_2 = 0$ . For clarity, we show only the arrows entering node  $\underline{y}_{2+\tau}$  for  $\tau = 1, 2, 3$ .

Eq.(93.173) expresses  $LL'_t(\theta)$  in terms of  $y_\tau$ 's and  $n_\tau$ 's, but the input data consist of only  $y_\tau$ 's. Luckily, Eq.(93.167) can be used to express all the  $n_{\leq t}$  in terms of the  $y_{\leq t}$ , assuming the input  $n_{\leq q} = 0$ . Next, we will explain how to do this. For definiteness and simplicity, we will assume  $q = 2$  and  $\nu_1 = \nu_2 = 1$ , and we will use Fig.93.17 as a pedagogical aid.

For  $q = 2$ , Eq.(93.167) gives  $\underline{y}_\tau$  as a linear combination of 3  $\underline{n}$  nodes,  $\underline{n}_\tau, \underline{n}_{\tau-1}$  and  $\underline{n}_{\tau-2}$ . But since it's a linear equation, it can be used to express the latest  $\underline{n}$  node, i.e.,  $\underline{n}_\tau$ , in terms of  $\underline{y}_\tau$  and the 2 previous  $\underline{n}$  nodes.

Hence, we see from Fig.93.17 that:

From  $\underline{n}_1 = \underline{n}_2 = 0$ , we get  $\underline{y}_1 = \underline{y}_2 = 0$ .

From the  $\tau = 1$  bnet, we get

$$\underline{n}_3 = \underline{y}_3 \quad (93.174)$$

From the  $\tau = 2$  bnet, we get

$$\underline{n}_4 = \underline{y}_4 - \underline{n}_3 \quad (93.175)$$

From the  $\tau = 3$  bnet, we get

$$\underline{n}_5 = \underline{y}_5 - \underline{n}_3 - \underline{n}_4 \quad (93.176)$$

### 93.15.3 PL of $ARMA(p, q)$

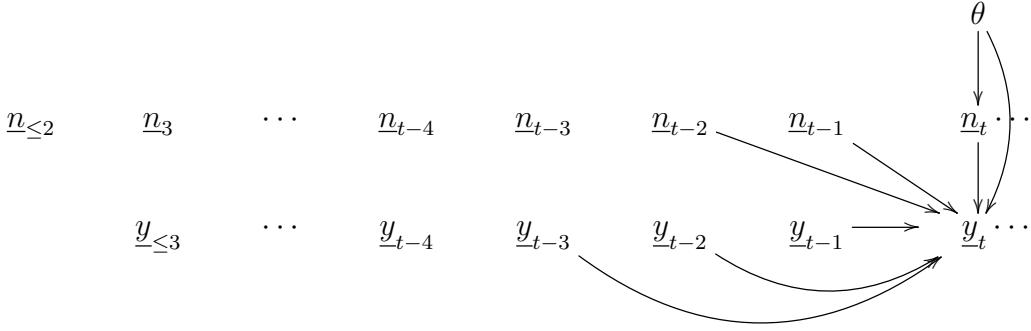


Figure 93.18: Bnet for PL of  $AR(3, 2)$ . For clarity, we show only the arrows entering nodes  $\underline{y}_t$  and  $\underline{n}_t$ .

Recall that if  $\{\underline{y}_t\}_{\forall t}$  is an  $AR(p, q)$  t-series, then

$$y_t = \sum_{j=1}^p \alpha_j y_{t-j} + n_t + \sum_{j=1}^q \nu_j y_{t-j} \quad (93.177)$$

Let  $\theta = (\sigma^2, \alpha_{[1,p]}, \nu_{[1,q]})$ . We want to learn the parameters  $\theta$  of the  $ARMA(p, q)$  bnet Fig.93.18, in which the TPMs, printed in blue, are as follows.

For  $t \geq \max(p+1, q+1)$ , let

$$P(y_t | y_{<t}, n_{\leq t}, \theta) = \mathbb{1} (y_t = \text{see Eq.(93.177)}) \quad (93.178)$$

$$P(n_t | \theta) = \frac{1}{\sigma \sqrt{2\pi}} \exp \left[ \frac{-(n_t)^2}{2\sigma^2} \right] \quad (93.179)$$

As we did for  $AR(p)$  and  $MA(q)$ , we can now calculate a log likelihood function and maximize it to obtain the parameters  $\theta$ . But first we will have to assume that  $n_{\leq q} = 0$  and  $y_{[1,t]}$  is known, and we will have to express the unknown  $n_{[q+1,t]}$  in terms of the known  $y_{[1,t]}$  using the t-series definition Eq.(93.177).

### 93.16 $VAR(p)$

Let  $\vec{x}_t = (\underline{x}_t^1, \underline{x}_t^2, \dots, \underline{x}_t^{nr})^T \in \mathbb{R}^{nr \times 1}$ . Thus,  $\vec{x}_t$  for each  $t$  is a column vector with  $nr$  rows. A **vector time series**, denoted variously by  $\{\vec{x}_1, \vec{x}_2, \dots, \vec{x}_{nt}\} = \{\vec{x}_t\}_{t=1}^{nt} = \{\vec{x}_t\}_{\forall t}$ , is a set of  $\mathbb{R}^{nr \times 1}$  vectors index by a discrete set of times  $\mathbb{Z}_{[0,nt]}$ .

Henceforth, we will use the Einstein summation convention for uppercase indices like  $A, B, C \in \mathbb{Z}_{[1,nr]}$ ; i.e., they should be summed over from 1 to  $nr$  if they are repeated in a product. For example,  $x^A y^A = \sum_{A=1}^{nr} x^A y^A$ .

By **vector white noise**  $\{\vec{n}_t\}_{\forall t} \sim WN(0, \Sigma)$ , where  $\Sigma \in \mathbb{R}^{nr \times nr}$ , we mean a vector t-series  $\{\vec{n}_t\}_{\forall t}$  that satisfies, for  $A, B \in \mathbb{Z}_{[1,nr]}$  and  $t, t' \in \mathbb{Z}_{[1,nt]}$ ,

$$E[\underline{n}_t^A] = 0 \quad (93.180)$$

$$\langle \underline{n}_t^A, \underline{n}_{t'}^B \rangle = \Sigma^{A,B} \delta(t, t') \quad (93.181)$$

Suppose  $\{\vec{y}_t\}_{\forall t}$  is a zero mean vector t-series. Hence  $\underline{y}_t^A = \underline{Y}_t^A - \mu^A$ ,  $E[\underline{Y}_t^A] = \mu^A$ ,  $E[\underline{y}_t^A] = 0$ . Suppose also that  $\{\vec{n}_t\}_{\forall t} \sim WN(0, \Sigma)$ . Then we define a **Vector Auto-Regressive t-series**  $VAR(p)$  by

$$\underline{y}_t^A = \sum_{j=1}^p \alpha_j^{A,B} \underline{y}_{t-j}^B + \underline{n}_t^A \quad (93.182)$$

The bnet for  $VAR(p)$  is the same as the bnet for  $AR(p)$  except that now, for all  $t$ , the nodes  $\underline{y}_t$  and  $\underline{n}_t$  are replaced by  $\vec{y}_t$  and  $\vec{n}_t$  and now the node weights  $\alpha_t$  are  $nr \times nr$  matrices with entries  $\alpha_t^{A,B}$ . For example, for  $nr = 2$ , we have

$$\begin{bmatrix} \underline{y}_t^1 \\ \underline{y}_t^2 \end{bmatrix} = \sum_{j=1}^p \begin{bmatrix} \alpha_j^{1,1} & \alpha_j^{1,2} \\ \alpha_j^{2,1} & \alpha_j^{2,2} \end{bmatrix} \begin{bmatrix} \underline{y}_{t-j}^1 \\ \underline{y}_{t-j}^2 \end{bmatrix} + \begin{bmatrix} \underline{n}_t^1 \\ \underline{n}_t^2 \end{bmatrix} \quad (93.183)$$

# Chapter 94

## Transfer Learning

Historically, the term Transfer Learning (TL) has been used in AI mostly by Artificial Neural Net (ANN) proponents (see the Wikipedia article on TL, Ref.[160]). Recently, however, a theory of causal TL has begun to emerge (see Chapter 96).

TL in AI is a fairly wide topic that is somewhat ambiguously defined. Some subjects that can be lumped under the heading of TL in AI are:

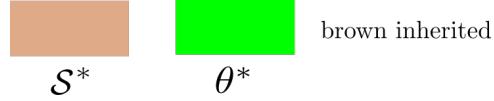
- data fusion/combining models
- model generalization
- transportability of causal knowledge, external validity (see Chapter 96)

Most AI researchers will agree that it is highly desirable to have TL in AI, because the human brain obviously does plenty of TL to great advantage. Although reams of papers have been written about the subject of TL in AI, a systematic theory of TL in AI that is universally accepted and popular remains elusive. The current theory of TL for ANN looks to me like a grab bag of heuristic approaches that are fragile, meaning they can be easily spoofed. The theory of TL for bnets (see Chapter 96) seems to me to be in much better shape: it's more elaborate, systematic, and it yields more robust results.

In this brief chapter, I will limit myself to describing a possible way of classifying, from a bnet perspective, the various approaches to TL in AI. Note that this method of classification even works for TL for ANNs, because ANNs can be viewed as bnets with deterministic nodes and a layered structure. One can describe TL in AI as a systematic way of defining a bnet  $\mathcal{B}^*$  using a bnet  $\mathcal{B}$  and other information. Bnet  $\mathcal{B}$  is associated with a dataset  $\mathcal{D}$ , and bnet  $\mathcal{B}^*$  is associated with a dataset  $\mathcal{D}^*$ . A bnet  $\mathcal{B} = (\mathcal{S}, \theta)$  comprises a DAG structure  $\mathcal{S}$  and a TPM for each node of the DAG. We'll denote the TPMs (a.k.a. parameters) of  $\mathcal{B}$  by  $\theta$ . So let's classify the various approaches to TL in AI by specifying what parts of the structure  $\mathcal{S}$  and parameters  $\theta$  of  $\mathcal{B}$  are transferred to the structure  $\mathcal{S}^*$  and parameters  $\theta^*$  of  $\mathcal{B}^*$ , and what parts of  $\mathcal{B}^* = (\mathcal{S}^*, \theta^*)$  are new.

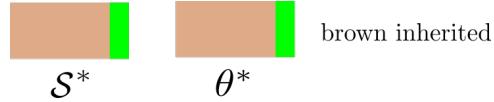
1. **Fine tune parameters.**  $\mathcal{S}^* = \mathcal{S}$ ,  $\theta^* \approx \theta$ .

In this approach, we use the dataset  $\mathcal{D}^*$  associated with bnet  $\mathcal{B}^*$  to adjust slightly the parameters from  $\theta$  to  $\theta^*$ .

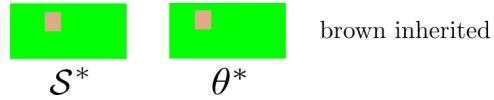


2. **Replace final layers of  $\mathcal{S}$  and of  $\theta$  by new ones.**  $\mathcal{S}^* = \mathcal{S}$  and  $\theta^* = \theta$  except for final layers,

For example, in an ANN, replace the final layers by new ones, and use  $\mathcal{D}^*$  to find the parameters of those new final layers.



3. **Transfer only the TPM of a single node  $y$  of  $\mathcal{B}$ .**  $\mathcal{S}^*$  and  $\theta^*$  are new except  $P^*(y|pa(y)) = P(y|pa(y))$ .



# Chapter 95

## Transformer Networks

The primary reference for this chapter is Ref.[81]. Ref.[81] is the highly influential 2017 paper entitled “Attention is all you need” that introduced **Transformer Networks** (tranets) and Attention into the AI vernacular. Besides Ref.[81], I also read blog posts such as Ref.[29] and the Wikipedia article on tranet (Ref. [161]). For a complete list of the large number of excellent blog post that I read to learn about this subject, see my open source software texnn (Ref.[80]).<sup>1</sup>

Transformer Networks (tranets) have been taking the fields of Natural Language Processing (NLP) and Large Language Models (LLM) by storm in recent years. They were introduced in 2017 and already are the basis of numerous LLMs. Two famous examples are, BERT (Bidirectional Encoder Representations from Transformers) and ChatGPT (Generative Pre-trained Transformer). Both of these have been trained with huge databases, of which all of the English Wikipedia ( $\sim 10^9$  words) is but a small part.

How well ChatGPT works was a huge surprise to most people, including experts in AI/ML. My conjecture is that this surprising LLM performance is due to causality. Let me explain. I believe tranets and the LLM that use them, are just curve-fitters (so are Least Squares, vanilla NNs, Convolutional NNs, etc.). But, we lucked out, because tranets are very good at fitting causal data, and the space of all human generated text, including math equations and computer code, is causally connected (i.e., has a **causally connected topology**.).

Normally, tranets are drawn as box diagrams that are somewhat cryptic and ambiguous, at least to me. In this chapter, instead of drawing them as box diagrams, I represent them as causal DAGs (bnets). This makes their causal nature more explicit than the box diagrams, and, in my opinion, also makes them less ambiguous and more understandable than the box diagrams.

Recurrent Neural Nets (RNNs) are discussed in Chapter 75. tranets are quickly displacing RNNs, an older method, in NLP. tranets are better than RNNs for doing

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<sup>1</sup>texnn is Python software that I wrote specifically for drawing the bnets of this chapter, but later I generalized it to a stand-alone app that can draw any bnet (including SCMs, NNs and tranets), not just a tranet bnet.

NLP in several important ways. Whereas RNNs analyze the tokens (words) of a sentence sequentially (like a Kalman Filter), tranets analyze them in parallel, and thus are more amenable to parallel computing. Also, because RNNs analyze the words of a sentence sequentially, they tend to give more importance to the end of a sentence than to its beginning. That's because RNNs start forgetting the beginning of a sentence by the time they reach its end, like a patient with Alzheimer's. tranets do not suffer from this malady.

Dynamical bnets are discussed in Chapter 25. In Chapter 75, we showed that RNNs are dynamical bnets. In this chapter we will show that tranets are dynamical bnets too.

In this chapter, we will use the Numpy-like tensor notation discussed in Section C.48. In particular, note that  $[n] = [0 : n] = \{0, 1, \dots, n - 1\}$  and that  $T^{[n], [m]}$  is an  $n \times m$  matrix.

## 95.1 Tensor Notation

Our tensor notation is discussed in Section C.48. Here is a quick review of some of the more salient facts in that section on tensors. Below, we will often accompany an equation in tensor component notation with the equivalent matrix equation, in parenthesis.

We use Greek letters for tensor indices.

Let  $\alpha \in [a]$ ,  $\beta \in [b]$ ,  $\gamma \in [c]$ ,  $\delta \in [d]$ ,  $\nu \in [n]$ ,  $\Delta \in [D]$ .

- **reshaping**

$$T^{\nu, \delta} \rightarrow T^\Delta \quad (T^{[n_h], [d]} \rightarrow T^{[D]}) \quad (95.1)$$

$$T^\Delta \rightarrow T^{\nu, \delta} \quad (T^{[D]} \rightarrow T^{[n_h], [d]}) \quad (95.2)$$

- **concatenation**

$$T^{[n]} = (T^0, T^1, \dots, T^{n-1}) = (T^\nu)_{\nu \in [n]} \quad (95.3)$$

- **Hadamard product (element-wise, entry-wise multiplication)**

$$T^{[n]} * S^{[n]} = (T^\nu S^\nu)_{\nu \in [n]} \quad (95.4)$$

- **Matrix multiplication**

$T^{[n]} = T^{[n], [1]}$  is a column vector.

$$(T^{[n]})^T S^{[n]} = \text{scalar} \quad (95.5)$$

$$T^{[a],[b]} S^{[b],[c]} = \left[ \sum_{\beta \in [b]} T^{\alpha,\beta} S^{\beta,\gamma} \right]_{\alpha \in [a], \gamma \in [c]} \quad (95.6)$$

Most treatments of tranets, including the “Attention is all you need” paper, order the operations chronologically from left to right (L2R). So if  $A$  occurs before  $B$ , they write  $AB$ . This is contrary to what is done in Linear Algebra, where one orders the operations chronologically from right to left (R2L), and one writes  $BA$ . In this chapter, will adhere to the Linear Algebra convention, since it is so prevalent and is the overwhelming precedent.

## 95.2 Recurrent Neural Net with Attention

### 95.2.1 Single Head Attention

Let

$\ell$  be the maximum number of words allowed in a sentence. Some words might be blanks (padding).

$d$  be the so called **hidden or embedding dimension**.

$e_\alpha^t \in \mathbb{R}^d$  be a  $d$ -dimensional column vector for word  $\alpha \in [\ell]$  at time  $t$ .

$W_q^t, W_k^t, W_v^t \in \mathbb{R}^{d \times d}$  be the weight matrices for time slice  $t$ . The letters  $Q, K, V$  stand for Query, Key and Value, respectively. These matrices are learned by training the net. They transform  $e_\alpha^t$  as follows

$$v_\alpha^t = W_v^t e_\alpha^t \quad (95.7)$$

$$q_\alpha^t = W_q^t e_\alpha^t \quad (95.8)$$

$$k_\alpha^t = W_k^t e_\alpha^t \quad (95.9)$$

Fig.95.1 represents a tranet of a 3-word sentence as a dynamical bnet. The TPMs (Transition Probability Matrices), printed in blue, for bnet Fig.95.1, are as follows:

$$P(v_\alpha^t | e_\alpha^t) = \mathbb{1}( v_\alpha^t = W_v^t e_\alpha^t ) \quad (95.10)$$

$$P(q_\alpha^t | e_\alpha^t) = \mathbb{1}( q_\alpha^t = W_q^t e_\alpha^t ) \quad (95.11)$$

$$P(k_\alpha^t | e_\alpha^t) = \mathbb{1}( k_\alpha^t = W_k^t e_\alpha^t ) \quad (95.12)$$

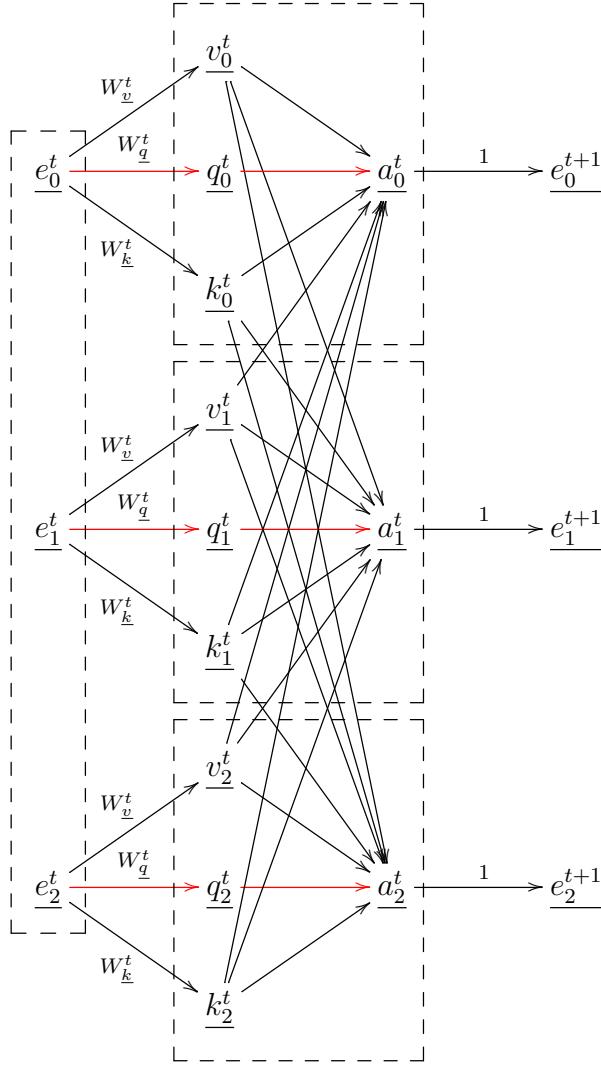


Figure 95.1: Dynamical bnet with single-head Attention for 3 words. Time-slice  $t$ . Note that  $k_\alpha^t$  for all  $\alpha$  points to  $a_{\alpha'}^t$  for all  $\alpha'$ . Likewise,  $v_\alpha^t$  for all  $\alpha$  points to  $a_{\alpha'}^t$  for all  $\alpha'$ . However,  $q_\alpha^t$  points only to  $a_\alpha^t$ .

$$P(e_\alpha^{t+1}|a_\alpha^t) = \mathbb{1}(e_\alpha^{t+1} = a_\alpha^t) \quad (95.13)$$

$$P(a_\alpha^{t+1}|v_\cdot^t, q_\alpha^t, k_\cdot^t) = \mathbb{1}(a_\alpha^{t+1} = \sum_{\alpha' \in [\ell]} v_{\alpha'}^t P(\alpha'|\alpha)) \quad (95.14)$$

where the conditional probability  $P(\alpha'|\alpha)$  is called defined as<sup>2</sup>

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<sup>2</sup>The reason sums over  $\delta \in [d]$  are divided by  $\sqrt{d}$  is to prevent the argument of the exponential

$$P(\alpha'|\alpha) = \text{softmax} \left[ \frac{1}{\sqrt{d}} \sum_{\delta \in [d]} (k^t)^{\delta, [\ell]} (q^t)^{\delta, \alpha} \right] (\alpha'|\alpha) \quad (95.15)$$

$$= \frac{\exp \left( \frac{1}{\sqrt{d}} (k_{\alpha'}^t)^T q_{\alpha}^t \right)}{\sum_{\alpha'' \in [\ell]} \exp \left( \frac{1}{\sqrt{d}} (k_{\alpha''}^t)^T q_{\alpha}^t \right)} \quad (95.16)$$

The right hand side of Eq.(95.14) constitutes an average over all the word vectors  $\{\underline{v}_{\alpha}^t : \alpha \in [\ell]\}$  in a sentence. This average is called the **Attention** (for a single head).<sup>3</sup>

$$\text{Attention}^{\delta, \alpha} ((v^t)^{[d], [\ell]}, (k^t)^{[d], [\ell]}, (q^t)^{[d], [\ell]}) = \sum_{\alpha' \in [\ell]} (v^t)^{\delta, \alpha'} P(\alpha'|\alpha) \quad (95.17)$$

On first encounter, the structure of an Attention bnet seems a bit mysterious. Then one realizes that this is an old friend. If the dashed boxes in Fig.95.1 are each “shrunk” to single nodes, then it becomes a TAN Bayes Net. Each of the 3 subgraphs  $e^t, (v^t, q^t, k^t), a^t$  also constitutes a TAN Bayes net.<sup>4</sup><sup>5</sup> In broad terms, Fig.95.1 can be described by saying that each word undergoes a special kind of 3-class (q,k,v) Naive Bayes classification, and the results of that classification are sent to the new version of every word (except the q class which only sends info to one word, not all of them).

It's also useful to think of Attention as a filter with input signal  $(e^t)^{[d], [\ell]}$  and output signal  $(e^{t+1})^{[d], [\ell]}$ .

Fig.95.1 can be “folded” (i.e., the 3 words can be represented by a single node). When folded, Fig.95.1 becomes Fig.95.2. Note that in Fig.95.2, we have started indicating the shapes of tensors by a superscript, using the tensor notation explained in Section C.48. We will continue doing this henceforth in this chapter.

The structural equations for Fig.95.2, printed in blue, are as follows.

$$(a^t)^{[d], [\ell]} = \text{Attention}((v^t)^{[d], [\ell]}, (k^t)^{[d], [\ell]}, (q^t)^{[d], [\ell]}) \quad (95.18a)$$

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from getting too large.

<sup>3</sup>Variations of this definition of Attention have been proposed. This particular one is the original one from the “Attention is all you need paper”. Some people call it the “scaled dot product Attention”.

<sup>4</sup>Tree Augmented Naive (TAN) Bayes nets were introduced in Chapter 9.

<sup>5</sup>A **reverse or upside down tree** is obtained by reversing the directions of all the arrows of a tree directed graph. A TAN Bayes net is normally defined as in Chapter 9, as a Naive Bayes net augmented with a tree. In an Attention bnet, the Naive Bayes Net is augmented with a reverse tree (RT) instead of a tree (T), so technically Attention bnets contain RTAN Bayes nets, not TAN Bayes nets.

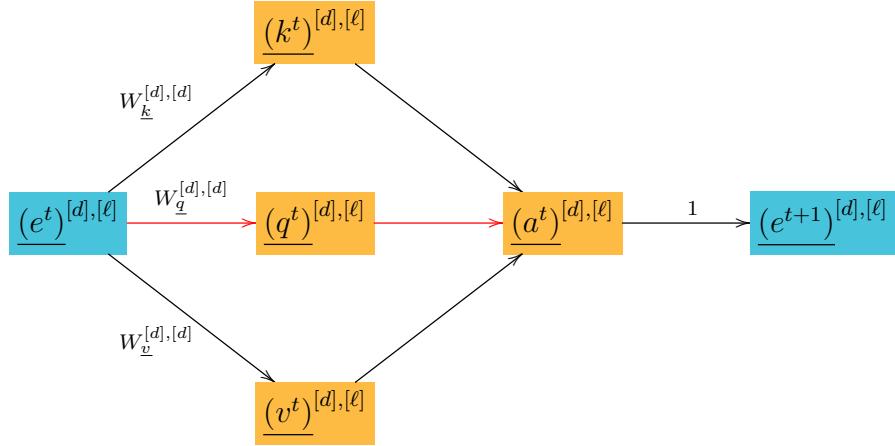


Figure 95.2: Folded version of Fig.95.1 when  $\ell = 3$ . Note that all orange nodes have the same tensor shape.

$$(e^t)^{[d],[\ell]} = \text{prior} \quad (95.18b)$$

$$(e^{t+1})^{[d],[\ell]} = (a^t)^{[d],[\ell]} \quad (95.18c)$$

$$(k^t)^{[d],[\ell]} = W_{\underline{k}}^{[d],[d]}(e^t)^{[d],[\ell]} \quad (95.18d)$$

$$(q^t)^{[d],[\ell]} = W_{\underline{q}}^{[d],[d]}(e^t)^{[d],[\ell]} \quad (95.18e)$$

$$(v^t)^{[d],[\ell]} = W_{\underline{v}}^{[d],[d]}(e^t)^{[d],[\ell]} \quad (95.18f)$$

### 95.2.2 Multi-Head Attention

In this section, we will generalize the single head Attention, as defined in the previous section, to multi-head Attention.

Let

$n_h$  = number of heads.  $\nu \in [n_h]$ .

$d$  = same as before, the hidden, embedding dimension.  $\delta \in [d]$

$D = n_h d$ .  $\Delta \in [D]$ . We will do some tensor reshaping:  $T^{[n_h], [d]} \rightarrow T^{[D]}$ , or, in component form,  $T^{\nu, \delta} \rightarrow T^\Delta$ .

Consider weight matrices  $W_{\underline{k}}^{[D], [d]}$ ,  $W_{\underline{q}}^{[D], [d]}$ , and  $W_{\underline{v}}^{[D], [d]}$  such that

$$(k^t)^{\nu, \delta, \alpha} = \sum_{\delta' \in [d]} W_{\underline{k}}^{\nu, \delta, \delta'} (e^t)^{\delta', \alpha} \quad (95.19)$$

$$(q^t)^{\nu, \delta, \alpha} = \sum_{\delta' \in [d]} W_{\underline{q}}^{\nu, \delta, \delta'} (e^t)^{\delta', \alpha} \quad (95.20)$$

$$(v^t)^{\nu, \delta, \alpha} = \sum_{\delta' \in [d]} W_{\underline{v}}^{\nu, \delta, \delta'} (e^t)^{\delta', \alpha} \quad (95.21)$$

We define the **Multi-head Attention** by

$$\boxed{\text{Attention}^{\nu, \delta, \alpha} ((v^t)^{[D], [\ell]}, (k^t)^{[D], [\ell]}, (q^t)^{[D], [\ell]}) = \sum_{\alpha' \in [\ell]} (v^t)^{\nu, \delta, \alpha'} P(\alpha' | \alpha, \nu)} \quad (95.22)$$

where

$$P(\alpha' | \alpha, \nu) = \text{softmax} \left[ \frac{1}{\sqrt{d}} \sum_{\delta \in [d]} (k^t)^{\nu, \delta, [\ell]} (q^t)^{\nu, \delta, \alpha} \right] (\alpha' | \alpha, \nu) \quad (95.23)$$

$$= \frac{\exp \left[ \frac{1}{\sqrt{d}} \sum_{\delta \in [d]} (k^t)^{\nu, \delta, \alpha'} (q^t)^{\nu, \delta, \alpha} \right]}{\sum_{\alpha'' \in [\ell]} \exp \left[ \frac{1}{\sqrt{d}} \sum_{\delta \in [d]} (k^t)^{\nu, \delta, \alpha''} (q^t)^{\nu, \delta, \alpha} \right]} \quad (95.24)$$

The structural equations, printed in blue, for the bnet Fig.95.3, are as follows. Note that  $\text{Attention}()$  always has the same tensor shape as its 3 arguments. Note also that the 3 weight matrices  $W_{\underline{k}}^{[D], [d]}$ ,  $W_{\underline{q}}^{[D], [d]}$ , and  $W_{\underline{v}}^{[D], [d]}$  raise the hidden dimension, whereas the weight matrix  $W_{\underline{a}}^{[d], [D]}$  lowers it.  $W_{\underline{a}}^{[d], [D]} = 1$  in the single head case.

$$(a^t)^{[D], [\ell]} = \text{Attention}((v^t)^{[D], [\ell]}, (k^t)^{[D], [\ell]}, (q^t)^{[D], [\ell]}) \quad (95.25a)$$

$$(e^t)^{[d], [\ell]} = \text{prior} \quad (95.25b)$$

$$(e^{t+1})^{[d], [\ell]} = W_{\underline{a}}^{[d], [D]} (a^t)^{[D], [\ell]} \quad (95.25c)$$

$$(k^t)^{[D], [\ell]} = W_{\underline{k}}^{[D], [d]} (e^t)^{[d], [\ell]} \quad (95.25d)$$

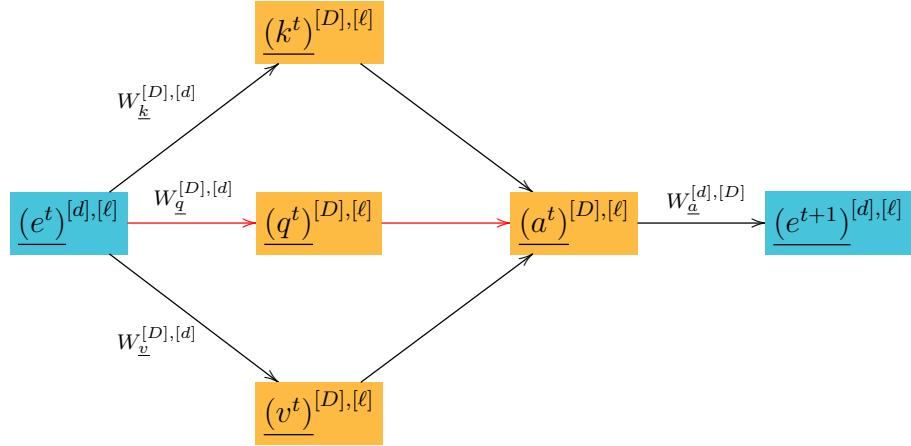


Figure 95.3: Dynamical bnet with single-head Attention for  $\ell$  words. Time-slice  $t$ . This is a generalization of the single head Attention of Fig.95.2. Note that all orange nodes have the same tensor shape.

$$(q^t)^{[D], [\ell]} = W_q^{[D], [d]}(e^t)^{[d], [\ell]} \quad (95.25e)$$

$$(v^t)^{[D], [\ell]} = W_v^{[D], [d]}(e^t)^{[d], [\ell]} \quad (95.25f)$$

### 95.3 Vanilla tranet

In this section, we will discuss the tranet of the “Attention is all you need” paper, Ref.[81]. As is common in the literature, we will refer to that tranet as the “Vanilla” tranet. Ref.[81] describes its tranet graphically with Fig.95.4. Our goal is to find a causal DAG (bnet) version of that figure.

Let

$\ell$  = maximum number of words in a sentence segment.  $\alpha \in [\ell]$ ,  $\ell \sim 100$

$L$  = number of words in vocabulary,  $\beta \in [L]$ ,  $L > \ell$

$d = d_q = d_k = d_v = 64$ , hidden dimension per head,  $\delta \in [d]$ .

$n_h = 8$ , number of heads,  $\nu \in [n_h]$

$D = n_h d = 8(64) = 512$ , hidden dimension for all heads,  $\Delta \in [D]$

$\Lambda = 6$ , number copies, connected in series, of boxed bnet,  $\lambda \in [\Lambda]$

Before we present the bnet version of Fig.95.4, we discuss some of the definitions needed to understand and motivate Fig.95.4.

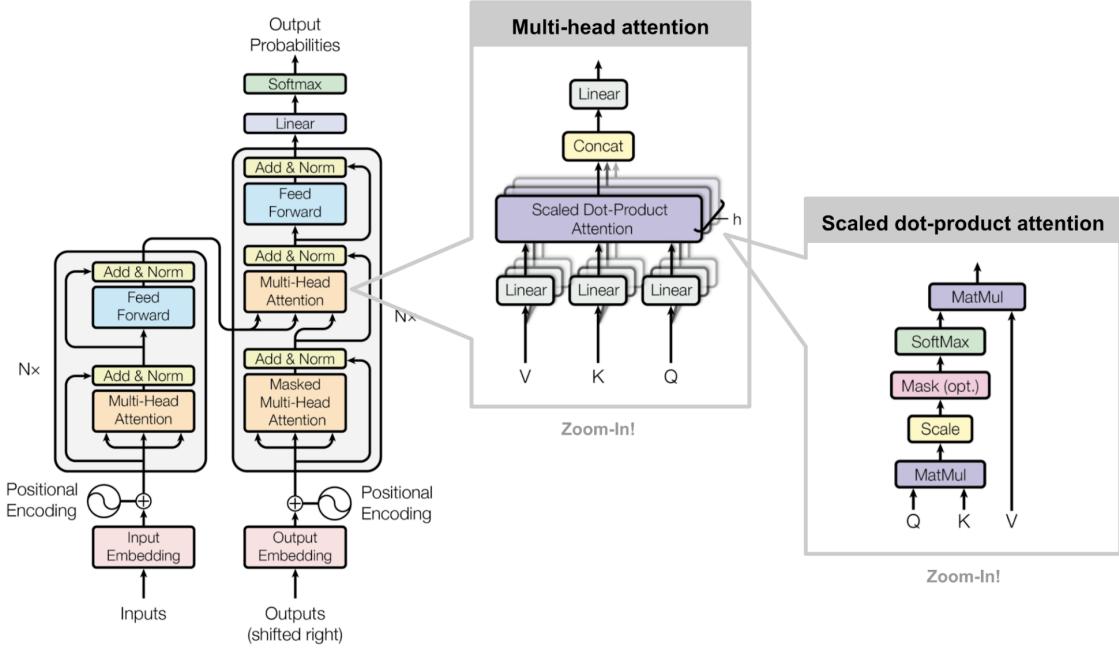


Figure 95.4: Vanilla tranet

- **Encoder Input**  $x^{\beta,\alpha}$

$$x^{\beta,\alpha} = \delta(\beta, \beta(\alpha)) \left( x^{[L],[\ell]} \text{ has one hot columns.} \right) \quad (95.26)$$

- **Embedding (a.k.a. encoding) Matrix**  $\mathcal{E}^{\delta,\beta}$

$$e^{\delta,\alpha} = \sum_{\beta} \mathcal{E}^{\delta,\beta} x^{\beta,\alpha} \quad (e^{[d],[\ell]} = \mathcal{E}^{[d],[L]} x^{[L],[\ell]}) \quad (95.27)$$

- **Weight matrices**  $W_q, W_k, W_v$

$$Q^{\nu,\delta,\alpha} = \sum_{\delta'} W_{\underline{q}}^{\nu,\delta,\delta'} e^{\delta',\alpha} \quad (Q^{[D],[\ell]} = W_{\underline{q}}^{[D],[d]} e^{[d],[\ell]}) \quad (95.28)$$

$$K^{\nu,\delta,\alpha} = \sum_{\delta'} W_{\underline{k}}^{\nu,\delta,\delta'} e^{\delta',\alpha} \quad (K^{[D],[\ell]} = W_{\underline{k}}^{[D],[d]} e^{[d],[\ell]}) \quad (95.29)$$

$$V^{\nu,\delta,\alpha} = \sum_{\delta'} W_{\underline{v}}^{\nu,\delta,\delta'} e^{\delta',\alpha} \quad (V^{[D],[\ell]} = W_{\underline{v}}^{[D],[d]} e^{[d],[\ell]}) \quad (95.30)$$

- **Multi-head Attention**

$$B^{\nu, \alpha', \alpha} = \frac{1}{\sqrt{d}} \sum_{\delta} K^{\nu, \delta, \alpha'} Q^{\nu, \delta, \alpha} \quad \left( B^{[n_h], [\ell], [\ell]} = \left[ \frac{1}{\sqrt{d}} (K^{\nu, [d], [\ell]})^T Q^{\nu, [d], [\ell]} \right]_{\nu \in [n_h]} \right) \quad (95.31)$$

$$A^{\nu, \delta, \alpha} = \sum_{\alpha'} V^{\nu, \delta, \alpha'} \underbrace{\text{softmax}(B^{\nu, [\ell], \alpha})(\alpha' | \alpha, \nu)}_{P(\alpha' | \alpha, \nu)} \quad (95.32)$$

$$\sum_{\alpha' \in [\ell]} P(\alpha' | \alpha, \nu) = 1 \quad (95.33)$$

$$A^{\nu, \delta, \alpha} \rightarrow A^{\Delta, \alpha} (A^{[n_h], [d], [\ell]} \rightarrow A^{[D], [\ell]}) \quad (95.34)$$

Column vector notation:

$$B^{\nu, \alpha', \alpha} = \frac{1}{\sqrt{d}} (K^{\nu, [d], \alpha'})^T Q^{\nu, [d], \alpha} \quad (95.35)$$

Important: Note that the softmax() makes the  $\alpha'$  component a probability, not the  $\alpha$  one!

For example, suppose  $\nu = 1$  (one head),  $\ell = 2$  (a 2 word segment), and  $d = 3$  (hidden dimension is 3). The  $Q^{[3], [2]}, K^{[3], [2]}, V^{[3], [2]}$  are  $3 \times 2$  matrices (i.e., two 3-dim column vectors). One uses the  $Q^{[3], [2]}$  and  $K^{[3], [2]}$  to arrive at a  $2 \times 2$  matrix  $P(\alpha' | \alpha)$  of probabilities. Then one uses that matrix of probabilities to replace

$$[V^{[3], 0}, V^{[3], 1}] \rightarrow [V^{[3], 0} P(0|0) + V^{[3], 1} P(1|0), V^{[3], 0} P(0|1) + V^{[3], 1} P(1|1)] \quad (95.36)$$

- **Positional Embedding Matrix  $\mathcal{E}_{pos}^{\delta, \beta}$**

$$\mathcal{E}_{pos}^{\delta, \beta} = \begin{cases} \sin\left(2\pi \frac{\beta}{(2\pi)10^{4\delta/d}}\right) = \sin(2\pi \frac{\beta}{\lambda(\delta)}) & \text{if } \delta \text{ is even} \\ \cos\left(2\pi \frac{\beta}{(2\pi)10^{4(\delta-1)/d}}\right) = \cos(2\pi \frac{\beta}{\lambda(\delta)}) & \text{if } \delta \text{ is odd} \end{cases} \quad (95.37)$$

$\mathcal{E}_{pos}^{\delta, \beta}$  changes in phase by  $\pi/2$  every time  $\delta$  changes by 1. Its wavelength  $\lambda$  is independent of  $\beta$ , but increases rapidly with  $\delta$ , from  $\lambda(\delta = 0) = 2\pi * 1$  to  $\lambda(\delta = d) = 2\pi * 10^4$ .

Total Embedding equals initial embedding plus positional embedding:

$$\mathcal{E}^{\delta,\beta} = \mathcal{E}_0^{\delta,\beta} + \mathcal{E}_{pos}^{\delta,\beta} \quad (95.38)$$

The purpose of positional embedding is to take  $e^{\beta,\alpha}$  to  $e^{\delta,\alpha} = \sum_{\beta} \mathcal{E}_{pos}^{\delta,\beta} e^{\beta,\alpha}$  where  $e^{\delta,\alpha}$  changes quickly as  $\delta$  (i.e., position) changes.

- **ReLU**

For a tensor  $T$  of arbitrary shape,

$$ReLU(T) = (T)_+ = \max(0, T) \quad (95.39)$$

max element-wise.

- **Feed Forward Neural Net**

$$F(e^{\delta,\alpha}) = \sum_{\Delta \in [n_{ff}]} W_2^{\delta,\Delta} ReLU \left( \sum_{\delta' \in [d]} W_1^{\Delta,\delta'} e^{\delta',\alpha} + b_1^{\Delta,\alpha} \right) + b_2^{\delta,\alpha} \quad (95.40)$$

$n_{ff}$  is called the `intermediate_size` in BERT.

- **Softmax**

`softmax()` takes a vector and returns a vector of probabilities of the same length

$$e^{[n]} \rightarrow P^{[n]} \quad (95.41)$$

where

$$P^{\alpha} = \frac{\exp(e^{\alpha})}{\sum_{\alpha \in [n]} \exp(e^{\alpha})} \quad \left( P^{[n]} = \frac{\exp(e^{[n]})}{\| \exp(e^{[n]}) \|_0} \right) \quad (95.42)$$

For example,

$$(1, 0, 0) \rightarrow (e, 1, 1)/norm \quad (95.43)$$

$$(10, 0, 0) \rightarrow (e^{10}, 1, 1)/norm \approx (1, 0, 0) \quad (95.44)$$

For any  $a \in \mathbb{R}$ ,

$$(a, a, a) \rightarrow \frac{1}{3}(1, 1, 1) \quad (95.45)$$

- **Skip Connection (Add & Normalize)**

A **skip connection** is when you split the input to a **filter** into two streams, one stream goes through the filter, the other doesn't. The one that doesn't is then merged with the output of the filter via a **add & normalize** node. The reason

for making skip connections is that the signal exiting a filter is usually full of jumps and kinks. By merging that filter output with some of the filter input, one smooths out the filter output to some degree. This makes back-propagation differentiation better behaved.

The filter might be a Multi-Head Attention or a Feed Forward NN.

Add & Normalize just means  $(A + B)/\text{norm}$  where  $A$  and  $B$  are the two input signals and “norm” is some norm of  $A + B$  (for instance,  $\| A + B \|_2$ ).

Normalization keeps the signal from growing too big and saturating the signal that will enter components upstream. Normalization can also involve subtracting the mean  $\langle X \rangle$  of the signal  $X$  so as to get a signal  $X - \langle X \rangle$  that has zero mean.

- **Redundancy**

For better results, the Encoder and Decoder both contain  $\Lambda$  copies, connected in series, of the boxed bnet.

Redundancy (see Chapter 79) has been used to avoid catastrophic failure at least as early as the dawn of the age of rocketry, when it was used to avoid the all too common occurrence of exploding rockets. There are 2 basic types of redundancy: in series connection (as in more layers in a feedforward NN), and in parallel connection (as in more tranet heads).

- **Right Shifted Outputs**

“Outputs (Shifted Right)” in Fig.95.4 refers to what is called **forced teaching** in the RNN (recurrent neural net) literature. We explain forced teaching in Fig.95.5.

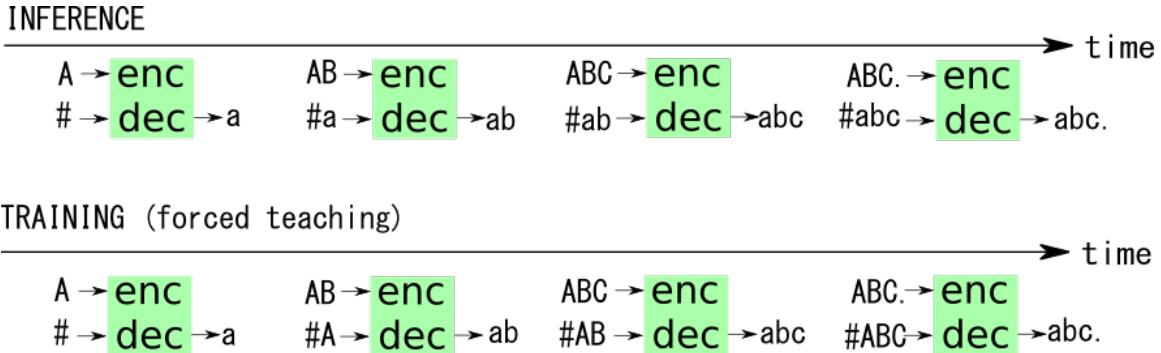


Figure 95.5: Training and Inference for vanilla transformer. “enc” and “dec” denote the encoder and decoder, respectively. A hash character represents the SOS (start of sentence) token, and a period represents the EOS (end of sentence) token. Capital letters represent ground truth tokens, and lower case ones represent predictions.

- Masked Attention

$$P(\alpha'|\alpha, \nu) = 0 \quad \text{if } \alpha' < \alpha \quad (95.46)$$

$\alpha$ , and  $\alpha'$  are sentence positions and  $\alpha'$  is in the future (downstream) compared to  $\alpha$ . So as to not violate causality, this condition enforces the constraint that no attention is paid to sentence positions in the future of  $\alpha$ .

### 95.3.1 Single Head Attention

Fig.95.6 gives a bnet representation of the “Single Head Attention” portion of Fig.95.4. The structural equations for that bnet, printed in blue, are as follows.

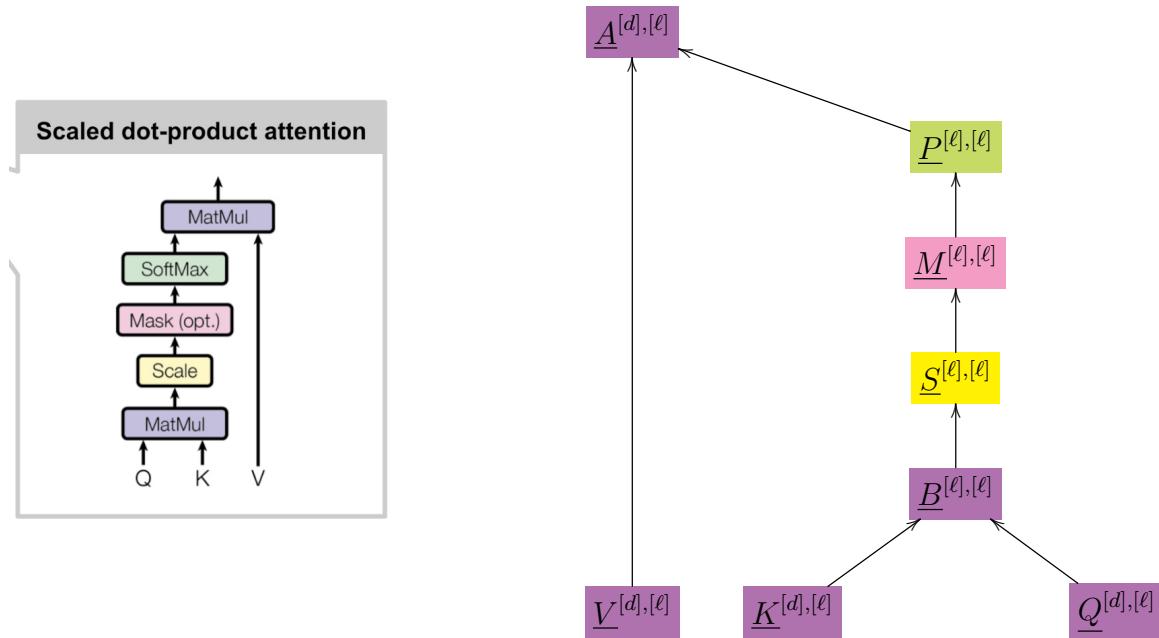


Figure 95.6: Single Head Attention. (Scaled Dot Product)

$$A^{[d],[\ell]} = V^{[d],[\ell]} P^{[\ell],[\ell]} \left( \text{Note that } \sum_{\alpha \in [\ell]} P^{\alpha,[\ell]} = 1 \right) \quad (95.47a)$$

$$B^{[\ell],[\ell]} = (K^{[d],[\ell]})^T Q^{[d],[\ell]} \quad (95.47b)$$

$$K^{[d],[\ell]} = \text{prior} \quad (95.47c)$$

$$M^{[\ell],[\ell]} = \text{mask}(S^{[\ell],[\ell]}) \quad (95.47\text{d})$$

$$P^{[\ell],[\ell]} = \text{softmax}(M^{[\ell],[\ell]}) \quad \left( \text{Note that } \sum_{\alpha \in [\ell]} P^{\alpha,[\ell]} = 1 \right) \quad (95.47\text{e})$$

$$Q^{[d],[\ell]} = \text{prior} \quad (95.47\text{f})$$

$$S^{[\ell],[\ell]} = \frac{B^{[\ell],[\ell]}}{\sqrt{d}} \quad (95.47\text{g})$$

$$V^{[d],[\ell]} = \text{prior} \quad (95.47\text{h})$$

### 95.3.2 Multi-Head Attention

Fig.95.7 gives a bnet representation of the “Multi-Head Attention” portion of Fig.95.4. The structural equations for that bnet, printed in blue, are as follows.

$$A^{[D],[\ell]} = [A_0^{[d],[\ell]} | A_1^{[d],[\ell]}] \quad (95.48\text{a})$$

$$A_0^{[d],[\ell]} = \text{Attention}(V_0^{[d],[\ell]}, K_0^{[d],[\ell]}, Q_0^{[d],[\ell]}) \quad (95.48\text{b})$$

$$A_1^{[d],[\ell]} = \text{Attention}(V_1^{[d],[\ell]}, K_1^{[d],[\ell]}, Q_1^{[d],[\ell]}) \quad (95.48\text{c})$$

$$K^{[D],[\ell]} = W_k^{[D],[d]} e^{[d],[\ell]} \quad (95.48\text{d})$$

$$K_0^{[d],[\ell]} = \text{linear}(K^{[D],[\ell]}) \quad (\text{split, then project a component}) \quad (95.48\text{e})$$

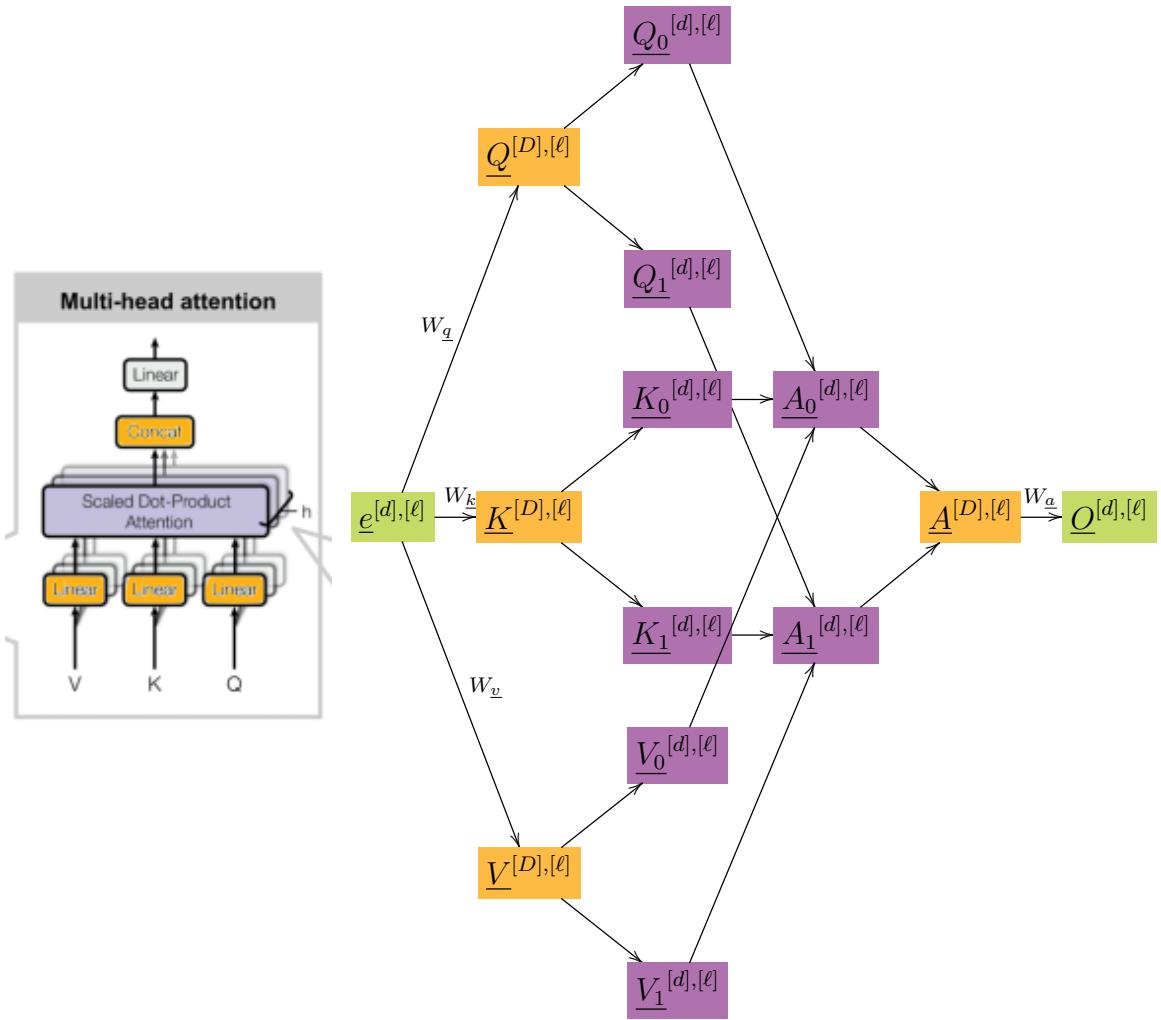


Figure 95.7: Multi-head Attention with 2 heads. Note that the orange nodes all have the same tensor shape.

$$K_1^{[d],[\ell]} = \text{linear}(K^{[D],[\ell]}) \quad (\text{split, then project a component}) \quad (95.48f)$$

$$O^{[d],[\ell]} = W_{\underline{a}}^{[d],[D]} A^{[D],[\ell]} \quad (95.48g)$$

$$Q^{[D],[\ell]} = W_q^{[D],[d]} e^{[d],[\ell]} \quad (95.48h)$$

$$Q_0^{[d],[\ell]} = \text{linear}(Q^{[D],[\ell]}) \text{ (split, then project a component)} \quad (95.48i)$$

$$Q_1^{[d],[\ell]} = \text{linear}(Q^{[D],[\ell]}) \text{ (split, then project a component)} \quad (95.48j)$$

$$V^{[D],[\ell]} = W_{\underline{v}}^{[D],[d]} e^{[d],[\ell]} \quad (95.48k)$$

$$V_0^{[d],[\ell]} = \text{linear}(V^{[D],[\ell]}) \text{ (split, then project a component)} \quad (95.48l)$$

$$V_1^{[d],[\ell]} = \text{linear}(V^{[D],[\ell]}) \text{ (split, then project a component)} \quad (95.48m)$$

$$e^{[d],[\ell]} = \text{prior} \quad (95.48n)$$

### 95.3.3 Encoder

Fig.95.8 gives a bnet representation of the “Encoder” portion of Fig.95.4. The structural equations for that bnet, printed in blue, are as follows.

$$A^{[D],[\ell]} = \text{Attention}(Q^{[D],[\ell]}, K^{[D],[\ell]}, V^{[D],[\ell]}) \quad (95.49a)$$

$$e^{[d],[\ell]} = \mathcal{E}^{[d],[L]} x^{[L],[\ell]} \quad (95.49b)$$

$$F^{[d],[\ell]} = \text{feed\_forward\_nn}(N^{[d],[\ell]}) \quad (95.49c)$$

$$K^{[D],[\ell]} = W_{\underline{k}}^{[D],[d]} e^{[d],[\ell]} \quad (95.49d)$$

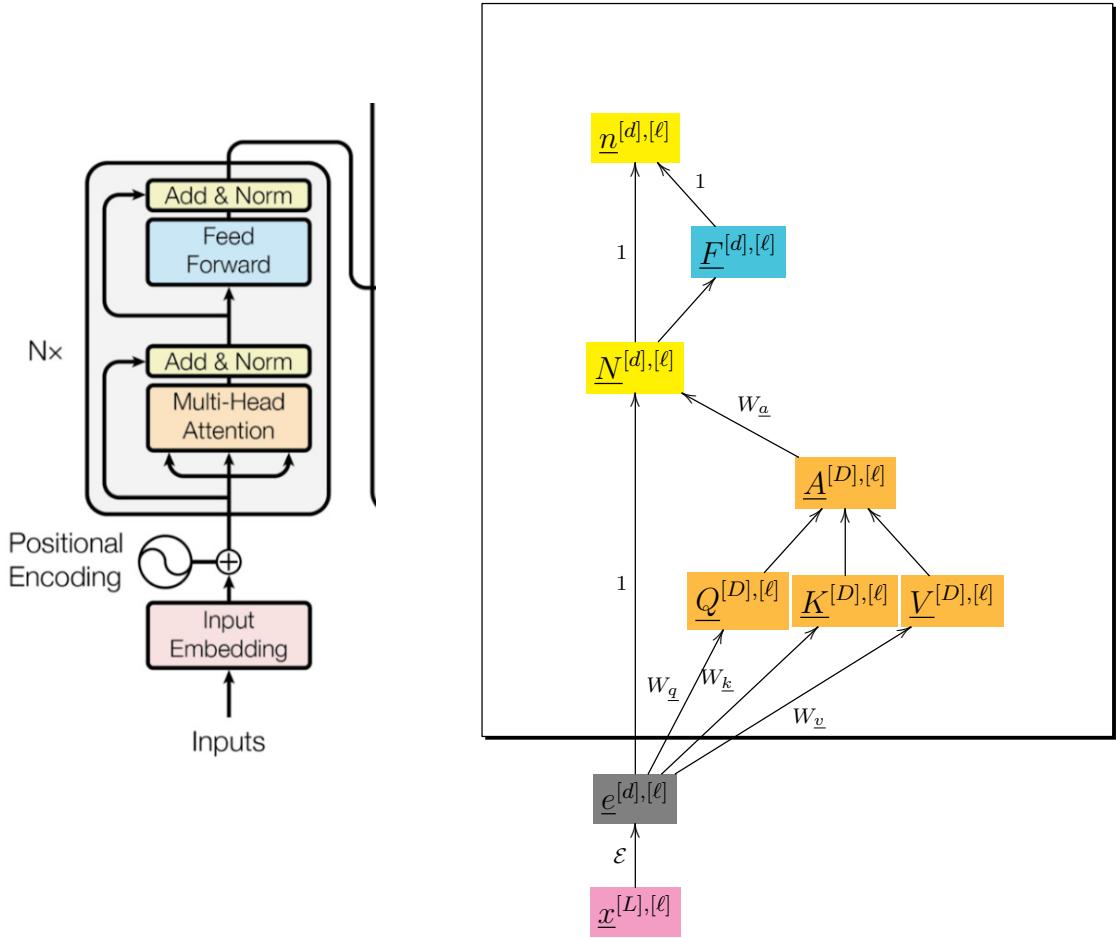


Figure 95.8: Encoder of Vanilla Transformer Net.  $\Lambda$  copies of the boxed part are connected in series.

$$n^{[d],[\ell]} = \text{normalize}(N^{[d],[\ell]} + F^{[d],[\ell]}) \quad (95.49e)$$

$$N^{[d],[\ell]} = \text{normalize}(e^{[d],[\ell]} + W_{\underline{a}}^{[d],[D]} A^{[D],[\ell]}) \quad (95.49f)$$

$$Q^{[D],[\ell]} = W_q^{[D],[d]} e^{[d],[\ell]} \quad (95.49g)$$

$$V^{[D],[\ell]} = W_{\underline{v}}^{[D],[d]} e^{[d],[\ell]} \quad (95.49h)$$

$$x^{[L],[\ell]} = \text{ prior} \quad (95.49i)$$

### 95.3.4 Decoder

Fig.95.9 gives a bnet representation of the “Decoder” portion of Fig.95.4. The structural equations for that bnet, printed in blue, are as follows.

$$a^{[D],[\ell]} = \text{Attention}(v^{[D],[\ell]}, k^{[D],[\ell]}, q^{[D],[\ell]}) \quad (95.50a)$$

$$A^{[D],[\ell]} = \text{Attention}(Q^{[D],[\ell]}, K^{[D],[\ell]}, V^{[D],[\ell]}) \quad (95.50b)$$

$$e^{[d],[\ell]} = \mathcal{E}^{[d],[L]} x^{[L],[\ell]} \quad (95.50c)$$

$$F^{[d],[\ell]} = \text{feed\_forward\_nn}(j^{[d],[\ell]}) \quad (95.50d)$$

$$I^{[L],[\ell]} = W_{fin}^{[L],[d]} Y^{[d],[\ell]} \quad (95.50e)$$

$$j^{[d],[\ell]} = \text{normalize}(U_{\underline{a}}^{[d],[D]} a^{[D],[\ell]} + J^{[d],[\ell]}) \quad (95.50f)$$

$$J^{[d],[\ell]} = \text{normalize}(W_{\underline{a}}^{[d],[D]} A^{[D],[\ell]} + e^{[d],[\ell]}) \quad (95.50g)$$

$$K^{[D],[\ell]} = W_k^{[D],[d]} e^{[d],[\ell]} \quad (95.50h)$$

$$k^{[D],[\ell]} = U_{\underline{k}}^{[D],[d]} n^{[d],[\ell]} \quad (95.50i)$$

$$n^{[d],[\ell]} = \text{ Prior coming from Encoder.} \quad (95.50j)$$

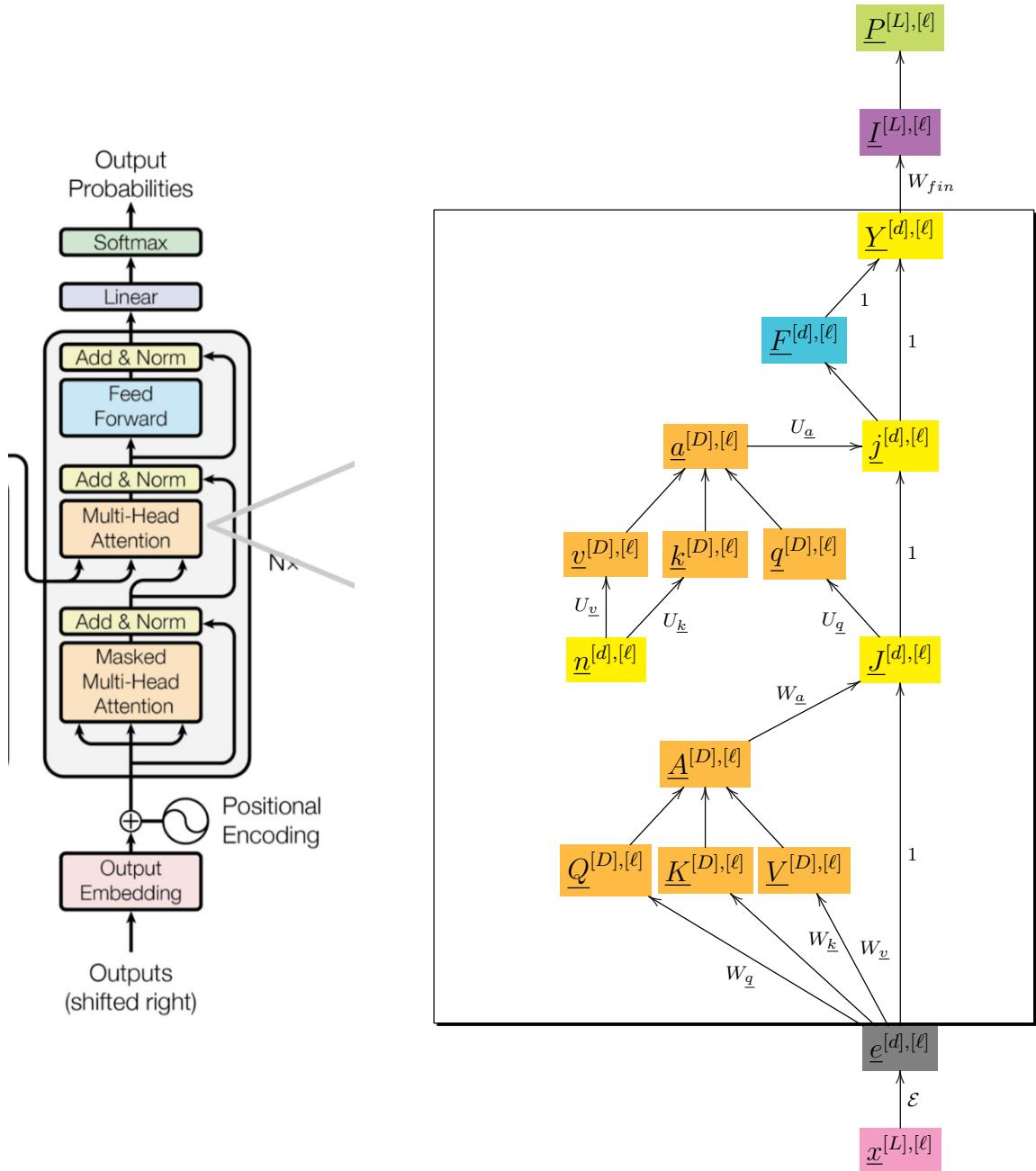


Figure 95.9: Decoder of Vanilla Transformer Net.  $\Lambda$  copies of the boxed part are connected in series.

$$P^{[L],[\ell]} = \text{softmax}(I^{[L],[\ell]}) \quad (\sum_{\alpha \in [\ell]} P^{[L],\alpha} = 1) \quad (95.50k)$$

$$q^{[D],[\ell]} = U_{\underline{q}}^{[D],[d]} J^{[d],[\ell]} \quad (95.50l)$$

$$Q^{[D],[\ell]} = W_{\underline{q}}^{[D],[d]} e^{[d],[\ell]} \quad (95.50m)$$

$$V^{[D],[\ell]} = W_v^{[D],[d]} e^{[d],[\ell]} \quad (95.50n)$$

$$v^{[D],[\ell]} = U_{\underline{v}}^{[D],[d]} n^{[d],[\ell]} \quad (95.50o)$$

$$x^{[L],[\ell]} = \text{ prior, right shifted output} \quad (95.50p)$$

$$Y^{[d],[\ell]} = \text{normalize}(F^{[d],[\ell]} + J^{[d],[\ell]}) \quad (95.50q)$$

## 95.4 BERT

BERT is a realization of the Encoder part of the Vanilla tranet.

	BERT base	BERT large
$\ell$	512?	512?
$L$ , vocab_size	30,522	30,522
$d$ , hidden_size	768	1024
$n_h$ , num_attention_heads	12	16
$\Lambda$ , num_hidden_layers	12	24
$D'$ , intermediate_size	3,072	3,072
number of parameters	110M	340M

Table 95.1: Some hyperparameters for BERT base and BERT large

# Chapter 96

## Transportability of Causal Knowledge

This chapter is mostly based on Refs.[54] and [41].

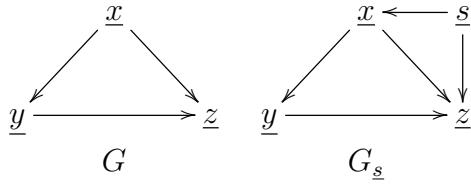


Figure 96.1: Example of selection bnet  $G_{\underline{s}}$  created from bnet  $G$ .

Suppose one wants to transfer causal knowledge from a **source population**  $\Sigma$  to a **target population**  $\Sigma^*$ .

Given a bnet  $G$ , define a **selection diagram**  $G_{\underline{s}}$  as a bnet formed by adding to  $G$  a new root node  $\underline{s}$  and new arrows pointing from **switch node** (a.k.a, **selection node**)  $\underline{s}$  to one or more **target nodes** of  $G$ . We'll call the set of target nodes of  $\underline{s}$  the **target set**  $T_{\underline{s}}$ .  $\underline{s} = 0$  corresponds to population  $\Sigma$  and  $\underline{s} = 1$  to population  $\Sigma^*$ . For bnet  $G$ , the TPM for a node  $\underline{x}$  with parents  $pa(\underline{x})$ , is given by:

$$P_G(\underline{x}|pa(\underline{x})) = P(\underline{x}|pa(\underline{x})) \quad (96.1)$$

For bnet  $G_{\underline{s}}$ , nodes  $\underline{x}$  with parents  $pa(\underline{x})$ , where  $\underline{s} \notin pa(\underline{x})$ , have TPMs:

$$P_{G_{\underline{s}}}(\underline{x}|pa(\underline{x})) = P(\underline{x}|pa(\underline{x})) . \quad (96.2)$$

Nodes  $\underline{x}$  with parents  $pa(\underline{x}) \cup \underline{s}$ , have TPMs:

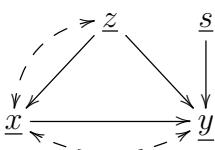
$$P_{G_{\underline{s}}}(\underline{x}|pa(\underline{x}), \underline{s}) = \begin{cases} P(\underline{x}|pa(\underline{x}), \underline{s} = 0) = P(\underline{x}|pa(\underline{x})) & \text{if } \underline{s} = 0 \\ P(\underline{x}|pa(\underline{x}), \underline{s} = 1) = P^*(\underline{x}|pa(\underline{x})) & \text{if } \underline{s} = 1 \end{cases} \quad (96.3)$$

Fig.96.1 shows an example of a selection diagram  $G_{\underline{s}}$ . In that figure, the target set of  $\underline{s}$  is  $\{\underline{x}, \underline{z}\}$ .

All this can be generalized so as to have more than one switch node, with the target sets of the switch nodes being disjoint, and such that a switch node can have more than 2 states.

### Do-transport formulae

**Claim 145** (*Trivial Memoryless Transportability, from Ref.[54]*)

If  where  $\underline{s} \in \{0, 1\}$  is a switch node, then

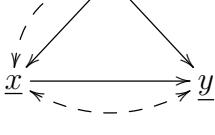
$$P^*(y|\mathcal{D}\underline{x} = x, z) = P^*(y|x, z) \quad (\text{replace } \mathcal{D} \text{ by } 1, \text{ keep } P^*) \quad (96.4)$$

$$\begin{array}{ccc} z & \xrightarrow{\underline{s}=1} & y \\ \mathcal{D}\underline{x} = x \longrightarrow & = & x \longrightarrow y \end{array} \quad (96.5)$$

**proof:** See Claim 49.

**QED**

**Claim 146** (*Direct Transportability, a.k.a. External Validity, from Ref.[54]*)

If  where  $\underline{s} \in \{0, 1\}$  is a switch node, then

$$P^*(y|\mathcal{D}\underline{x} = x, z) = P(y|\mathcal{D}\underline{x} = x, z) \quad (\text{replace } P^* \text{ by } P, \text{ keep } \mathcal{D}) \quad (96.6)$$

$$\begin{array}{ccc} \underline{s}=1 \longrightarrow z & & z \\ \mathcal{D}\underline{x} = x \longrightarrow y & = & \mathcal{D}\underline{x} = x \longrightarrow y \end{array} \quad (96.7)$$

Furthermore,

$$P^*(y|\mathcal{D}\underline{x} = x) = \sum_z P(y|\mathcal{D}\underline{x} = x, z)P^*(z) \quad (96.8)$$

$$\begin{array}{ccc} \underline{s}=1 & & \underline{s}=1 \longrightarrow \sum z \\ \mathcal{D}\underline{x} = x \longrightarrow y & = & \mathcal{D}\underline{x} = x \longrightarrow y \end{array} \quad (96.9)$$

**proof:** See Claim 50.

**QED**

**Claim 147** (*S-Admissible Transportability, from Ref.[54]*)

If  $\underline{s} \xrightarrow{\text{---}} \underline{z} \xrightarrow{\text{---}} \underline{a}$  where  $\underline{s} \in \{0, 1\}$  is a switch node, then

$$P^*(y|\mathcal{D}\underline{x} = x) = \sum_a P(y|\mathcal{D}\underline{x} = x, a)P^*(a) \quad (96.10)$$

$$\begin{array}{ccc} \underline{s} = 1 & & \underline{s} = 1 \longrightarrow \sum a \\ \searrow & & \downarrow \\ \mathcal{D}\underline{x} = x \longrightarrow y & = & \mathcal{D}\underline{x} = x \longrightarrow y \end{array} \quad (96.11)$$

**proof:** See Claim 51.

**QED**

**Claim 148** (*Non-transportability, from Ref.[54]*)

If  $\underline{s} \xrightarrow{\text{---}} \underline{h} \xrightarrow{\text{---}} \underline{z}$  where  $\underline{s} \in \{0, 1\}$  is a switch node, then

$$P^*(y|\mathcal{D}\underline{x} = x) = P^*(y|\mathcal{D}\underline{x} = x) \quad (96.12)$$

$$\begin{array}{ccc} \underline{s} = 1 & & \\ \downarrow & & \\ \mathcal{D}\underline{x} = x \longrightarrow y & = & \text{same} \end{array} \quad (96.13)$$

**proof:** See Claim 52.

**QED**

**Claim 149** (*from Ref.[54]*)

If  $\underline{s} \xrightarrow{\text{---}} \underline{h} \xrightarrow{\text{---}} \underline{z}$  where  $\underline{s} \in \{0, 1\}$  is a switch node, then

$$P^*(y|\mathcal{D}\underline{x} = x) = P(y|\mathcal{D}\underline{x} = x) \quad (96.14)$$

$$\begin{array}{ccc} \underline{s} = 1 & & (96.15) \\ & \searrow & \\ \mathcal{D}\underline{x} = x & \longrightarrow & y = \mathcal{D}\underline{x} = x \longrightarrow y \end{array}$$

**proof:** See Claim 53.

**QED**

**Claim 150** (*from Ref.[54]*)

If  $\underline{s}$  is a switch node, then

$$P^*(y|\mathcal{D}\underline{x} = x) = \sum_z P(y|\mathcal{D}\underline{x} = x, z)P^*(z|x) \quad (96.16)$$

$$\begin{array}{ccccc} \underline{s} = 1 & \mathcal{D}\underline{x} = x & \underline{s} = 1 & \mathcal{D}\underline{x} = x & (96.17) \\ \searrow & \downarrow & \searrow & \downarrow & \\ y & = & x \longrightarrow \sum z \longrightarrow y & & \end{array}$$

**proof:** See Claim 54.

**QED**

# Chapter 97

## Turbo Codes

This chapter is based on Ref.[39].

In this chapter, vectors with  $n$  components will be indicated by an  $n$  superscript. For example,  $a^n = (a_0, a_1, \dots, a_{n-1})$ .

Consider an  $n$ -letter message  $u^n = (u_0, u_1, \dots, u_{n-1})$ , where for all  $i$ ,  $u_i \in \mathcal{A}$  is an element of an alphabet  $\mathcal{A}$ , and where for all  $i$ , the  $u_i$  are i.i.d.. Suppose  $u^n$  is encoded deterministically in two different ways,  $e_1(u^n)$  and  $e_2(u^n)$ . After passing through the same memoryless channel, the variables  $u^n, e_1, e_2$  become  $\tilde{u}^n, \tilde{e}_1, \tilde{e}_2$ , respectively. The letter  $u$  stands for unencoded, and  $e$  for encoded. Quantities with a tilde  $\tilde{u}^n, \tilde{e}_1, \tilde{e}_2$  occur after channel passage and are visible (measurable). Quantities without a tilde  $u^n, e_1, e_2$  are hidden (unmeasurable).

The situation just described can be represented by the bnet Fig.97.1, or by its abridged version Fig.97.2. But note that the abridged version does not show explicitly that the  $u_i$  are i.i.d. or that the channel is memoryless (i.e., that the  $u_i$  for all  $i$  pass independently through the channel).

Define

$$x = (u^n, e_1, e_2) \quad (97.1)$$

and

$$\tilde{x} = (\tilde{u}^n, \tilde{e}_1, \tilde{e}_2) . \quad (97.2)$$

Fig.97.1 implies that

$$P(x, \tilde{x}) = P(\tilde{u}^n | u^n) \left[ \prod_{r=1,2} P(\tilde{e}_r | e_r) P(e_r | u^n) \right] P(u^n) . \quad (97.3)$$

Because the  $u^n$  are i.i.d.,

$$P(u^n) = \prod_i P(u_i) . \quad (97.4)$$

Because the channel is memoryless,

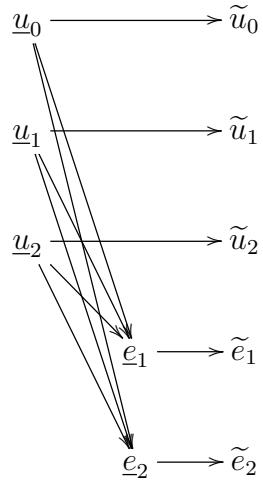


Figure 97.1: Turbo coding Bnet representing a message being encoded two different ways and then the original message and the 2 encodings pass through a memoryless channel.

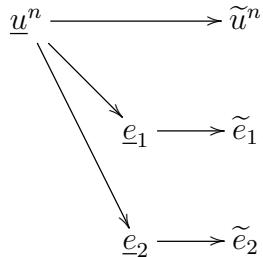


Figure 97.2: Abridged version of Fig.97.1.

$$P(\tilde{u}^n | u^n) = \prod_i P(\tilde{u}_i | u_i) . \quad (97.5)$$

Because the encoding is deterministic, we must have for  $r = 1, 2$

$$P(e_r | u^n) = \delta(e_r, e_r(u^n)) . \quad (97.6)$$

Define the belief functions

$$BEL_i = BEL_i(\underline{u}_i = a) = P(\underline{u}_i = a | \tilde{x}) . \quad (97.7)$$

The best estimate of  $u_j$  given all visible evidence  $\tilde{x}$  is

$$\hat{u}_i = \operatorname{argmax}_{u_i} BEL_i(u_i) . \quad (97.8)$$

Define the probability functions

$$\pi_i = \pi_i(u_i) = P(u_i) , \quad (97.9)$$

and the likelihood functions

$$\lambda_i = \lambda_i(u_i) = P(\tilde{u}_i|u_i) . \quad (97.10)$$

For  $r = 1, 2$ , define the Kernel functions

$$K_r = K_r(u^n) = P(\tilde{e}_r|e_r = e_r(u^n)) . \quad (97.11)$$

In this book,  $\mathcal{N}(!a)$  denotes a normalization constant that does not depend on  $a$ . Define

$$\mathcal{N}_i = \mathcal{N}(!u_i) . \quad (97.12)$$

### Claim 151

$$BEL_i = \mathcal{N}_i \lambda_i \pi_i \mathcal{T}_i^{K_1 K_2} [\prod_{j \neq i} \lambda_j \pi_j] , \quad (97.13)$$

where  $\mathcal{T}_i^K(\cdot)$  with  $K = K_1 K_2$  is an operator (transform) that acts on functions of  $u^n$ :

$$\mathcal{T}_i^K(\cdot) = \sum_{u^n} \delta(u_i, a) K(u^n)(\cdot) . \quad (97.14)$$

**proof:**

$$\begin{aligned} P(\underline{u}_i = a | \tilde{x}) &= \\ &= \sum_x \delta(u_i, a) P(x | \tilde{x}) \end{aligned} \quad (97.15)$$

$$= \sum_x \delta(u_i, a) \frac{P(\tilde{x}|x)P(x)}{P(\tilde{x})} \quad (97.16)$$

$$= \mathcal{N}(!a) \sum_x \delta(u_i, a) P(\tilde{x}|x)P(x) \quad (97.17)$$

$$= \mathcal{N}(!a) \sum_x \delta(u_i, a) P(u^n) \left[ \prod_{r=1,2} P(\tilde{e}_r|e_r) \delta(e_r, e_r(u^n)) \right] \prod_j P(\tilde{u}_j|u_j) \quad (97.18)$$

$$= \mathcal{N}(!a) \lambda_i(a) \pi_i(a) R , \quad (97.19)$$

where

$$R = \sum_{u^n} \delta(u_i, a) \left[ \prod_{r=1,2} P(\tilde{e}_r | e_r(u^n)) \right] \prod_{j \neq i} P(\tilde{u}_j | u_j) P(u_j) \quad (97.20)$$

$$= \sum_{u^n} \delta(u_i, a) \left[ \prod_{r=1,2} K_r(u^n) \right] \prod_{j \neq i} \lambda_j(u_j) \pi_j(u_j) \quad (97.21)$$

$$= \mathcal{T}_i^{K_1 K_2} \left[ \prod_{j \neq i} \lambda_j(u_j) \pi_j(u_j) \right]. \quad (97.22)$$

Hence

$$BEL_i(a) = \mathcal{N}(!a) \lambda_i(a) \pi_i(a) \mathcal{T}_i^{K_1 K_2} \left[ \prod_{j \neq i} \lambda_j(u_j) \pi_j(u_j) \right]. \quad (97.23)$$

**QED**

## 97.1 Decoding Algorithm

The Turbo algorithm for decoding the encode message is as follows. For  $m = 0$ , let

$$\pi_j^{(0)}(u_j) = \frac{1}{n_{\underline{u}_j}}. \quad (97.24)$$

Then for  $m = 1, 2, \dots$ , let

$$\pi_i^{(m)} = \mathcal{N}_i \mathcal{T}_i^{K_m \% 2} \left[ \prod_{j \neq i} \lambda_j \pi_j^{(m-1)} \right], \quad (97.25)$$

where  $m \% 2 = 1$  if  $m$  is odd and  $m \% 2 = 2$  if  $m$  is even. Furthermore, for  $m > 0$ , let

$$BEL_i^{(m)} = \mathcal{N}_i \lambda_i \pi_i^{(m-1)} \pi_i^{(m)} \quad (97.26)$$

$$= \mathcal{N}_i \lambda_i \pi_i^{(m-1)} \mathcal{T}_i^{K_m \% 2} \left[ \prod_{j \neq i} \lambda_j \pi_j^{(m-1)} \right]. \quad (97.27)$$

As  $m \rightarrow \infty$ ,  $BEL_i^{(m)}$  given by Eq.(97.27) is expected to converge to the the exact  $BEL_i$  given by Eq.(97.13).

Turbo decoding can be represented by the bnets Figs.97.3 and 97.4.

The TPMs, printed in blue, for bnet Fig.97.3, are as follows.

$$P(d_i^{(m)} = a | \tilde{u}^n, \tilde{e}_{m \% 2}) = BEL_i^{(m)}(a). \quad (97.28)$$

The TPMs, printed in blue, for bnet Fig.97.4, are as follows.

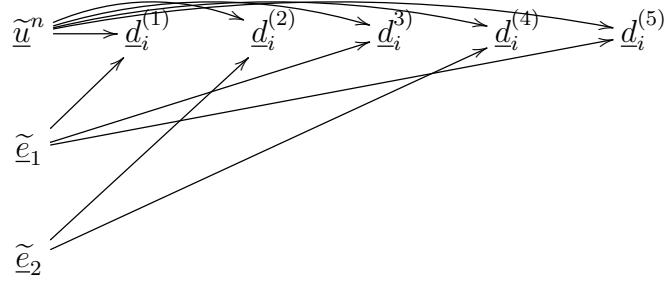


Figure 97.3: Bnet describing Turbo code generation of  $BEL_i^{(m)}(a)$  for  $m = 1, 2, \dots$

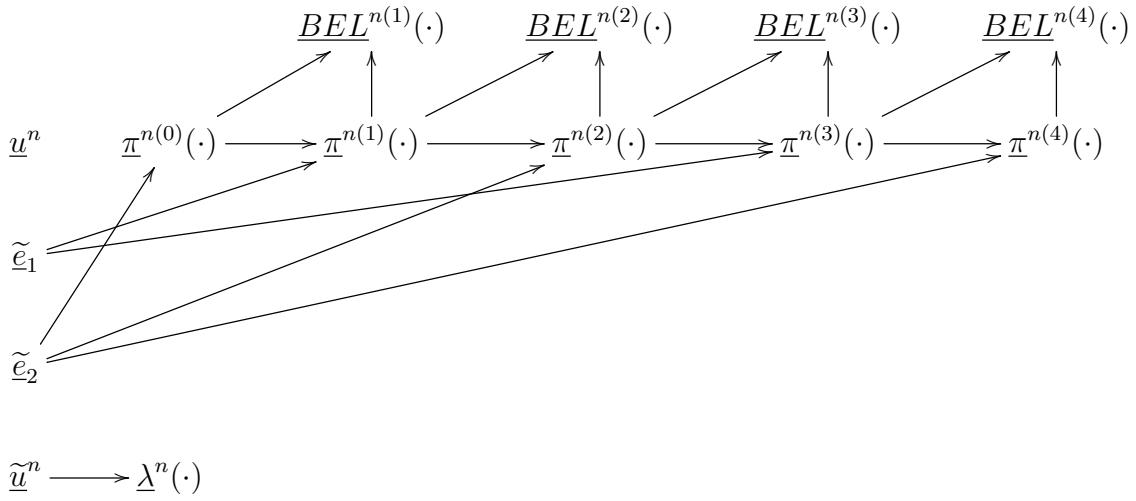


Figure 97.4: Bnet describing Turbo code generation of  $BEL^{n(m)}(\cdot)$  and  $\pi^{n(m)}(\cdot)$  for  $m = 0, 1, 2, \dots$ . The following arrows were not drawn for clarity: Arrows pointing from node  $\underline{\lambda}^n(\cdot)$  to nodes  $\underline{\pi}^{n(m)}(\cdot)$  and  $\underline{BEL}^{n(m)}(\cdot)$  for  $m = 0, 1, 2, \dots$

$$P((\lambda^n)'(\cdot) | \tilde{u}^n) = \delta((\lambda^n)'(\cdot), \lambda^n(\cdot)) \quad (97.29)$$

$$P(\pi^{n(m)}(\cdot) | \lambda^n(\cdot), \pi^{n(m-1)}(\cdot), \tilde{e}_{m \% 2}) = \prod_i \prod_{u_i} \delta(\pi_i^{(m)}(u_i), \mathcal{N}_i \mathcal{T}_i^{K_m \% 2} [\prod_{j \neq i} \lambda_j \pi_j^{(m-1)}]) \quad (97.30)$$

$$P(BEL^{n(m)}(\cdot) | \lambda^n(\cdot), \pi^{n(m)}(\cdot), \pi^{n(m-1)}(\cdot)) = \prod_i \prod_{u_i} \delta(BEL_i(u_i), \mathcal{N}_i \lambda_i \pi_i^{(m-1)} \pi_i^{(m)}) \quad (97.31)$$

## 97.2 Message Passing Interpretation of Decoding Algorithm

Ref.[39] shows that the Turbo code decoding algo can be interpreted as an application of Message Passing. We leave all talk of Message Passing to a separate chapter, Chapter 56.

# Chapter 98

## Uplift Modelling

This chapter is based on many references, including Ref.[19, 15, 162, 60].

Uphill Modelling (UP) deals with the application of Rubin’s Theory of Potential Outcomes (PO) to advertisement and marketing.

PO, which is discussed in Chapter 72, is a subset of Pearl’s Causal Inference. Besides UP, other applications of PO theory that are discussed in this book are: Regression Discontinuity (Chapter 76), Difference-in-Differences (Chapter 18) and Synthetic Controls (Chapter 91).

In UP, each **participant person** is interrogated at two well anticipated, fairly closely spaced times  $t_0$  and  $t_1$  (as opposed to Difference-in-Differences (DID), where  $t_0$  and  $t_1$  might be years apart, and long before the DID analysis is attempted.). In between those two times, a treatment which we will refer to as the **UP diagnostic test** is applied. For example, at times  $t_0$  and  $t_1$ , every participant might be asked how important he/she rates climate change on a scale of 1 to 10. In between times  $t_0$  and  $t_1$ , every participant might be sent a brochure on climate change. In UP, as in all other PO applications, each **sample**  $\sigma$  is in the treated or control groups, but not both. But in UP, the same participant can be in both the treated and control groups. If so, that participant is considered two different samples  $\sigma$ ; for example,  $\sigma = \text{treatedBob}, \text{controlBob}$ . In UP, the samples are aware of which of those groups they are in, so they are not “treatment blind”.

### 98.1 UP types

Let  $y_t^B \in \mathbb{R}$  for  $t = t_0, t_1$  be the treatment response at time  $t$  for participant  $B$ . (We are using here the same notation as in Chapter 72). Call  $\delta^B = y_{t_1}^B - y_{t_0}^B$  the **participant uplift** for participant  $B$ . As shown in Fig.98.1, UP classifies participants into 4 **UP-types**: Persuadables, SureThings, LostCauses, and SleepyDogs. The UP-type of a participant depends on the changes that are induced on that participant by an **UP-diagnostic-test**.

- For a **Persuadable** participant,  $\delta^B > 0$ .

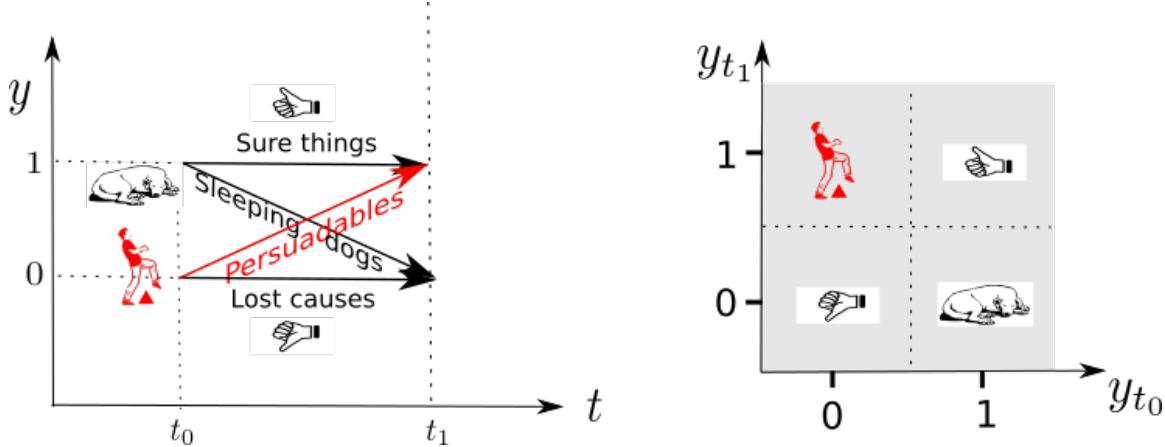


Figure 98.1: UP diagnostic test can be used to classify all participants of the population into 4 UP-types. This figure assumes  $y \in \{0, 1\}$ . More generally,  $y \in \mathbb{R}$ .  $t$  represents time.  $t = t_0$  corresponds to  $d = 0 = \text{untreated}$ , and  $t = t_1$  corresponds to  $d = 1 = \text{treated}$ .

- For a **SleepyDogs** participant,  $\delta^B < 0$ .
- For a **SureThings** participant,  $\delta^B \approx 0$  and  $y_{t_0}^B$  is high.
- For a **LostCauses** participant,  $\delta^B \approx 0$  and  $y_{t_0}^B$  is low.

Suppose  $B$  belongs to stratum  $A_x$ . What is commonly called the **uplift** is the **stratum-uplift**  $\delta_x = ACE_x$ . Strata can also be classified into the 4 UP-types, depending on the sign and size of their  $\delta_x$ . A participant may not be typical for his stratum and may have different **participant and stratum UP-types**. For example, he may have positive participant uplift and therefore have a Persuadable participant UP-type, but his stratum-uplift might be negative, so he has the SleepyDogs stratum UP-type.

Advertisers are very interested in finding the Persuadable strata in a population so as to focus their resources on them. For example, UP was used very successfully during the Obama presidential campaigns. Team Obama conducted UP-diagnostic tests much like the climate change one described earlier. This allowed them to identify voters who might be sitting on the fence on whether to vote for Obama or not. Then Team Obama spent the lion share of resources on those fence-sitters.

## 98.2 Some Relevant Technical Formulas from Chapter 72

Recall the following technical formulae that were proven in Chapter 72:

- Recall Eq.(72.143):

$$ACE = \sum_x P(x) \underbrace{\sum_y y [P(y|d=1, x) - P(y|d=0, x)]}_{ACE_x} \quad (98.1)$$

If  $y \in \{0, 1\}$ , then

$$\underbrace{ACE_x}_{\delta_x} = \underbrace{\frac{P_{y|\underline{d}, \underline{x}}(1|1, x)}{Y_x^1}} - \underbrace{\frac{P_{y|\underline{d}, \underline{x}}(1|0, x)}{Y_x^0}} . \quad (98.2)$$

- Recall Eq.(72.158):

$$\widehat{ACE}_x = \underbrace{\frac{1}{N_x} \sum_{\sigma \in A_x} \frac{d^\sigma y^\sigma}{g_{1|x^\sigma}}}_{Y_x^1} - \underbrace{\frac{1}{N_x} \sum_{\sigma \in A_x} \frac{(1-d^\sigma)y^\sigma}{g_{0|x^\sigma}}}_{Y_x^0} \quad (98.3)$$

### 98.3 UP Analysis

The input to UP is a PO dataset  $DS = \{(\sigma, d^\sigma, x^\sigma, y^\sigma) : \sigma = 0, 1, 2, \dots, nsam - 1\}$ . where  $d^\sigma \in \{0, 1\}$ ,  $x^\sigma \in S_{\underline{x}}$ ,  $y^\sigma \in \mathbb{R}$ . A participant  $B$  is assigned two different  $\sigma$  if he/she belongs to both the treated and control groups. We will assume  $S_{\underline{x}}$  is a finite set. In general,  $x = (x_0, x_1, \dots, x_{n-1})$  is an  $n$  dimensional vector of features  $x_i$ . If any of the  $x_i$  is a priori continuous, we will assume it has been binned into a finite number of bins.

Starting with  $DS$ , UP performs the following steps. Fig.98.2 is a pictorial representation of the quantities that are calculated during these steps.

1. Find  $A_x$  for each observed  $x \in S_{\underline{x}}$ . Set  $A_x = \emptyset$  for unobserved  $x \in S_{\underline{x}}$ .
2. Calculate  $\delta_x$  for each  $x \in S_{\underline{x}}$ . Set  $\delta_x = 0$  if  $A_x = \emptyset$ .
3. Calculate the set

$$\{\Delta_c\}_{c=0,1,\dots,nc-1} = \{\delta_x : x \in S_{\underline{x}}\} \quad (98.4)$$

of distinct uplifts  $\delta_x$ . The class labels  $c$  should be assigned so that the sequence of  $\Delta_c$  is monotonic and non-increasing; i.e.,

$$\Delta_0 \geq \Delta_1 \geq \dots \geq \Delta_{nc-1} . \quad (98.5)$$

Now calculate

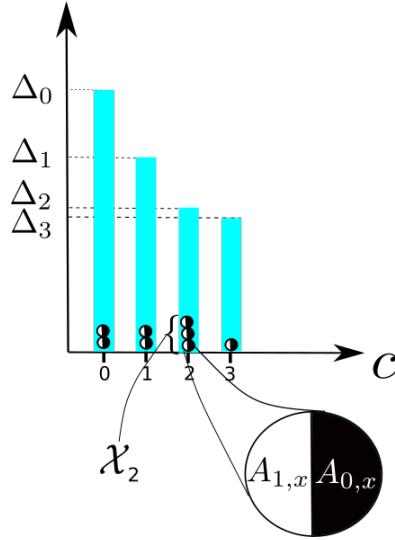


Figure 98.2: Pictorial representation of the sequence  $\{(\mathcal{X}_c, \Delta_c)\}_{c=0,1,\dots,nc-1}$ .

$$\mathcal{X}_c = \{x : \delta_x = \Delta_c\} \quad (98.6)$$

for each  $c$ . By the end of this step, we will have calculated  $\{(\mathcal{X}_c, \Delta_c)\}_{c=0,1,\dots,nc-1}$ . We will refer to the  $\mathcal{X}_c$  as **strata-bins**. Note that

$$\Delta_c = \frac{1}{|\mathcal{X}_c|} \sum_{x \in \mathcal{X}_c} \delta_x \quad (98.7)$$

$$= \underbrace{\frac{1}{|\mathcal{X}_c|} \sum_{x \in \mathcal{X}_c} Y_x^1}_{Y_c^1} - \underbrace{\frac{1}{|\mathcal{X}_c|} \sum_{x \in \mathcal{X}_c} Y_x^0}_{Y_c^0} . \quad (98.8)$$

4. For each  $c$ , calculate

$$\Sigma_{d,c} = \cup_{x \in \mathcal{X}_c} A_{d,x} \quad (98.9)$$

for  $d \in \{0, 1\}$  and

$$\Sigma_c = \Sigma_{0,c} \cup \Sigma_{1,j} . \quad (98.10)$$

Fig.98.3 is a way of plotting the results of UP in an intuitive way that even a business type can understand. UP software often plots something called a Qini curve, but I find Qini curves opaque, confusingly defined in the literature, unnecessary and not very well motivated. So I don't use them.

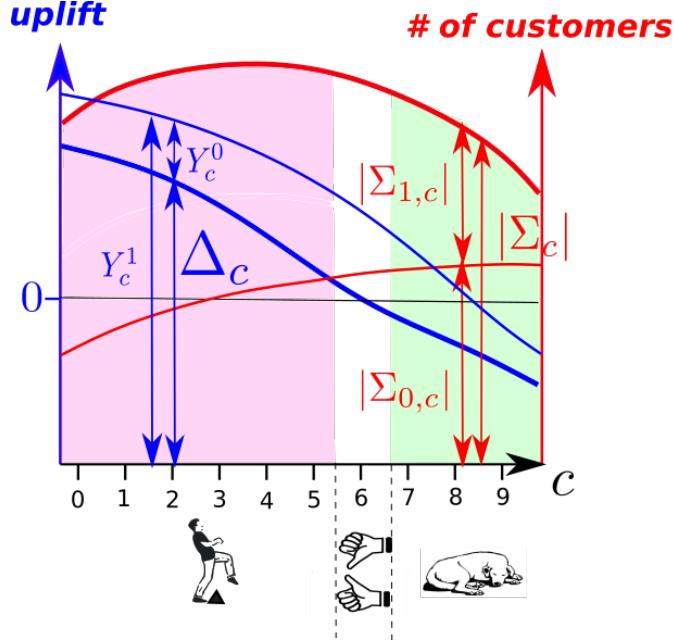


Figure 98.3: Plot of UP results. Alternative to Qini curves.

## 98.4 UP Decision Trees

In this section, we will describe how to build UP decision trees (UP dtrees), and explain why they are needed for UP.

Generic dtrees are described in Chapter 16. This section complements rather than replaces that chapter so the reader is advised to read that chapter first.

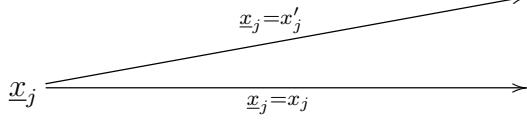
Ref.[60] is an excellent paper on the use of dtrees in UP.

The analysis described previously in Section 98.3, although theoretically correct, will work very poorly in practice. The strata-bins of Section 98.3 correspond to the classification classes of a dtree. But strata-bins are very specific so they severely overfit the data. Although dtrees can also suffer from overfitting, there are known methods of preventing or mitigating overfitting in dtrees.

There are also tasks that dtrees can do well and the methods explained so far cannot do well. For example, suppose we have a classless dataset  $DS^- = \{(\sigma, x^\sigma) : \sigma \in \Sigma^-\}$  and we want to predict the class  $c^\sigma$  and uplift  $\Delta_{c^\sigma}$  for each of these individuals  $\sigma \in \Sigma^-$ . A dtree can easily do that. The alternative is to use the classy dataset  $DS = \{(\sigma, x^\sigma, c^\sigma) : \sigma \in \Sigma\}$  to prepare a dictionary that orders the elements of  $S_x$  and gives a class  $c$  and an uplift value  $\Delta_c$  for each feature vector  $x \in S_x$ . But such a dictionary overfits and says nothing for feature vectors  $x$  that do not show up in the classy dataset  $DS$ ; i.e., the dictionary doesn't guess (interpolate). Dtrees, on the other hand, do guess.

So, without further ado, let us describe how to modify the results of Chapter 16 on generic dtrees to the case of UP dtrees. The main difference, as we will explain

in detail next, is that the Information Gain metric used for generic dtrees needs to be replaced by another metric.



$$\{N_j^d(c, x_j)\}_{c \in S_c, x_j \in S_{\underline{x}_j}}$$

$$\sum_{c \in S_c} N_j^d(c, x_j) = N_j^d(x_j)$$

$$\sum_{x_j \in S_{\underline{x}_j}} N_j^d(c, x_j) = N_j^d(c) \quad \sum_{c \in S_c} N_j^d(c) = \sum_{x_j \in S_{\underline{x}_j}} N_j^d(x_j) = N_j^d$$

Figure 98.4: Fig.16.4 with  $d$  dependence added.  $d \in \{0, 1\}$  is the treatment dose.

Fig.98.4 was obtained from Fig.16.4 by adding  $d$  dependence.  $d \in \{0, 1\}$  is the treatment dose. Note that in UP, we build a dtree in which every node carries a double ( $d = 0, 1$ ) TPV. This is in contrast to the generic dtrees built in Chapter 16, in which each node carries a single TPV.  $N_j^d(c, x_j)$  is the number of individuals  $\sigma$  in the population that reaches node  $\underline{x}_j$  with  $d \in \{0, 1\}$ , belonging to class  $c \in S_c$  and having  $x_j = x_j$ . From these population numbers, we can define the bnet in Fig.98.5. The TPMs, printed in blue, for the (non-root) nodes of this bnet, are as follows

$$P(c|x_j, j, d) = \frac{N_j^d(c, x_j)}{N_j^d(x_j)} \quad (98.11)$$

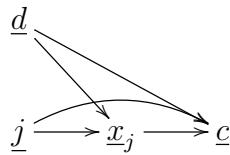


Figure 98.5: Bnet derived from population numbers in Fig.98.4

$$P(x_j|j, d) = \frac{N^d(x_j)}{N_j^d} \quad (98.12)$$

In Chapter 16, we used Information Gain (a mutual information) as the SAM (Separation Ability Measure) in SL (Structure Learning) of dtrees (Decision Trees). Information Gain is a bad SAM for SL of UP dtrees, because it knows nothing about  $d = 0, 1$  and the double TPVs of nodes in UP dtrees. For UP dtrees, we need a SAM specifically designed to separate  $d = 0, 1$ , and generate classes that are uplift bins (i.e., uplift intervals).

Ref.[60] proposes and studies the following 3 SAMs for doing SL of UP dtrees.

### 1. SAM\_DD (DD=Delta Delta)

For  $d \in \{0, 1\}$  and  $c, c' \in S_{\underline{c}}$ , define the increments

$$\partial_d f(d) = f(1) - f(0) \quad (98.13)$$

and

$$\partial_{c',c} f(c) = f(c') - f(c) . \quad (98.14)$$

Let

$$\Delta_{c|j} = P(c|j, 1) - P(c|j, 0) \quad (98.15)$$

$$= \partial_d P(c|j, d) \quad (98.16)$$

$$SAM\_DD_j = \max_{c,c'} |\partial_{c',c} \partial_d P(c|j, d)| \quad (98.17)$$

$$= \max_{c,c'} |\partial_{c',c} \Delta_{c|j}| \quad (98.18)$$

### 2. SAM\_KL (KL=Kullback Leibler)

$$SAM\_KL_j = \left[ \sum_{x_j \in S_{\underline{x}_j}} P(x_j|j) D_{KL}(P_{\underline{c}|x_j,j,1} \| P_{\underline{c}|x_j,j,0}) \right] - D_{KL}(P_{\underline{c}|j,1} \| P_{\underline{c}|j,0}) \quad (98.19)$$

$$= \left[ \sum_{x_j \in S_{\underline{x}_j}} P(x_j|j) \sum_{c \in S_{\underline{c}}} P(c|x_j, j, 1) \ln \frac{P(c|x_j, j, 1)}{P(c|x_j, j, 0)} \right] - \sum_{c \in S_{\underline{c}}} P(c|j, 1) \ln \frac{P(c|j, 1)}{P(c|j, 0)} \quad (98.20)$$

$SAM\_KL_j$  can be negative.

### 3. SAM\_E (E=Euclidean)

$SAM\_E_j$  is defined the same way as  $SAM\_KL_j$  except with the KL divergence  $D_{KL}(P \parallel Q)$  in  $SAM\_KL$  replaced by the Euclidean distance squared.

$$D(P, Q) = \sum_x (P(x) - Q(x))^2 \quad (98.21)$$

The intuitive reason for using these quantities as SAMs is that they maximize the change in uplift between successive tree levels, so that the uplift increases as quickly as possible as we descend down the UP tree. In the case of generic dtrees for which we use Information Gain as SAM, we are maximizing the correlation between classes and nodes as we descend down the tree. These two goals are related. In fact, in the limit where the number of control individuals becomes zero,  $SAM\_KL_j$  and  $IG_j$  become the same, as will be shown later.

Next we show that  $SAM\_KL_j$  satisfies the following 3 axioms<sup>1</sup>

**Claim 152 .**

1.  $SAM\_KL_j$  is minimum iff  $P(c|x_j, j, 0) = P(c|x_j, j, 1)$  for all  $c$  and  $x_j$ .
2. If  $P(c|j, d) = P(c|d)$  for all  $c, d$ , then  $SAM\_KL_j = 0$ .
3. Suppose  $N_r^0 = 0$  for all nodes  $r \in J_0$  (i.e., no control population) and we use the Laplace Correction when warranted. Then

$$SAM\_KL_j = H(\underline{c} : \underline{x}_j | j, 1) \quad (98.22)$$

$$= IG_j \quad \text{for treated population .} \quad (98.23)$$

**proof:**

The proof of items 1 and 2 follow by inspection of Eq.(98.20). Item 3 is proven in Claim 153 below.

**QED**

Let  $N_{\underline{c}} = |S_{\underline{c}}|$ . Define the uniform probability distribution

$$U_{\underline{c}}(c) = \frac{1}{N_{\underline{c}}} \quad (98.24)$$

for all  $c \in S_{\underline{c}}$ .

Eq.(98.11) for the TPM of node  $\underline{c}$  in the bnet Fig.98.5 can be "Laplace Corrected" as follows so that it is no longer undefined when its denominator vanishes:

---

<sup>1</sup>We won't show it here, but according to Ref.[60],  $SAM\_E_j$  also satisfies these 3 axioms, but  $SAM\_DD_j$  satisfies only the first two.

$$P(c|j, d) = \begin{cases} \frac{N_j^d(c)}{N_j^d} & \text{if } N_j^d > 0 \\ U_{\underline{c}}(c) & \text{if } N_j^d = 0 \text{ (Laplace Correction)} \end{cases} \quad (98.25)$$

**Claim 153** Suppose  $N_r^0 = 0$  for all dtree nodes  $r \in J_0$  and we use the Laplace Correction when warranted. Then

$$SAM\_KL_j = H(\underline{c} : \underline{x}_j | j, 1) . \quad (98.26)$$

**proof:**

For all nodes  $r \in J_0$ , we must have

$$P_{\underline{c}|r,0} = U_{\underline{c}} \quad (98.27)$$

so

$$D_{KL}(P_{\underline{c}|r,1} \| P_{\underline{c}|r,0}) = D_{KL}(P_{\underline{c}|r,1} \| U_{\underline{c}}) \quad (98.28)$$

$$= \ln(N_{\underline{c}}) - H(\underline{c}|r, 1) . \quad (98.29)$$

For all  $x_j \in S_{\underline{x}_j}$ , we must also have

$$N_j = N_j^1, N(x_j) = N^1(x_j) \quad (98.30)$$

so

$$P(x_j | j) = P(x_j | j, 1) . \quad (98.31)$$

Now using Eqs.(98.29) and (98.31), we get

$$SAM\_KL_j = - \left[ \sum_{x_j \in S_{\underline{x}_j}} P(x_j | j) H(\underline{c} | x_j, j, 1) \right] + H(\underline{c} | j, 1) \quad (98.32)$$

$$= - \left[ \sum_{x_j \in S_{\underline{x}_j}} P(x_j | j, 1) H(\underline{c} | x_j, j, 1) \right] + H(\underline{c} | j, 1) \quad (98.33)$$

$$= -H(\underline{c} | x_j, j, 1) + H(\underline{c} | j, 1) \quad (98.34)$$

$$= H(\underline{c} : \underline{x}_j | j, 1) \quad (98.35)$$

**QED**

### 98.4.1 Appendix, connection between $\Delta_c$ and $\Delta_{c|j}$

Recall Eq.(98.8):

$$\Delta_c = \underbrace{\frac{1}{|\mathcal{X}_c|} \sum_{x \in \mathcal{X}_c} Y_x^1 - \frac{1}{|\mathcal{X}_c|} \sum_{x \in \mathcal{X}_c} Y_x^0}_{Y_c^1 - Y_c^0} \quad (98.36)$$

$$= \partial_d Y_c^d. \quad (98.37)$$

Compare that to Eq.(98.16):

$$\Delta_{c|j} = P(c|j, 1) - P(c|j, 0) \quad (98.38)$$

$$= \partial_d P(c|j, d) \quad (98.39)$$

What is the connection between these 2 deltas,  $\Delta_c$  and  $\Delta_{c|j}$ ? Are they equal?

First off, notice that  $\Delta_{c|j}$  is defined for all nodes  $j$  of the dtree. Let  $j(c)$  be the leaf node for which  $\Delta_c \approx \Delta_{c|j(c)}$ . Assume  $y^\sigma \in \{0, 1\}$ . Then

$$P(c|j = j(c), d) = \frac{N_{j(c)}^d(c)}{N_{j(c)}^d} \approx Y_c^d \quad (98.40)$$

So the two deltas are indeed approximately equal when  $y^\sigma \in \{0, 1\}$  and  $j = j(c)$ .

# Chapter 99

## Variational Bayesian Approximation for Medical Diagnosis

This chapter is based on Ref.[27].

A Variational Bayesian Approximation (VBA) is when we approximate a probability distribution by another probability distribution that depends on a continuous “variational parameter”. This parameter is adjusted within its range of possible values, to make the approximation as good as possible. There are many VBA methods. VBA methods are inspired by ancient methods used in Calculus of Variations applied to Physics and Engineering problems.

In this chapter, we do VBA via Jensen’s inequality and convex/concave dual functions.

Ref.[27], on which this chapter is based, applies VBA methods to the problem of diagnostic inference using the Quick Medical Reference (QMR) bipartite Bayesian Network. According to Ref.[27] the maximal clique size of the QMR bnet is 150 nodes, which rules out exact methods of inference like the Junction Tree Algorithm (see Chapter 43). For such high complexity cases, one is forced to use either a VBA or a Monte Carlo method.

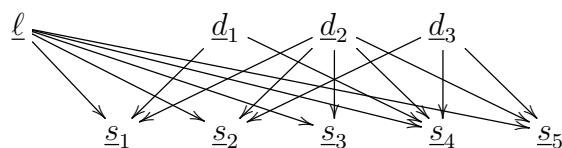


Figure 99.1: Typical bnet (bipartite, 2 level graph) for medical diagnosis to which we will apply VBA methods. In this case,  $nd = 3$  and  $ns = 5$ . According to Ref.[27], for QMR,  $nd \approx 600$  and  $ns \approx 4000$ .

Fig.99.1 gives a typical bnet for medical diagnosis to which we will apply VBA methods.  $\underline{d}_i \in \{0, 1\}$  for  $i = 1, 2, \dots, nd$  are the possible diseases,  $\underline{s}_\sigma \in \{0, 1\}$  for

$\sigma = 1, 2, \dots, ns$  are the possible symptoms, and  $\underline{\ell} \in \{0, 1\}$  is the leakage due to possible error in the parents of the symptoms. Note that the arrows point from diseases to symptoms because diseases precede in time the symptoms.

Let

$$\mathbb{Z}_{[1,n]} = \{1, 2, \dots, n\} \quad (99.1)$$

$$pa_\sigma = \{i \in \mathbb{Z}_{[1,nd]} : \underline{d}_i \in pa(\underline{s}_\sigma)\} = \text{parents of } \underline{s}_\sigma \quad (99.2)$$

Note that  $pa_\sigma$  does not include  $\underline{\ell}$ , which is also a parent of  $\underline{s}_\sigma$ .

$$ch_i = \{\sigma \in \mathbb{Z}_{[1,ns]} : \underline{s}_\sigma \in ch(\underline{d}_i)\} = \text{children of } \underline{d}_i \quad (99.3)$$

$$\underline{d}_A = \{\underline{d}_k : k \in A\} \quad (99.4)$$

$$\underline{d}^{nd} = \{\underline{d}_k : k \in \mathbb{Z}_{[1,nd]}\} \quad (99.5)$$

$$\underline{d}_{\setminus j} = \{\underline{d}_k : k \in \mathbb{Z}_{[1,nd]} - \{j\}\} \quad (99.6)$$

The TPMs, printed in blue, for the bnet Fig.99.1, are as follows:

$$P(\underline{d}_j) = \text{ given} \quad (99.7)$$

$$P(\underline{\ell}) = \text{ given} \quad (99.8)$$

$$P(\underline{s}_\sigma = 0 | d_{pa_\sigma}, \underline{\ell}) = \underbrace{P(\underline{s}_\sigma = 0 | \underline{\ell})}_{e^{-\theta_{\sigma|0}}} \prod_{j \in pa_\sigma} \underbrace{P(\underline{s}_\sigma = 0 | d_j)}_{e^{-\theta_{\sigma|j} d_j}} \quad (99.9)$$

$$= e^{-\theta_{\sigma|0} - \sum_{j \in pa_\sigma} \theta_{\sigma|j} d_j} \quad (99.10)$$

where  $\theta_{\sigma|0}, \theta_{\sigma|j} > 0$ . This  $P(\underline{s}_\sigma = 0 | d_{pa_\sigma}, \underline{\ell})$  corresponds to the noisy-or model (See Chapter 65.).

$$P(\underline{s}_\sigma = 1 | d_{pa_\sigma}) = 1 - e^{-\theta_{\sigma|0} - \sum_{j \in pa_\sigma} \theta_{\sigma|j} d_j} \quad (99.11)$$

Define

$$x_\sigma = \theta_{\sigma|0} + \sum_{j \in pa_\sigma} \theta_{\sigma|j} d_j \quad (99.12)$$

Suppose  $A \subset \mathbb{Z}_{[1,ns]}$ ,  $A^c = \mathbb{Z}_{[1,ns]} - A$ . Then

$$P(d_j | \underline{s}_A = 0, \underline{s}_{A^c} = 1) = \frac{P(\underline{s}_A = 0, \underline{s}_{A^c} = 1 | d_j) P(d_j)}{P(\underline{s}_A = 0, \underline{s}_{A^c} = 1)} \quad (99.13)$$

$$= \mathcal{N}(!d_j) \sum_{d_{!j}} P(\underline{s}_A = 0, \underline{s}_{A^c} = 1 | d^{nd}) P(d^{nd}) \quad (99.14)$$

$$= \mathcal{N}(!d_j) \sum_{d_{!j}} P(\underline{s}_{A^c} = 1 | d^{nd}) P(\underline{s}_A = 0 | d^{nd}) P(d^{nd}) \quad (99.15)$$

$$= \mathcal{N}(!d_j) \sum_{d_{!j}} \left\{ \begin{array}{l} \text{call } \mathcal{P}_\sigma \\ \frac{\prod_{\sigma \in A^c} (1 - e^{-x_\sigma})}{\prod_{\sigma \in A} e^{-\theta_{\sigma|0}} \prod_{j \in pa_\sigma} [e^{-\theta_{\sigma|j}}]^{d_j}} \\ \prod_{j \in \mathbb{Z}_{[1, nd]}} P(d_j) \end{array} \right\} \quad (99.16)$$

Summing over  $d_{!j}$  seems crazy, because  $nd \gg 1$ , but we will approximate the summand so that the sum can be done in closed form.

Define

$$f(x_\sigma) = \ln(1 - e^{-x_\sigma}) \quad (99.17)$$

and

$$\mathcal{P}_\sigma = 1 - e^{-x_\sigma} = e^{f(x_\sigma)} \quad (99.18)$$

$f(x_\sigma)$  is a concave function. See Fig.C.24 for a plot of it.

Next, we shall find a lower and upper bound for  $\mathcal{P}_\sigma$ .

To find the upper bound, we will use dual functions, which are discussed in Section C.47.

Let  $\tilde{f}(p_\sigma)$  be the dual function of  $f(x_\sigma) = \ln(1 - e^{-x_\sigma})$ . In Section C.47, we show that

$$\tilde{f}(p_\sigma) = \min_{x_\sigma} (x_\sigma p_\sigma - f(x_\sigma)) \quad (99.19)$$

$$= -p_\sigma \ln p_\sigma + (1 + p_\sigma) \ln(1 + p_\sigma) \quad (99.20)$$

and

$$f(x_\sigma) \leq x_\sigma p_\sigma - \tilde{f}(p_\sigma). \quad (99.21)$$

Therefore

$$\mathcal{P}_\sigma = e^{f(x_\sigma)} \quad (99.22)$$

$$\leq e^{x_\sigma p_\sigma - \tilde{f}(p_\sigma)} \quad (99.23)$$

$$= e^{-\tilde{f}(p_\sigma)} e^{-\theta_{\sigma|0} p_\sigma} \underbrace{\prod_{j \in pa_\sigma} [e^{-\theta_{\sigma|j} p_\sigma}]^{d_j}}_{\text{call } \mathcal{B}(p_\sigma)} \quad (99.24)$$

To find a lower bound for  $P_\sigma$ , we will use Jensen's inequality, which is discussed in Section C.42. Let  $q_{j|\sigma} \in [0, 1]$  satisfy  $\sum_j q_{j|\sigma} = 1$ . Then

$$\mathcal{P}_\sigma = e^{f(x_\sigma)} \quad (99.25)$$

$$= e^{f(\theta_{\sigma|0} + \sum_j \theta_{\sigma|j} d_j)} \quad (99.26)$$

$$= e^{f\left(\theta_{\sigma|0} + \sum_j q_{j|\sigma} \frac{\theta_{\sigma|j} d_j}{q_{j|\sigma}}\right)} \quad (99.27)$$

$$\geq e^{\sum_j q_{j|\sigma} f\left(\theta_{\sigma|0} + \frac{\theta_{\sigma|j} d_j}{q_{j|\sigma}}\right)} \quad (99.28)$$

$$= e^{\sum_j q_{j|\sigma} \left[ d_j f\left(\theta_{\sigma|0} + \frac{\theta_{\sigma|j} d_j}{q_{j|\sigma}}\right) + (1-d_j) f(\theta_{\sigma|0}) \right]} \quad (99.29)$$

$$= \underbrace{e^{f(\theta_{\sigma|0}) + \sum_j q_{j|\sigma} d_j \left[ f\left(\theta_{\sigma|0} + \frac{\theta_{\sigma|j} d_j}{q_{j|\sigma}}\right) - f(\theta_{\sigma|0}) \right]}}_{\text{call } \mathcal{A}(q_{.|\sigma})} \quad (99.30)$$

In conclusion,

$$\boxed{\mathcal{A}(q_{.|\sigma}) \leq \mathcal{P}_\sigma \leq \mathcal{B}(p_\sigma)} \quad (99.31)$$

with variational parameters  $q_{.|\sigma}$  and  $p_\sigma$ .

# Chapter 100

## Variational Bayesian Approximation via $D_{KL}$

For more info and references about this topic, see Ref.[163].

A Variational Bayesian Approximation (VBA) is when we approximate a probability distribution by another probability distribution that depends on a continuous “variational parameter”. This parameter is adjusted within its range of possible values, to make the approximation as good as possible. There are many VBA methods. VBA methods are inspired by ancient methods used in Calculus of Variations applied to Physics and Engineering problems.

In this chapter, we do VBA via the Kullback-Leibler divergence  $D_{KL}$ . We approximate the probability distribution  $P(h|\vec{x})$ , where  $h$  are the hidden variables and  $\vec{x}$  is the data. More precisely, suppose  $\underline{h} \in S_{\underline{h}}$  and  $\underline{q} \in S_{\underline{h}}$ . Suppose  $\underline{\vec{x}} \in S_{\underline{x}}^{nsam}$  is a vector of  $nsam$  samples and the samples  $\underline{x}[\sigma] \in S_{\underline{x}}$  are i.i.d.. The VBA is simply an approximation  $P_{\underline{q}|\underline{\vec{x}}}$  to  $P_{\underline{h}|\underline{\vec{x}}}$ :

$$P_{\underline{h}|\underline{\vec{x}}}(h|\vec{x}) \approx P_{\underline{q}|\underline{\vec{x}}}(h|\vec{x}) \quad (100.1)$$

obtained by minimizing the Kullback-Leibler divergence  $D_{KL}(P_{\underline{q}|\underline{\vec{x}}} \parallel P_{\underline{h}|\underline{\vec{x}}})$  over all  $P_{\underline{q}|\underline{\vec{x}}}$ . The minimization is usually subject to some constraints on the admissible forms of  $P_{\underline{q}|\underline{\vec{x}}}$ .

$D_{KL}(Q \parallel P) \neq D_{KL}(P \parallel Q)$ ; i.e.,  $D_{KL}$  is not symmetric. So why do we use  $D_{KL}(P_{\underline{q}|\underline{\vec{x}}} \parallel P_{\underline{h}|\underline{\vec{x}}})$  instead of  $D_{KL}(P_{\underline{h}|\underline{\vec{x}}} \parallel P_{\underline{q}|\underline{\vec{x}}})$ ? Because  $D_{KL}(P_{\underline{h}|\underline{\vec{x}}} \parallel P_{\underline{q}|\underline{\vec{x}}})$  requires knowledge of  $P_{\underline{h}|\underline{\vec{x}}}$ , but calculating  $P_{\underline{h}|\underline{\vec{x}}}$  is what we are trying to do in the first place.

See Fig.100.1 for some intuition on what minimizing  $D_{KL}(P_{\underline{q}|\underline{\vec{x}}} \parallel P_{\underline{h}|\underline{\vec{x}}})$  means.

Suppose  $\underline{h} = (\underline{h}_0, \underline{h}_1, \dots, \underline{h}_{nh-1})$  and  $\underline{q} = (\underline{q}_0, \underline{q}_1, \dots, \underline{q}_{nh-1})$  where  $\underline{h}_i \in S_{\underline{h}_i}$  and  $\underline{q}_i \in S_{\underline{h}_i}$  for all  $i$ . We say  $\underline{q}$  and  $\underline{h}$  have  $nh$  mirroring components and those of  $\underline{q}$  are independent at fixed  $\underline{\vec{x}}$  if

$$P_{\underline{q}|\underline{\vec{x}}}(h|\vec{x}) = \prod_i P_{\underline{q}_i|\underline{\vec{x}}}(h_i|\vec{x}) . \quad (100.2)$$

The bnet Fig.100.2 describes the scenario that we have in mind: The samples  $\underline{x}[\sigma]$  are

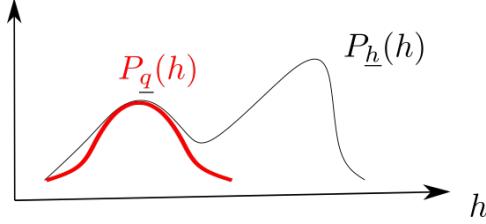


Figure 100.1: If  $P_{\underline{q}}(h)$  is Gaussian shaped and  $P_{\underline{h}}(h)$  has multiple bumps (modes) then  $D_{KL}(P_{\underline{q}} \parallel P_{\underline{h}})$  is minimized when  $P_{\underline{q}}$  fits one of the modes of  $P_{\underline{h}}$ . That is because  $D_{KL}(P_{\underline{q}} \parallel P_{\underline{h}}) = \sum_h P_{\underline{q}}(h) \ln \frac{P_{\underline{q}}(h)}{P_{\underline{h}}(h)}$  is a weighted average with weights  $P_{\underline{q}}$ , so nothing going on outside the support of  $P_{\underline{q}}$  influences much the final average.

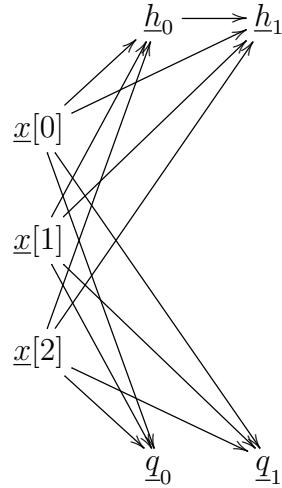


Figure 100.2:  $\underline{q}$  and  $\underline{h}$  have  $nh = 2$  mirroring components and those of  $\underline{q}$  are independent at fixed  $\vec{x}$ .

i.i.d.. Each component  $\underline{h}_i$  of  $\underline{h}$  has a mirroring component  $\underline{q}_i$  in  $\underline{q}$ . The components of  $\underline{h}$  are correlated whereas those of  $\underline{q}$  are independent at fixed  $\vec{x}$ .

**Claim 154** *If  $\underline{q}$  and  $\underline{h}$  have  $nh$  mirroring components and those of  $\underline{q}$  are independent at fixed  $\vec{x}$  and  $\bar{D}_{KL}(P_{\underline{q}|\vec{x}} \parallel P_{\underline{h}|\vec{x}})$  is minimum over all  $P_{\underline{q}|\vec{x}}$ , then*

$$P_{\underline{q}_i|\vec{x}}(q_i|\vec{x}) = \mathcal{N}(!q_i) e^{E_{(q_j)_{j \neq i}} [\ln P_{\underline{h}|\vec{x}}(\underline{h}=\underline{q}|\vec{x})]} \quad (100.3)$$

$$= \mathcal{N}(!q_i) e^{E_{(q_j)_{j \neq i}} [\ln P_{\underline{h},\vec{x}}(\underline{h}=\underline{q}, \vec{x})]} \quad (100.4)$$

for all  $i$ .

**proof:**

Since all quantities in Eq.(100.3) are conditioned on  $\vec{x}$ , let us omit all mention of  $\vec{x}$  in this proof.

Let

$$\mathcal{L} = \mathcal{L}_0 + \mathcal{L}_1 \quad (100.5)$$

where

$$\mathcal{L}_0 = D_{KL}(P_{\underline{q}} \| P_{\underline{h}}) \quad (100.6)$$

$$= \sum_h P_{\underline{q}}(h) \ln \frac{P_{\underline{q}}(h)}{P_{\underline{h}}(h)} \quad (100.7)$$

$$= \sum_h P_{\underline{q}}(h) \ln P_{\underline{q}}(h) - \sum_h P_{\underline{q}}(h) \ln P_{\underline{h}}(h) \quad (100.8)$$

$$= \sum_i \sum_{h_i} P_{\underline{q}_i}(h_i) \ln P_{\underline{q}_i}(h_i) - \sum_h P_{\underline{q}}(h) \ln P_{\underline{h}}(h) \quad (100.9)$$

and

$$\mathcal{L}_1 = \sum_i \lambda_i \left[ \sum_{h_i} P_{\underline{q}_i}(h_i) - 1 \right]. \quad (100.10)$$

Then

$$\delta \mathcal{L} = \sum_i \sum_{h_i} \delta P_{\underline{q}_i}(h_i) \left[ \ln P_{\underline{q}_i}(h_i) + 1 + \lambda_i - \frac{1}{nh} \sum_{(h_j)_{j \neq i}} \prod_{(h_j)_{j \neq i}} \{P_{\underline{q}_j}(h_j)\} \ln P_{\underline{h}}(h) \right]. \quad (100.11)$$

Hence,

$$P_{\underline{q}_i}(h_i) = \mathcal{N}(!h_i) e^{\sum_{(h_j)_{j \neq i}} \left\{ \prod_{(h_j)_{j \neq i}} P_{\underline{q}_j}(h_j) \right\} \ln P_{\underline{h}}(h)}. \quad (100.12)$$

**QED**

Note that Eq.(100.3) yields a system of  $nh$  nonlinear equations in  $nh$  unknowns  $(P_{\underline{q}_i|\vec{x}})_{i=0,1,\dots,nh-1}$ . This system is usually solved recursively.

## 100.1 Free Energy $\mathcal{F}(\vec{x})$

To simplify the notation below, let us introduce the following abbreviations:

$$P(h|\vec{x}) = P_{\underline{h}|\vec{x}}(h|\vec{x}) \quad (100.13)$$

$$P(h, \vec{x}) = P_{\underline{h}, \vec{x}}(h, \vec{x}) \quad (100.14)$$

$$P(\vec{x}) = P_{\vec{x}}(\vec{x}) \quad (100.15)$$

Note that

$$D_{KL}(P_{\underline{q}|\vec{x}} \| P_{\underline{h}|\vec{x}}) = \sum_h P_{\underline{q}|\vec{x}}(h|\vec{x}) \ln \frac{P_{\underline{q}|\vec{x}}(h|\vec{x})}{P(h|\vec{x})} \quad (100.16)$$

$$= \sum_h P_{\underline{q}|\vec{x}}(h|\vec{x}) \ln \frac{P_{\underline{q}|\vec{x}}(h|\vec{x})}{P(h, \vec{x})} + \ln P(\vec{x}) \quad (100.17)$$

$$= \mathcal{F}(\vec{x}) + \ln P(\vec{x}) \quad (100.18)$$

Hence, the **Free energy**  $\mathcal{F}(\vec{x})$  is defined as

$$\mathcal{F}(\vec{x}) = \sum_h P_{\underline{q}|\vec{x}}(h|\vec{x}) \ln \frac{P_{\underline{q}|\vec{x}}(h|\vec{x})}{P(h, \vec{x})} \quad (100.19)$$

$$= E_{\underline{q}|\vec{x}} \left[ \ln \frac{P_{\underline{q}|\vec{x}}(q|\vec{x})}{P_{\underline{h}, \vec{x}}(q, \vec{x})} \right]. \quad (100.20)$$

The name free energy is justified because

$$\mathcal{F}(\vec{x}) = \underbrace{- \sum_h P_{\underline{q}|\vec{x}}(h|\vec{x}) \ln P_{\underline{h}, \vec{x}}(h, \vec{x})}_{U, \text{ Internal Energy}} + \underbrace{\sum_h P_{\underline{q}|\vec{x}}(h|\vec{x}) \ln P_{\underline{q}|\vec{x}}(h|\vec{x})}_{-S, \text{ minus Entropy}}. \quad (100.21)$$

It is also common to define a quantity called "ELBO" to be the negative of the free energy.

$$ELBO(\vec{x}) = -\mathcal{F}(\vec{x}) \quad (100.22)$$

ELBO stands for "Evidence Lower BOund". That name is justified because

$$\underbrace{\ln P_{\vec{x}}(\vec{x})}_{\text{evidence} \leq 0} = \underbrace{D_{KL}(P_{\underline{q}|\vec{x}} \| P_{\underline{h}|\vec{x}})}_{\geq 0} - |ELBO(\vec{x})|. \quad (100.23)$$

Some properties of  $\mathcal{F}$  are:

- $\mathcal{F}$  is **non-negative**.

$$\underbrace{D_{KL}(P_{\underline{q}|\vec{x}} \| P_{\underline{h}|\vec{x}})}_{\geq 0} + \underbrace{\ln \frac{1}{P_{\vec{x}}(\vec{x})}}_{\geq 0} = \mathcal{F}(\vec{x}) \quad (100.24)$$

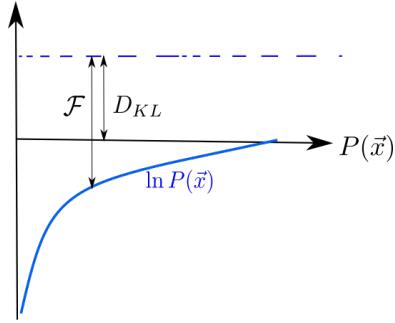


Figure 100.3:  $D_{KL} + \ln \frac{1}{P(\vec{x})} = \mathcal{F}$ .

- KL divergence is min iff  $\mathcal{F}$  is min at fixed  $P(\vec{x})$ .

During a variation  $\delta$  that holds  $P(\vec{x})$  fixed, the KL divergence and  $\mathcal{F}$  change by the same amount:

$$\delta D_{KL}(P_{\underline{g}|\vec{x}} \parallel P_{h|\vec{x}}) = \delta \mathcal{F}(\vec{x}) \quad (100.25)$$

# Chapter 101

## XGBoost

This chapter is based on the original XGBoost paper Ref.[8] and the excellent StatQuest videos (highly recommended) [65].

Extreme Gradient Boosting (XGBoost) (Chen, Guestrin, 2016) improves gradient boosting (Friedman, 1999) in a number of ways, such as by using a quadratic rather than linear approximation for the variational function.

In XGBoost, one calculates a sequence of functions where each function tries to correct the errors of the previous function. Then a series (i.e., linear combination) of those functions yields an estimate  $\hat{y}^\sigma$  of the target attribute  $y^\sigma$ . As will be shown in this chapter, XGBoost can be used in two cases: Regression (continuous target attribute) and Binary Classification (binary target attribute)<sup>1</sup>. An implementation of the XGBoost algorithm is available as open source. It's written in C++, with Python and R interfaces.

Boosting (see this chapter on XGBoost and Chapter 1 on AdaBoost) and bagging (see Chapter 74 on Random Forest) are two methods of building a classifier function from an ensemble of classifier functions. These two methods are most commonly applied to dtrees: Boosting for an ensemble of small dtrees, and Bagging for a random forest (which is an ensemble of dtrees that are usually much more complicated than small dtrees).

### 101.1 Divergences

To set up a cost function for XGBoost, we begin by defining 2 types of "divergences" and calculating the first and second derivatives of those divergences:

- **Divergence for regression** (i.e., continuous classification, continuous target attribute). For  $x, y \in \mathbb{R}$

$$D_{reg}(x, y) = \frac{1}{2}(x - y)^2 \quad (101.1)$$

---

<sup>1</sup>XGBoost can also be used for classification into more than two classes, as long as a suitable Divergence function can be defined.

- **Divergence for binary classification** (i.e., binary target attribute). For  $p, q \in [0, 1]$ .

$$D_{bc}(p, q) = -\{p \ln q + (1-p) \ln(1-q)\} \quad (101.2)$$

$$= CE(\{p, 1-p\} \| \{q, 1-q\}) \quad (101.3)$$

The cross-entropy  $CE()$  is defined in Chapter C.

**Claim 155**

$$\partial_{\hat{y}} D_{reg}(y, \hat{y}) = \hat{y} - y \quad (101.4)$$

$$\partial_{\hat{y}}^2 D_{reg}(y, \hat{y}) = 1 \quad (101.5)$$

$$D(y, \hat{y} + h) \approx D(y, \hat{y}) + (\hat{y} - y)h + \frac{1}{2}h^2 \quad (101.6)$$

**proof:** Obvious.

**QED**

Recall from Section C.21 in Chapter C that

$$\hat{y} = \text{smoid}(\text{lodds}(\hat{y})) \quad (101.7)$$

Let us abbreviate  $s() = \text{smoid}()$  and  $l() = \text{lodds}()$  so

$$\hat{y} = s(l(\hat{y})). \quad (101.8)$$

**Claim 156** <sup>2</sup>

$$\partial_l D(y, \hat{y}(l)) = \hat{y} - y \quad (101.9)$$

$$\partial_l^2 D(y, \hat{y}(l)) = \hat{y}(1 - \hat{y}) \quad (101.10)$$

$$D(y, \hat{y}(l + \Delta l)) \approx D(y, \hat{y}(l)) + (\hat{y} - y)\Delta l + \frac{1}{2}\hat{y}(1 - \hat{y})(\Delta l)^2 \quad (101.11)$$

**proof:**

---

<sup>2</sup>Note that  $D_{bc}(y, \hat{y}) \neq D_{bc}(\hat{y}, y)$ ; i.e.,  $D_{bc}$  is not symmetric in its two arguments. Normally  $0 < \hat{y} < 1$  and  $y \in \{0, 1\}$ . Since the log is applied only to the second argument, to avoid logs of zero, it is better to have  $\hat{y}$  as the second argument.

$$\frac{\partial D(y, s)}{\partial s} = -\partial_s \{y \ln s + (1 - y) \ln(1 - s)\} \quad (101.12)$$

$$= -\frac{y}{s} + \frac{1-y}{1-s} \quad (101.13)$$

$$= \frac{-y(1-s) + (1-y)s}{s(1-s)} \quad (101.14)$$

$$= \frac{-y+s}{s(1-s)} \quad (101.15)$$

Recall that  $\text{smoid}'(l) = \text{smoid}(l)[1 - \text{smoid}(l)]$  so

$$\frac{\partial s}{\partial l} = s(1 - s). \quad (101.16)$$

$$\frac{\partial D(y, s)}{\partial l} = \frac{\partial s}{\partial l} \frac{\partial D(y, s)}{\partial s} = -y + s = -y + \hat{y} \quad (101.17)$$

$$\frac{\partial^2 D(y, s)}{\partial l^2} = \frac{\partial s}{\partial l} = s(1 - s) \quad (101.18)$$

**QED**

## 101.2 Minimizing Cost function for single tree

Let

$\sigma \in \Sigma$  be an individual in a population  $\Sigma$

$x^\sigma \in S_{\underline{x}}$  be a feature vector  $x^\sigma = (x_i^\sigma)_{i=0,1,\dots,nf-1}$

$t \in \{0, 1, \dots, nt - 1\}$  be the tree index

$\mathcal{L}_t$  be the set of leafs of tree  $t$

$\ell \in \mathcal{L}_t$  be a leaf in tree  $t$

$w_t^\ell \in \mathbb{R}$

$f_t : S_{\underline{x}} \rightarrow \mathbb{R}$

$\ell_t : \Sigma \rightarrow \mathcal{L}_t$ ,  $\ell_t(\Sigma) = \mathcal{L}_t$ .

$\ell_t(\sigma)$  be the leaf of individual  $\sigma$  in tree  $t$

$\Sigma_t^\ell = \{\sigma \in \Sigma : \ell_t(\sigma) = \ell\}$

Define the function  $f_t$  by

$$f_t(x^\sigma) = \sum_{\ell \in \mathcal{L}_t} w_t^\ell \mathbb{1}(\sigma \in \Sigma_t^\ell) = w_t^{\ell_t(\sigma)}. \quad (101.19)$$

$f_t(x^\sigma)$  gives the output value for tree  $t$  and feature vector  $x^\sigma$ .

Define the **cost function** for tree  $t$  as follows

$$\mathcal{C}_t = \sum_{\sigma} D(\hat{y}_t^{\sigma}, y^{\sigma}) + \underbrace{\sum_{\ell \in \mathcal{L}_t} \left[ \gamma + \frac{\lambda}{2} (w_t^{\ell})^2 \right]}_{\text{regulator}}, \quad (101.20)$$

where  $\gamma > 0, \lambda > 0$  are regulator parameters.

The estimate  $\hat{y}_t^{\sigma}$ , using trees from 0 to  $t$ , of the target attribute  $y^{\sigma}$ , is defined by

$$\hat{y}_0^{\sigma} = f_0(x^{\sigma}) = \text{arbitrary constant, XGBoost default for this is 0.5} \quad (101.21)$$

$$\hat{y}_1^{\sigma} = f_0(x^{\sigma}) + f_1(x^{\sigma}) \quad (101.22)$$

$$\hat{y}_2^{\sigma} = f_0(x^{\sigma}) + f_1(x^{\sigma}) + f_2(x^{\sigma}) \quad (101.23)$$

$$\vdots \quad (101.24)$$

$$\hat{y}_t^{\sigma} = \sum_{t' \leq t} f_{t'}(x^{\sigma}) = \hat{y}_{t-1}^{\sigma} + f_t(x^{\sigma}) \quad (101.25)$$

In the cost function  $\mathcal{C}_t$ , we approximate the divergence  $D()$  by a second order Taylor approximation:

$$D(y^{\sigma}, \hat{y}_t^{\sigma}) = D(y^{\sigma}, \hat{y}_{t-1}^{\sigma} + \underbrace{f_t(x^{\sigma})}_{\delta}) \quad (101.26)$$

$$\approx D(y^{\sigma}, \hat{y}_{t-1}^{\sigma}) + a_t^{\sigma} \delta + \frac{1}{2} b_t^{\sigma} \delta^2 \quad (101.27)$$

$$= D(y^{\sigma}, \hat{y}_{t-1}^{\sigma}) + a_t^{\sigma} w_t^{\ell_t(\sigma)} + \frac{1}{2} b_t^{\sigma} (w_t^{\ell_t(\sigma)})^2, \quad (101.28)$$

where

$$a_t^{\sigma} = [\partial_{\hat{y}} D(y^{\sigma}, \hat{y})]_{\hat{y}=\hat{y}_{t-1}^{\sigma}}, \quad (101.29)$$

$$b_t^{\sigma} = [\partial_{\hat{y}}^2 D(y^{\sigma}, \hat{y})]_{\hat{y}=\hat{y}_{t-1}^{\sigma}}. \quad (101.30)$$

$a_t^{\sigma}$  is called  $g$  for gradient and  $b_t^{\sigma}$  is called  $h$  for Hessian in Ref.[8]. Table 101.1 gives the values for  $a_t^{\sigma}$  and  $b_t^{\sigma}$  for Regression (reg) and Binary classification (bc).

Define the **residual** for tree  $t$  and individual  $\sigma$  by

$$r_t^{\sigma} = y^{\sigma} - \hat{y}_{t-1}^{\sigma}. \quad (101.31)$$

Note that

$$\sum_{\sigma} = \sum_{\ell \in \mathcal{L}_t} \sum_{\sigma \in \Sigma_t^{\ell}}. \quad (101.32)$$

Define

	Regression ( $y^\sigma \in \mathbb{R}$ , $\hat{y}_t^\sigma \in \mathbb{R}$ , $D = D_{reg}$ )	Binary Classification ( $y^\sigma \in \{0, 1\}$ , $\hat{y}_t^\sigma \in [0, 1]$ , $D = D_{bc}$ )
$a_t^\sigma$	$\hat{y}_{t-1}^\sigma - y^\sigma = \text{neg.residual}$	$\hat{y}_{t-1}^\sigma - y^\sigma = \text{neg.residual}$
$b_t^\sigma$	1	$\hat{y}_{t-1}^\sigma(1 - \hat{y}_{t-1}^\sigma)$

Table 101.1: The first ( $a_t^\sigma$ ) and second ( $b_t^\sigma$ ) derivatives for Regression (reg) and Binary classification (bc).

$$A_t^\ell = \sum_{\sigma \in \Sigma_t^\ell} a_t^\sigma \quad (101.33)$$

and

$$B_t^\ell = \sum_{\sigma \in \Sigma_t^\ell} b_t^\sigma. \quad (101.34)$$

Now we can rewrite the cost function as

$$\mathcal{C}_t = \underbrace{\sum_{\sigma} D(\hat{y}_{t-1}^\sigma, y^\sigma)}_{\mathcal{K}} + \sum_{\ell \in \mathcal{L}_t} \left[ A_t^\ell w_t^\ell + \frac{1}{2} B_t^\ell (w_t^\ell)^2 \right] + \sum_{\ell \in \mathcal{L}_t} \left[ \gamma + \frac{\lambda}{2} (w_t^\ell)^2 \right] \quad (101.35)$$

$$= \sum_{\ell \in \mathcal{L}_t} \left[ \gamma + A_t^\ell w_t^\ell + \frac{1}{2} (B_t^\ell + \lambda) (w_t^\ell)^2 \right] \quad (\text{absorbed } \mathcal{K} \text{ into } \gamma) \quad (101.36)$$

The cost function  $\mathcal{C}_t$  can be minimized over  $w_t^\ell$ :

$$0 = \delta \mathcal{C}_t = \sum_{\ell \in \mathcal{L}_t} \delta w_t^\ell \left[ A_t^\ell + (B_t^\ell + \lambda) w_t^\ell \right] \quad (101.37)$$

Therefore, the cost is minimized when

$$w_t^\ell = \frac{-A_t^\ell}{B_t^\ell + \lambda}. \quad (101.38)$$

The optimum cost is

$$\mathcal{C}_t = \sum_{\ell \in \mathcal{L}_t} \underbrace{\left[ \gamma - \frac{(A_t^\ell)^2}{2(B_t^\ell + \lambda)} \right]}_{\mathcal{C}_t^\ell} \quad (101.39)$$

$\mathcal{C}_t^\ell$  is called the **similarity score** for leaf  $\ell$  and tree  $t$ . Note that an increase in similarity decreases the cost.

## 101.3 Leaf Splitting

Suppose leaf  $\ell_0$  splits into leafs  $\ell_L$  and  $\ell_R$ . Then

$$\Sigma_t^{\ell_0} = \Sigma_t^{\ell_L} \cup \Sigma_t^{\ell_R}, \quad \Sigma_t^{\ell_L} \cap \Sigma_t^{\ell_R} = \emptyset \quad (101.40)$$

so

$$A_t^{\ell_0} = A_t^{\ell_L} + A_t^{\ell_R} \quad (101.41)$$

and

$$B_t^{\ell_0} = B_t^{\ell_L} + B_t^{\ell_R}. \quad (101.42)$$

Hence,

$$\mathcal{C}_t^{\ell_j} = \gamma - \frac{(A_t^{\ell_j})^2}{2(B_t^{\ell_j} + \lambda)} \quad \text{for } j = L, R \quad (101.43)$$

$$\mathcal{C}_t^{\ell_0} = \gamma - \frac{(A_t^{\ell_L} + A_t^{\ell_R})^2}{2(B_t^{\ell_L} + B_t^{\ell_R} + \lambda)} \quad (101.44)$$

Define the **XGBoost branch Gain** for a binary tree branch by

$$Gain_{XGB} = \mathcal{C}_t^{\ell_0} - \mathcal{C}_t^{\ell_L} - \mathcal{C}_t^{\ell_R} \quad (101.45)$$

$$= \underbrace{\left\{ SS_t^{\ell_L} + SS_t^{\ell_R} - SS_t^{\ell_0} \right\}}_{\Delta SS_t} - \gamma \quad (101.46)$$

By splitting a leaf, we create a new binary branch with 2 new leafs. We successively add new branches to the tree until some stopping criterion is satisfied. We continue adding branches to the tree as long as they have a positive gain, and as long as the number of levels is smaller than an upper bound input parameter (XGBoost's default maximum number of tree levels is six). XGBoost also rules out leafs that have a denominator quantity  $B_t^\ell$  (called the **cover**) smaller than a lower bound input parameter. This branching process is illustrated in Figs.101.1 and 101.2.

## 101.4 Pruning

If we raise  $\gamma$  or raise  $\lambda$ , branches that previously had positive gain may acquire a negative gain. Get rid of branches from highest level that now have negative gain. This will generate new branches. Get rid of new branches from the highest level that have negative gain. Continue this process until all highest level branches have positive gain. This may reduce a tree to a single node or even rule out the entire tree.

$\lambda$  measures **level of insensitivity** to observations, and  $\gamma$  measures **level of tree simplicity**.

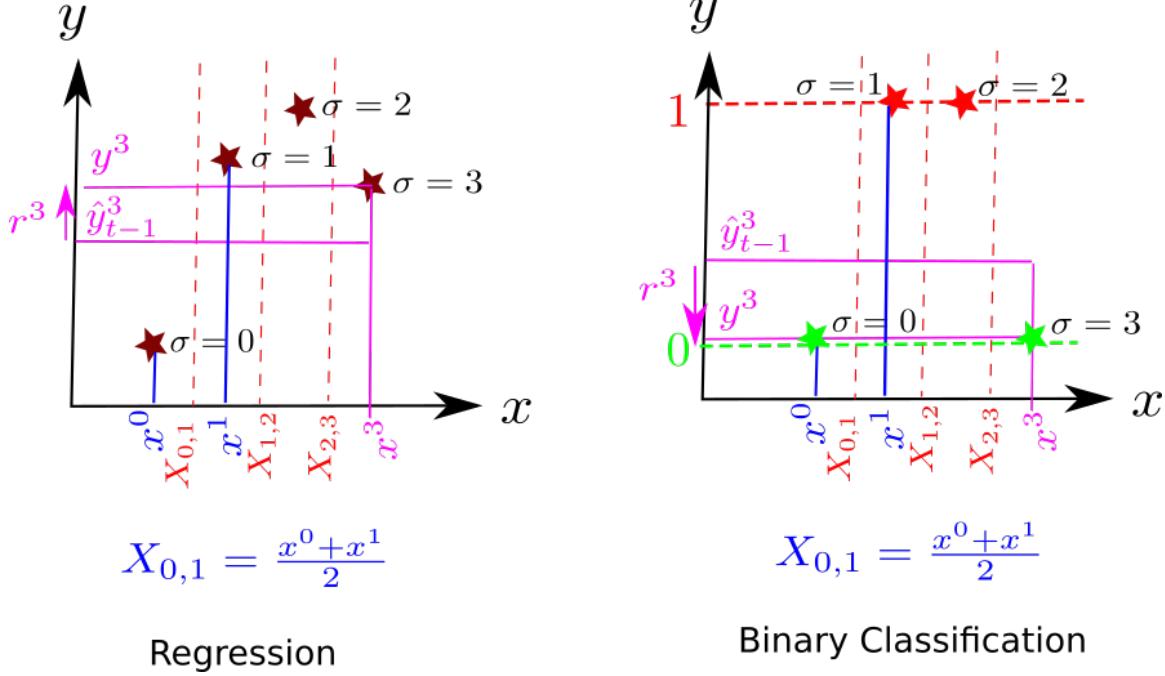
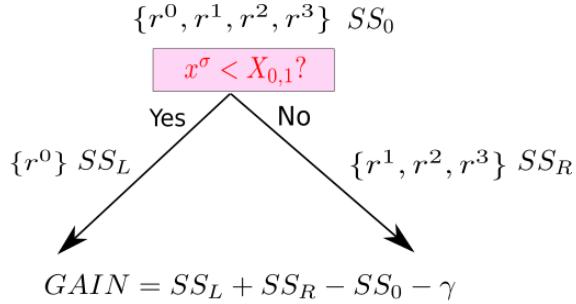


Figure 101.1: Plot of target attribute  $y^\sigma$  versus a feature vector  $x^\sigma$  with a single component. More generally, the feature vector  $x^\sigma = (x_j^\sigma)_{j=0,1,\dots,nf-1}$  can have multiple components called features or attributes. The left plot refers to a population of 4 individuals and regression so  $y^\sigma, \hat{y}^\sigma \in \mathbb{R}$ . The right plot refers to a population of 4 individuals and binary classification so  $y^\sigma \in \{0, 1\}, \hat{y}^\sigma \in [0, 1]$ .  $X_{j,j+1}$  for  $j = 0, 1, 2$  is the average between 2 adjacent values of  $x^\sigma$ .



Repeat for  $x^\sigma < X_{1,2}$ ? and  $x^\sigma < X_{2,3}$ ?  
Choose inequality with highest GAIN

Figure 101.2: This figure refers to the situation of Fig.101.1. Out of all allowed tree branches, we choose the one with the highest gain.

## 101.5 Feature Binning

For really large population sizes  $|\Sigma|$ , it is convenient to bin the set  $\{x_i^\sigma : \sigma \in \Sigma\}$  for each  $i$ .

A common bin type is quantiles. Quantiles are bins  $[X_{j-1}, X_j]$  for  $j = 0, 1, \dots, nbins - 1$  that all contain approximately the same number of points. For example, in Fig.101.2, with 1 point quantile bins, use  $[X_{j-1}, X_j]$  for  $j = 0, 1, 2, 3$ . With 2 point quantile bins, use  $[X_{j-1}, X_j]$  for  $j = 0, 1$ .

Use the right edge of each bin as the  $X_j$  in the question  $x^\sigma < X_j?$ , and choose the question which yields the highest gain.

## 101.6 Final estimate of target attribute

In this section, we will give a formula for the final estimate of the target attribute. Previously, we set the learning rate  $\eta$  to one. Here we restore  $\eta$  to an arbitrary value between 0 and 1.

Instead of using

$$f(x^\sigma) = \sum_{t=0}^{nt-1} f_t(x^\sigma), \quad (101.47)$$

we will use

$$f(x^\sigma) = \sum_{t=0}^{nt-1} (\eta)^t f_t(x^\sigma), \quad (101.48)$$

where  $\eta \in [0, 1]$  is called the **learning rate**. This has the effect of compensating for the  $f_t$ 's with  $t > nt - 1$  that would have been included had we used an infinite series. Also, think of Eq.(101.47) as an approximation (a truncated Taylor expansion in powers of  $\Delta x$ ) of a function  $f(x + \Delta x)$ , and think of Eq.(101.48) as an analogous approximation of the function  $f(x + \eta\Delta x)$ .

For the case of Regression, we get:

$$f(x^\sigma) = \sum_t (\eta)^t \left( \frac{-A_t^{\ell_t(\sigma)}}{B_t^{\ell_t(\sigma)} + \lambda} \right). \quad (101.49)$$

For the case of Binary Classification, we get

$$f(x^\sigma) = \sum_{t=0}^{nt-1} (\eta)^t \underbrace{\text{smoid} \left( \frac{-A_t^{\ell_t(\sigma)}}{B_t^{\ell_t(\sigma)} + \lambda} \right)}_{\substack{\text{lodds(probability)} \\ \text{probability}}}. \quad (101.50)$$

## 101.7 Bnet for XGBoost

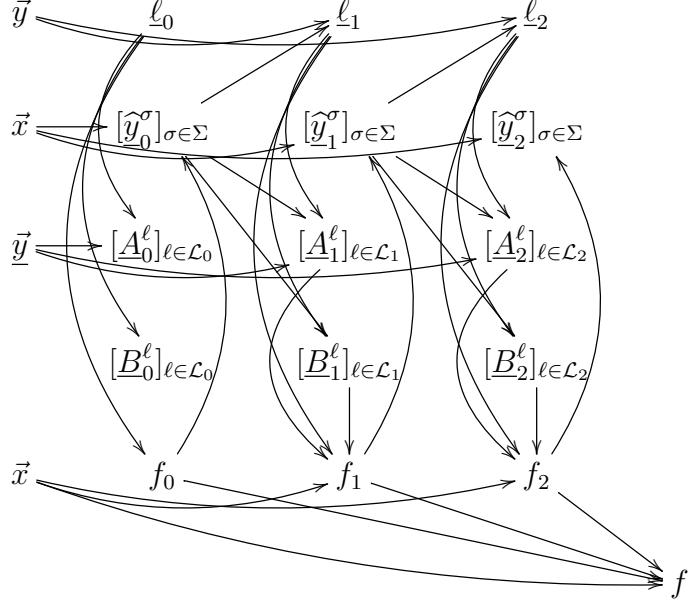


Figure 101.3: Bnet for XGBoost assuming  $nt = 3$ . Nodes that appear multiple times (namely  $\vec{x}$  and  $\vec{y}$ ) should be considered the same node, drawn multiple times for clarity. The parameters  $\lambda, \gamma, \eta$  are taken to be global. Recall that  $\ell_t : \Sigma \rightarrow \mathcal{L}_t$ . From the function  $\ell_t()$ , we can derive its range  $\mathcal{L}_t = \{\ell_t(\sigma) : \sigma \in \Sigma\}$ , and  $\Sigma_t^\ell = \{\sigma \in \Sigma : \ell_t(\sigma) = \ell\}$  for all  $\ell \in \mathcal{L}_t$ .

Fig.101.3 gives our bnet for the XGBoost algo assuming  $nt = 3$ . The TPMs, printed in blue, for this bnet, are as follows:

For  $t = 0$ ,  $\ell_0$  describes a single node “tree” such that  $\ell_0(x^\sigma) = f_0(x^\sigma) = 0.5$  for all  $\sigma \in \Sigma$ . For  $t \geq 1$ ,

$$P(\ell_t | \vec{y}, [\hat{y}_{t-1}^\sigma]_\sigma) = \begin{array}{l} \text{build tree } \ell_t \text{ using } y^\sigma \text{ and } \hat{y}_{t-1}^\sigma \text{ for all } \sigma \in \Sigma. \\ \lambda \text{ and } \gamma \text{ are used here.} \end{array} \quad (101.51)$$

$$P([\hat{y}_t^\sigma]_\sigma | f_t, \vec{x}) = \prod_{\sigma \in \Sigma} \mathbb{1}(\hat{y}_t^\sigma = f_t(x^\sigma)) \quad (101.52)$$

$$P([A_t^\ell]_{\ell \in \mathcal{L}_t} | \vec{y}, [\hat{y}_{t-1}^\sigma]_\sigma, \ell_t) = \prod_{\ell \in \mathcal{L}_t} \mathbb{1}(A_t^\ell = - \sum_{\sigma \in \Sigma_t^\ell} \underbrace{(y^\sigma - \hat{y}_{t-1}^\sigma)}_{r_t^\sigma}) \quad (101.53)$$

$$P(B_t^\ell | \ell \in \mathcal{L}_t | [\hat{y}_{t-1}^\sigma]_\sigma, \ell_t) = \prod_{\ell \in \mathcal{L}_t} \mathbb{1}(B_t^\ell = \sum_{\sigma \in \Sigma_t^\ell} \left\{ \begin{array}{ll} 1 & \text{if reg.} \\ \hat{y}_{t-1}^\sigma (1 - \hat{y}_{t-1}^\sigma) & \text{if b.c.} \end{array} \right\}) \quad (101.54)$$

$$P(f_t | [A_t^\ell]_{\ell \in \mathcal{L}_t}, [B_t^\ell]_{\ell \in \mathcal{L}_t}, \ell_t, \vec{x}) = \prod_{\sigma \in \Sigma} \mathbb{1}\left(f_t(x^\sigma) = \left\{ \begin{array}{ll} 1 & \text{if reg.} \\ \text{smoid} & \text{if b.c.} \end{array} \right\} \frac{-A^{\ell_t(\sigma)}}{2(B^{\ell_t(\sigma)} + \lambda)} \right) \quad (101.55)$$

$$P(f | [f_t]_t, \vec{x}) = \prod_{\sigma \in \Sigma} \mathbb{1}(f(x^\sigma) = \sum_t (\eta)^t f_t(x^\sigma)) \quad (101.56)$$

# Chapter 102

## Zero Information Transmission (Graphoid Axioms)

This chapter assumes that you have read Chapter 23 on d-separation.

The following quantities play a very prominent role in the d-separation Theorem that we enunciated in Chapter 23.

- the mutual information (MI)  
(a.k.a. information transmission)  $H(\underline{a} : \underline{b})$
- the conditional mutual information (CMI)  
(a.k.a. conditional information transmission)  $H(\underline{a} : \underline{b} | \underline{c})$

MI can be viewed as the special case of CMI, when the set of variables being conditioned on is empty. Particularly prominent in d-separation discussions are probability distributions for which CMI vanishes. The goal of this chapter is to study such probability distributions.

Recall that CMI is non-negative and symmetric in its first two variables (i.e.,  $H(\underline{a} : \underline{b} | \underline{c}) = H(\underline{b} : \underline{a} | \underline{c})$ ). Another very useful property of CMI is its chain rule

**Claim 157** (*Chain Rule for CMI*)

$$H(\underline{y} : \underline{x}^n) = \sum_i H(\underline{y} : \underline{x}_i | \underline{x}_{<i}), \quad (102.1)$$

where  $\underline{x}^n = (\underline{x}_0, \underline{x}_1, \dots, \underline{x}_{n-1})$  and  $\underline{x}_{<i} = (\underline{x}_0, \underline{x}_1, \dots, \underline{x}_{i-1})$ .

**proof:**

$$\frac{P(y|x_{<i+1})}{P(y)} = \frac{P(y|x_i, x_{<i})}{P(y|x_{<i})} \cdot \frac{P(y|x_{<i})}{P(y)} \quad (102.2)$$

Therefore,

$$\ln \frac{P(y|x_{<i+1})}{P(y)} = \ln \frac{P(y|x_i, x_{<i})}{P(y|x_{<i})} + \ln \frac{P(y|x_{<i})}{P(y)} \quad (102.3)$$

If we now apply  $\sum_{y,x^n} P(y, x^n)$  to both sides, we get

$$H(\underline{y} : \underline{x}_{<i+1}) = H(\underline{y} : \underline{x}_i | \underline{x}_{<i}) + H(\underline{y} : \underline{x}_{<i}) \quad (102.4)$$

**QED**

A trivial but very useful consequence of the chain rule for CMI is:

$$\boxed{H(\underline{y} : \underline{x}^n) = 0 \iff H(\underline{y} : \underline{x}_i | \underline{x}_{<i}) = 0 \text{ for all } i}. \quad (102.5)$$

## 102.1 Consequences of Eq.(102.5)

Table 102.1 gives a set of statements about CMI referred to as the Graphoid Axioms in chapter 1 of Ref.[52]. See Ref.[52] to learn the history of these axioms. The purpose of this section is to prove that the graphoid axioms are all a simple consequence of Eq.(102.5).

Symmetry	$\underline{a} \perp_P \underline{b} \implies \underline{b} \perp_P \underline{a}$ $H(\underline{a} : \underline{b}) = 0 \implies H(\underline{b} : \underline{a}) = 0$
Decomposition	$\underline{a} \perp_P \underline{b}, \underline{c} \implies \underline{a} \perp_P \underline{b} \text{ and } \underline{a} \perp_P \underline{c}$ $H(\underline{a} : \underline{b}, \underline{c}) = 0 \implies H(\underline{a} : \underline{b}) = 0 \text{ and } H(\underline{a} : \underline{c}) = 0$
Weak Union	$\underline{a} \perp_P \underline{b}, \underline{c} \implies \underline{a} \perp_P \underline{b} \underline{c} \text{ and } \underline{a} \perp_P \underline{c} \underline{b}$ $H(\underline{a} : \underline{b}, \underline{c}) = 0 \implies H(\underline{a} : \underline{b} \underline{c}) = 0 \text{ and } H(\underline{a} : \underline{c} \underline{b}) = 0$
Contraction	$\underline{a} \perp_P \underline{b} \underline{c} \text{ and } \underline{a} \perp_P \underline{c} \implies \underline{a} \perp_P \underline{b}, \underline{c}$ $H(\underline{a} : \underline{b} \underline{c}) = 0 \text{ and } H(\underline{a} : \underline{c}) = 0 \implies H(\underline{a} : \underline{b}, \underline{c}) = 0$
Intersection	$\underline{a} \perp_P \underline{b} \underline{c}, \underline{d} \text{ and } \underline{a} \perp_P \underline{d} \underline{c}, \underline{b} \implies \underline{a} \perp_P \underline{b}, \underline{d} \underline{c}$ $H(\underline{a} : \underline{b} \underline{c}, \underline{d}) = 0 \text{ and } H(\underline{a} : \underline{d} \underline{c}, \underline{b}) = 0 \implies H(\underline{a} : \underline{b}, \underline{d} \underline{c}) = 0$

Table 102.1: Graphoid Axioms

**Claim 158** *Table 102.1 is true.*

**proof:**

- **Symmetry**

Follows trivially from  $H(\underline{a} : \underline{b}) = H(\underline{b} : \underline{a})$ .

- **Decomposition**

From the chain rule for CMI, we have

$$H(\underline{a} : \underline{b}, \underline{c}) = H(\underline{a} : \underline{b}|\underline{c}) + H(\underline{a} : \underline{c}), \quad (102.6)$$

and

$$H(\underline{a} : \underline{b}, \underline{c}) = H(\underline{a} : \underline{c}|\underline{b}) + H(\underline{a} : \underline{b}) . \quad (102.7)$$

Hence,

$$H(\underline{a} : \underline{b}, \underline{c}) = 0 \quad (102.8)$$

implies

$$H(\underline{a} : \underline{b}|\underline{c}) = H(\underline{a} : \underline{c}) = 0 , \quad (102.9)$$

and

$$H(\underline{a} : \underline{c}|\underline{b}) = H(\underline{a} : \underline{b}) = 0 . \quad (102.10)$$

- **Weak Union**

Already proven in proof of Decomposition.

- **Contraction**

From chain rule for CMI, we have

$$H(\underline{a} : \underline{b}, \underline{c}) = H(\underline{a} : \underline{b}|\underline{c}) + H(\underline{a} : \underline{c}) . \quad (102.11)$$

- **Intersection**

From the chain rule for CMI, we have

$$H(\underline{a} : \underline{b}, \underline{d}|\underline{c}) = H(\underline{a} : \underline{b}|\underline{d}, \underline{c}) + H(\underline{a} : \underline{d}|\underline{c}) , \quad (102.12)$$

and

$$H(\underline{a} : \underline{b}, \underline{d}|\underline{c}) = H(\underline{a} : \underline{d}|\underline{b}, \underline{c}) + H(\underline{a} : \underline{b}|\underline{c}) . \quad (102.13)$$

Thus,

$$H(\underline{a} : \underline{b}, \underline{d}|\underline{c}) = 0 \quad (102.14)$$

implies

$$H(\underline{a} : \underline{b}|\underline{d}, \underline{c}) = H(\underline{a} : \underline{d}|\underline{c}) = 0 , \quad (102.15)$$

and

$$H(\underline{a} : \underline{d}|\underline{b}, \underline{c}) = H(\underline{a} : \underline{b}|\underline{c}) = 0 . \quad (102.16)$$

**QED**

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