

Bayesuvius,
a small visual dictionary of Bayesian Networks

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Figure 1: View of Mount Vesuvius from Pompeii

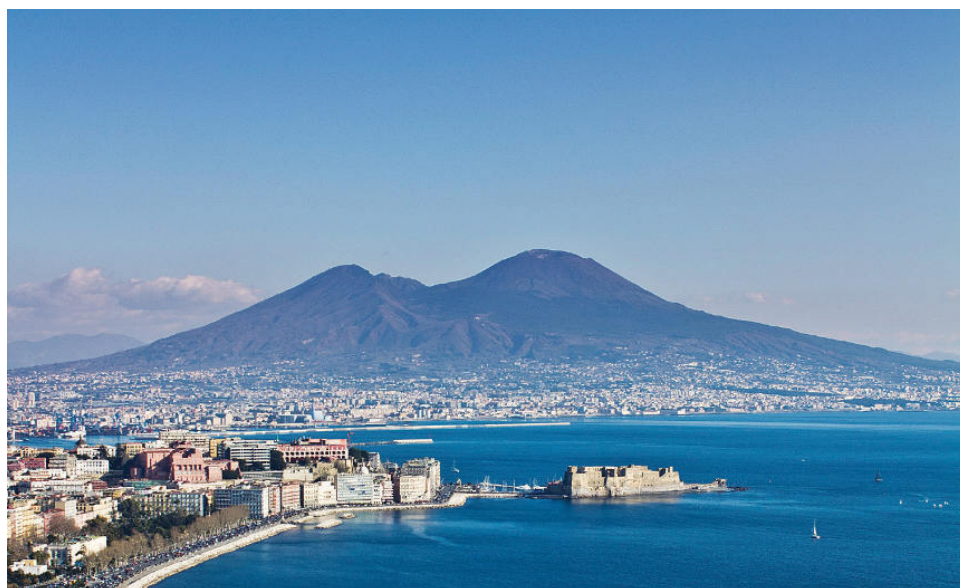


Figure 2: Mount Vesuvius and Bay of Naples

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Notational Conventions and Preliminaries

0.1 Some abbreviations frequently used throughout this book.

- bnet= B net= Bayesian Network
- CPT = Conditional Probabilities Table, same as TPM
- DAG = Directed Acyclic Graph
- i.i.d.= independent identically distributed.
- RCT= Randomized Controlled Trial, aka A/B testing.
- TPM= Transition Probability Matrix, same as CPT

0.2 $\mathcal{N}(!a)$

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

0.3 One hot

A **one hot** vector of zeros and ones is a vector with all entries zero with the exception of a single entry which is one. A **one cold** vector has 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.

0.4 Special sets

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

For $a < b$, define $I_{\mathbb{Z}}$ 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).

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

0.5 Kronecker delta function

For x, y in discrete set S ,

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

0.6 Dirac delta function

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

$$\int_{-\infty}^{+\infty} dx \delta(x - y) f(x) = f(y) \quad (2)$$

0.7 Indicator function (aka Truth function)

$$\mathbb{1}(\mathcal{S}) = \begin{cases} 1 & \text{if } \mathcal{S} \text{ is true} \\ 0 & \text{if } \mathcal{S} \text{ is false} \end{cases} \quad (3)$$

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

0.8 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.

0.9 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 (aka cardinality) of that set. Hence,

$$\sum_{x \in S_{\underline{x}}} P_{\underline{x}}(x) = 1 \quad (4)$$

$$P_{\underline{x}, \underline{y}}(x, y) = P(\underline{x} = x, \underline{y} = y) = P(x, y) \quad (5)$$

$$P_{\underline{x}|\underline{y}}(x|y) = P(\underline{x} = x|\underline{y} = y) = P(x|y) = \frac{P(x, y)}{P(y)} \quad (6)$$

0.10 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 Δx . 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

$$\frac{1}{(b-a)} \int_{[a,b]} dx f(x) \rightarrow \frac{\Delta x}{(b-a)} \sum_{x \in S_{\underline{x}}} f(x) = \frac{1}{n_{\underline{x}}} \sum_{x \in S_{\underline{x}}} f(x) . \quad (7)$$

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

$$\int_{[a,b]} dx \delta(x - y) f(x) = f(y) \rightarrow \sum_{x \in S_{\underline{x}}} \delta(x, y) f(x) = f(y) . \quad (8)$$

0.11 Samples, i.i.d. variables

$$\vec{x} = (x[0], x[1], x[2] \dots, x[nsam(\vec{x}) - 1]) = x[:] \quad (9)$$

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

$$x[\sigma] \sim P_{\underline{x}} \text{ (i.e. } P_{\underline{x}[\sigma]} = P_{\underline{x}}) \quad (10)$$

$$P(\underline{x} = x) = \frac{1}{nsam(\vec{x})} \sum_{\sigma} \mathbb{1}(x[\sigma] = x) \quad (11)$$

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

$$\sum_x P(\underline{x} = x) f(x) = \frac{1}{nsam(\vec{x})} \sum_{\sigma} f(x[\sigma]) \quad (12)$$

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

$$P(\vec{x}) = \prod_{\sigma} P(x[\sigma]) \quad (13)$$

$$\sum_{\vec{x}} = \prod_{\sigma} \sum_{x[\sigma]} \quad (14)$$

$$\partial_{\vec{x}} = [\partial_{x[0]}, \partial_{x[1]}, \partial_{x[2]}, \dots, \partial_{x[nsam(\vec{x})-1]}] \quad (15)$$

$$P(\vec{x}) \approx \left[\prod_x P(x)^{P(x)} \right]^{nsam(\vec{x})} \quad (16)$$

$$= e^{nsam(\vec{x}) \sum_x P(x) \ln P(x)} \quad (17)$$

$$= e^{-nsam(\vec{x}) H(P_{\underline{x}})} \quad (18)$$

0.12 Normal Distribution

For $x, \mu, \sigma \in \mathbb{R}$, $\sigma > 0$

$$\mathcal{N}(x; \mu, \sigma^2) = \frac{1}{\sigma\sqrt{2\pi}} e^{-\frac{1}{2}\left(\frac{x-\mu}{\sigma}\right)^2} \quad (19)$$

0.13 Uniform Distribution

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

$$\mathcal{U}(x; a, b) = \frac{1}{b-a} \quad (20)$$

0.14 Sigmoid and logit functions

The sigmoid function $\text{sig}:\mathbb{R} \rightarrow [0, 1]$ is defined by

$$\text{sig}(x) = \frac{1}{1 + e^{-x}} \quad (21)$$

$\text{sig}()$ is monotonically increasing with $\text{sig}(-\infty) = 0$ and $\text{sig}(+\infty) = 1$.

The logit or log-odds function $\text{logit}:[0, 1] \rightarrow \mathbb{R}$ is defined by

$$\text{logit}(p) = \ln \frac{p}{1-p} \quad (22)$$

$\text{logit}()$ is the inverse of $\text{sig}()$:

$$\text{logit}[\text{sig}(x)] = x \quad (23)$$

0.15 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

$$E_{\underline{x}}[f(\underline{x})] = E_{x \sim P(x)}[f(x)] = \sum_x P(x) f(x) \quad (24)$$

$$\text{Var}_{\underline{x}}[f(\underline{x})] = E_{\underline{x}}[(f(\underline{x}) - E_{\underline{x}}[f(\underline{x})])^2] \quad (25)$$

$$= E_{\underline{x}}[f(\underline{x})^2] - (E_{\underline{x}}[f(\underline{x})])^2 \quad (26)$$

$$E[\underline{x}] = E_{\underline{x}}[\underline{x}] \quad (27)$$

$$\text{Var}[\underline{x}] = \text{Var}_{\underline{x}}[\underline{x}] \quad (28)$$

0.16 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

$$E_{\underline{x}|\underline{y}}[f(\underline{x}, \underline{y})] = \sum_x P(x|\underline{y})f(x, \underline{y}) , \quad (29)$$

$$E_{\underline{x}|\underline{y}=\underline{y}}[f(\underline{x}, \underline{y})] = E_{\underline{x}|\underline{y}}[f(\underline{x}, \underline{y})] = \sum_x P(x|\underline{y})f(x, \underline{y}) . \quad (30)$$

Note that

$$E_{\underline{y}}[E_{\underline{x}|\underline{y}}[f(\underline{x}, \underline{y})]] = \sum_{x,y} P(x|\underline{y})P(\underline{y})f(x, \underline{y}) \quad (31)$$

$$= \sum_{x,y} P(x, \underline{y})f(x, \underline{y}) \quad (32)$$

$$= E_{\underline{x}, \underline{y}}[f(\underline{x}, \underline{y})] . \quad (33)$$

0.17 Law of Total Variance

Claim 1 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

$$\text{Var}_{\underline{x}, \underline{y}}(f) = E_{\underline{y}}[\text{Var}_{\underline{x}|\underline{y}}(f)] + \text{Var}_{\underline{y}}(E_{\underline{x}|\underline{y}}[f]) . \quad (34)$$

In particular,

$$\text{Var}_{\underline{x}}(x) = E_{\underline{y}}[\text{Var}_{\underline{x}|\underline{y}}(x)] + \text{Var}_{\underline{y}}(E_{\underline{x}|\underline{y}}[x]) . \quad (35)$$

proof:

Let

$$A = \sum_y P(y) \left(\sum_x P(x|\underline{y})f \right)^2 . \quad (36)$$

Then

$$Var_{\underline{x}, \underline{y}}(f) = \sum_{x,y} P(x,y) f^2 - \left(\sum_{x,y} P(x,y) f \right)^2 \quad (37)$$

$$= \left\{ \begin{array}{l} \sum_{x,y} P(x,y) f^2 - A \\ + \left(A - \left(\sum_{x,y} P(x,y) f \right)^2 \right) \end{array} \right. \quad (38)$$

$$E_{\underline{y}}[Var_{\underline{x}|\underline{y}}(f)] = \sum_y P(y) \left(\sum_x P(x|y) f^2 - \left(\sum_x P(x|y) f \right)^2 \right) \quad (39)$$

$$= \sum_{x,y} P(x,y) f^2 - A \quad (40)$$

$$Var_{\underline{y}}(E_{\underline{x}|\underline{y}}[f]) = \sum_y P(y) \left(\sum_x P(x|y) f \right)^2 - \left(\sum_y P(y) \sum_x P(x|y) f \right)^2 \quad (41)$$

$$= A - \left(\sum_{x,y} P(x,y) f \right)^2 \quad (42)$$

QED

0.18 Notation for covariances

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

- Mean value of \underline{x}

$$\langle \underline{x} \rangle = E_{\underline{x}}[\underline{x}] \quad (43)$$

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

$$\Delta \underline{x} = \underline{x} - \langle \underline{x} \rangle \quad (44)$$

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

$$Cov(\underline{x}, \underline{y}) = \langle \underline{x}, \underline{y} \rangle = \langle \Delta \underline{x} \Delta \underline{y} \rangle = \langle \underline{x} \underline{y} \rangle - \langle \underline{x} \rangle \langle \underline{y} \rangle \quad (45)$$

$\langle \underline{x}, \underline{y} \rangle$ is bilinear.

- Variance of \underline{x}

$$Var(\underline{x}) = \langle \underline{x}, \underline{x} \rangle \quad (46)$$

- Standard deviation or \underline{x}

$$\sigma_{\underline{x}} = \sqrt{\langle \underline{x}, \underline{x} \rangle} \quad (47)$$

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

$$\rho_{\underline{x}, \underline{y}} = \frac{\langle \underline{x}, \underline{y} \rangle}{\sqrt{\langle \underline{x}, \underline{x} \rangle \langle \underline{y}, \underline{y} \rangle}} \quad (48)$$

0.19 Linear regression, Ordinary Least Squares (OLS)

Wikipedia articles

1. Linear Regression (LR)

- linear regression, Ref.[56]
- simple linear regression, Ref.[70]
- errors in variable, Ref.[43]

2. Least squares (LS)

- least squares, Ref.[55]
- ordinary least squares (OLS), Ref.[67]

In LR, the **dependent variables** y equal a linear combination of some **independent variables** x plus some external noise variables ϵ called the **residuals**.

Below, we consider two types of LR:

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

Once one assumes that certain variables are random, a “model” (i.e., a bnet) for the random variables must be specified.

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.

OLS provides a cost function which when minimized, yields LR. The term OLS is often used to refer to LR of type 1.

0.19.1 LR, assuming x_σ are non-random

Let

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

$y_\sigma \in \mathbb{R}$: dependent variables

$x_{\sigma j} \in \mathbb{R}$: independent variables

$\epsilon_\sigma \in \mathbb{R}$: residuals

β_0, β_j : real coefficients

$$y_\sigma = \beta_0 + \sum_{j=1}^n x_{\sigma j} \beta_j + \epsilon_\sigma \quad (49)$$

If we define

$$x_{\sigma 0} = 1 \quad (50)$$

for all σ , then

$$y_\sigma = \sum_{j=0}^n x_{\sigma j} \beta_j + \epsilon_\sigma . \quad (51)$$

If y and ϵ are $nsam \times 1$ column vectors and β is an $(n + 1) \times 1$ column vector, then can write previous equation in matrix form as:

$$y = X\beta + \epsilon . \quad (52)$$

Define the **projection matrices**

$$\wedge = X(X^T X)^{-1} X^T , \quad \vee = 1 - \wedge \quad (53)$$

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

$$\vee \wedge = \wedge \vee = 0 \quad (54)$$

and

$$\wedge X = X , \quad \vee X = 0 . \quad (55)$$

One has

$$\beta = (X^T X)^{-1} X^T (y - \epsilon) . \quad (56)$$

Define

$$\hat{\beta} = (X^T X)^{-1} X^T y = B y , \quad (57a)$$

$$\hat{y} = X \hat{\beta} = \wedge y , \quad (57b)$$

and

$$\hat{\epsilon} = y - X\hat{\beta} = y - \hat{y} = (1 - \wedge)y = \vee y . \quad (57c)$$

\wedge 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 $\{X, y, \hat{y}, \epsilon, \hat{\epsilon}\}$ are all of order 1 under scaling, $\{\beta, \hat{\beta}, \wedge, \vee\}$ are all of order 0 under scaling, and B is of order -1 under scaling. Thus, the estimator variables (i.e, those with a hat) scale the same way as the variables without a hat that they are estimating. Furthermore, β , its estimator $\hat{\beta}$, and the projection matrices \wedge, \vee are invariant ($\mathcal{O} = 0$) under scaling.

Fig.3 illustrates that y can be expressed as a sum of 2 estimators:

$$y = \underbrace{\hat{y}}_{\wedge y} + \underbrace{\hat{\epsilon}}_{\vee y} . \quad (58)$$

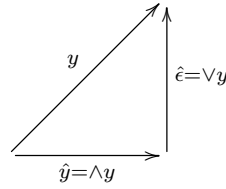


Figure 3: Decomposition of y into sum of two estimators, \hat{y} and $\hat{\epsilon}$.

model dependent results:

Assume the components of ϵ are random over σ and

$$E_{\sigma}[\underline{\epsilon}] = \langle \underline{\epsilon} \rangle = 0 \quad (59)$$

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

$$\langle \underline{y} \rangle = X\beta \quad (60)$$

$$\langle \underline{\hat{y}} \rangle = \wedge \langle \underline{y} \rangle = \langle \underline{y} \rangle \quad (61a)$$

$$\langle \underline{\hat{\epsilon}} \rangle = \vee \langle \underline{y} \rangle = 0 \quad (61b)$$

$$\langle \underline{\hat{\beta}} \rangle = \beta \quad (61c)$$

So far, we have assumed a zero mean value for ϵ . Next, assume “**homoscedasticity**” (**HS**), which means that

$$\langle \underline{\epsilon}, \underline{\epsilon}^T \rangle = \xi^2 I_{nsam} \quad (61d)$$

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

$$\langle \underline{y}, \underline{y}^T \rangle = \langle \underline{\epsilon}, \underline{\epsilon}^T \rangle = \xi^2 I_{nsam} , \quad (62)$$

$$\langle \hat{\underline{\epsilon}}, \hat{\underline{\epsilon}}^T \rangle = \vee \langle \underline{y}, \underline{y}^T \rangle \vee^T = \xi^2 \vee , \quad (63)$$

$$\langle \hat{\underline{y}}, \hat{\underline{y}}^T \rangle = \wedge \langle \underline{y}, \underline{y}^T \rangle \wedge^T = \xi^2 \wedge \quad (64)$$

and

$$\langle \hat{\underline{\beta}}, \hat{\underline{\beta}}^T \rangle = B \langle \underline{y}, \underline{y}^T \rangle B^T = \xi^2 (X^T X)^{-1} . \quad (65)$$

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

$$R^2 = \frac{\| \underline{\hat{y}} - \langle \underline{\hat{y}} \rangle \|^2}{\| \underline{y} - \langle \underline{y} \rangle \|^2} = \frac{\text{tr} \langle \underline{\hat{y}}, \underline{\hat{y}}^T \rangle}{\text{tr} \langle \underline{y}, \underline{y}^T \rangle} \quad (66)$$

If HS holds, then R^2 reduces to

$$R^2 = \frac{\text{tr} \wedge}{nsam} . \quad (67)$$

0.19.2 LR, assuming x_{σ} are random and i.i.d.

Let

\underline{y} = true value
 $\underline{\hat{y}}$ = estimator
 $\underline{\epsilon}$ = residual

$$\underline{\hat{y}} = \beta_0 + \sum_{j=1}^n \beta_j \underline{x}_j \quad (68)$$

$$\underline{y} = \underline{\hat{y}} + \underline{\epsilon} \quad (69)$$

Assume

$$\langle \underline{\epsilon} \rangle = 0 \quad (70)$$

and

$$\langle \underline{x}_j, \underline{\epsilon} \rangle = 0 \quad (71)$$

for all j .

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

$$\langle \underline{x}_k, \underline{y} \rangle = \sum_{j=1}^n \beta_j \langle \underline{x}_k, \underline{x}_j \rangle . \quad (72)$$

Let \underline{x}^n and β^n be column vectors. Then

$$\langle \underline{x}^n, \underline{y} \rangle = \langle \underline{x}^n, (\underline{x}^n)^T \rangle \beta^n , \quad (73)$$

$$\beta^n = \langle \underline{x}^n, (\underline{x}^n)^T \rangle^{-1} \langle \underline{x}^n, \underline{y} \rangle . \quad (74)$$

$$\beta_0 = \langle \underline{y} \rangle - (\beta^n)^T \langle \underline{x}^n \rangle \quad (75)$$

0.20 Short Summary of Boolean Algebra.

See Ref.[38] for more info about this topic.

Suppose $x, y, z \in \{0, 1\}$. Define

$$x \text{ or } y = x \vee y = x + y - xy , \quad (76)$$

$$x \text{ and } y = x \wedge y = xy , \quad (77)$$

and

$$\text{not } x = \bar{x} = 1 - x , \quad (78)$$

where we are using normal addition and multiplication on the right hand sides.¹

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.

Since $x \in \{0, 1\}$,

$$P(\bar{x}) = 1 - P(x) . \quad (79)$$

Clearly, from analyzing the simple event space $(x, y) \in \{0, 1\}^2$,

$$P(x \vee y) = P(x) + P(y) - P(x \wedge y) . \quad (80)$$

¹Note the difference between \vee and modulus 2 addition \oplus . For \oplus (aka 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 1: Boolean Algebra Identities

0.21 Entropy, Kullback-Liebler divergence

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

- Entropy:

$$H(p) = - \sum_x p(x) \ln p(x) \geq 0 \quad (81)$$

- Kullback-Liebler divergence:

$$D_{KL}(p \parallel q) = \sum_x p(x) \ln \frac{p(x)}{q(x)} \geq 0 \quad (82)$$

- Cross entropy:

$$CE(p \rightarrow q) = - \sum_x p(x) \ln q(x) \quad (83)$$

$$= H(p) + D_{KL}(p \parallel q) \quad (84)$$

0.22 Definition of various entropies used in Shannon Information Theory

- (plain) Entropy of \underline{x}

$$H(\underline{x}) = - \sum_x P(x) \ln P(x) \quad (85)$$

This quantity measures the spread of $P_{\underline{x}}$.

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

$$H(\underline{y}|\underline{x}) = - \sum_{x,y} P(x,y) \ln P(y|x) \quad (86)$$

$$= H(\underline{y}, \underline{x}) - H(\underline{x}) \quad (87)$$

This quantity measures the conditional spread of \underline{y} given \underline{x} .

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

$$H(\underline{y} : \underline{x}) = \sum_{x,y} P(x,y) \ln \frac{P(x,y)}{P(x)P(y)} \quad (88)$$

$$= H(\underline{x}) + H(\underline{y}) - H(\underline{y}, \underline{x}) \quad (89)$$

This quantity measures the correlation between \underline{x} and \underline{y} .

- Conditional Mutual Information (CMI)² of \underline{x} and \underline{y} given $\underline{\lambda}$

$$H(\underline{y} : \underline{x}|\underline{\lambda}) = \sum_{x,y,\lambda} P(x,y,\lambda) \ln \frac{P(x,y|\lambda)}{P(x|\lambda)P(y|\lambda)} \quad (90)$$

$$= H(\underline{x}|\underline{\lambda}) + H(\underline{y}|\underline{\lambda}) - H(\underline{y}, \underline{x}|\underline{\lambda}) \quad (91)$$

This quantity measures the conditional correlation of \underline{x} and \underline{y} given $\underline{\lambda}$.

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

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

$$D_{KL}(P_{\underline{x}} \parallel P_{\underline{y}}) = \sum_x P_{\underline{x}}(x) \ln \frac{P_{\underline{x}}(x)}{P_{\underline{y}}(x)} \quad (92)$$

This measures a non-symmetric distance between the probability distributions $P_{\underline{x}}$ and $P_{\underline{y}}$. $D_{KL}(P_{\underline{x}} \parallel P_{\underline{y}})$ is non-negative and equals zero iff $P_{\underline{x}} = P_{\underline{y}}$.

²CMI can be read as “see me”.

Chapter 10

Difference-in-Differences

This chapter is based on Ref.[3].

This chapter assumes that the reader has read Chapter 38 on Potential Outcomes. DID theory applies the basic single-time PO theory described in Chapter 38 to 2 well separated times in which different conditions prevail.

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** (aka a **natural experiment**. See Ref.[65]) 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.

10.1 John Snow, DID and a cholera transmission pathway

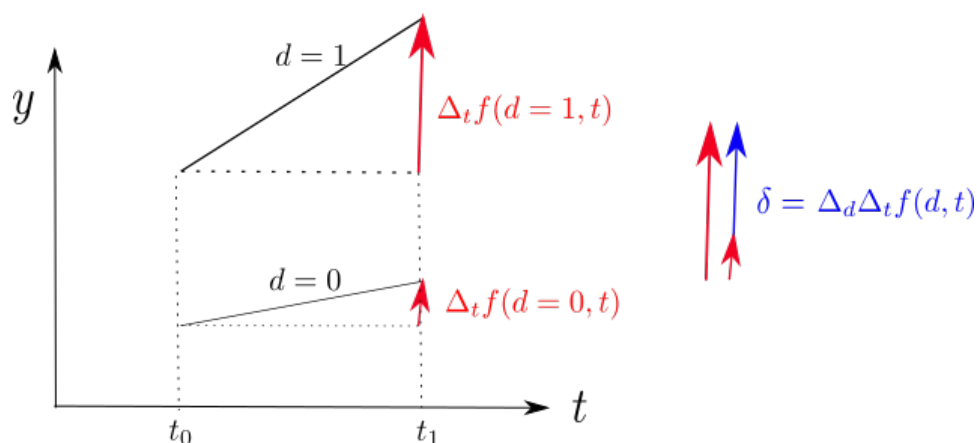


Figure 10.1: Pictorial representation of Difference-in-differences (DID) as a difference of two differences (i.e., a difference of two slopes).

Let

$$\begin{aligned}
d &\in \{0, 1\} \\
t &\in \{t_0, t_1\}, t_0 < t_1 \\
y &= f(d, t) \in \mathbb{R}
\end{aligned}$$

$$\Delta_t f(d, t) = f(d, t_1) - f(d, t_0) \quad (10.1)$$

$$\Delta_d f(d, t) = f(1, t) - f(0, t) \quad (10.2)$$

$$DID = \delta = \Delta_d \Delta_t f(d, t) \quad (10.3)$$

DID is illustrated in Fig.10.1.

A **time series** is any function of time (the domain of the function is usually a discrete set of times).

In DID, one calculates the slope, over the same time interval, of two time series. One of the time series ($d = 0$) is for the control (i.e., untreated) population and the other ($d = 1$) is for the treated population. Then the difference δ of those 2 slopes is taken. The idea is that if there is no causal difference between the 2 time series, then both time series will have the same slope, and δ will be zero.

	$t = t_0$ (1849)	$t = t_1$ (1854)
$\tilde{d} = 1$ (town 1)	85 deaths, polluted DW	19 death, unpolluted DW
$\tilde{d} = 0$ (town 0)	135 deaths, polluted DW	147 deaths, polluted DW

Table 10.1: 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).

A condensation of the data collected by John Snow in 1854 is given in Table 10.1. From that data, we find that

$$\delta = \Delta_d \Delta_t f(d, t) = (19 - 85) - (147 - 135) = -66 - 12 = -78 \quad (10.4)$$

10.2 PO analysis

In this section, we show how to analyze DID using the formalism of PO theory.

We will speak of a treatment outcome $\underline{y}^\sigma(\underline{d}, x^\sigma; t, g^\sigma)$ for individual σ that depends, not just on the treatment dose $\tilde{d}^\sigma \in \{0, 1\}$ and the confounder state x^σ , 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 σ). Actually, we will assume $g^\sigma = \tilde{d}^\sigma$, so we will just speak of $\underline{y}^\sigma(\underline{d}, x^\sigma; t)$ with no explicit g^σ dependence. As usual for PO theory, we will consider expected values of y^σ :

$$E_{\sigma|\underline{d}, x}[y^\sigma(\tilde{d}^\sigma, x^\sigma; t)] = E_{y|\underline{d}, x}[\underline{y}(\underline{d}, x; t)] = \mathcal{Y}_{\underline{d}|x}(t) \quad (10.5)$$

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.10.2. The TPMs, printed in blue, for the two bnets $G(t_0)$ and $G(t_1)$ shown in Fig.10.2, are as follows. Note that the TPMs for the bnets $G(t_0)$ and $G(t_1)$ are defined in terms of the TPMs for the bnet G .

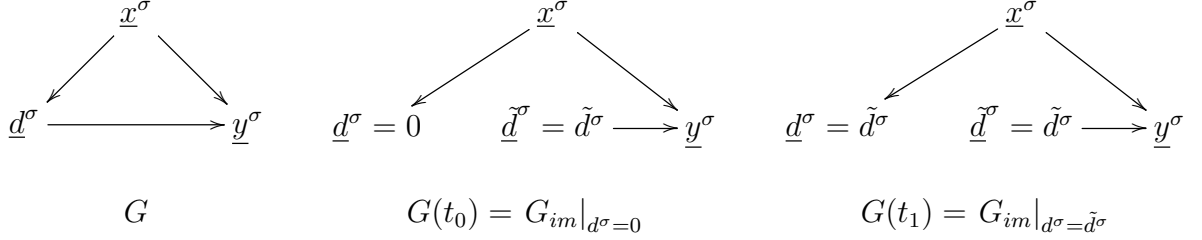


Figure 10.2: Bnet $G_{im} = \kappa_{\underline{d}^\sigma \rightarrow \underline{y}^\sigma}(\tilde{d}^\sigma)G$ is obtained by applying the imagine operator to arrow $\underline{d}^\sigma \rightarrow \underline{y}^\sigma$ of bnet G . Bnet $G_{im}(t_0)$ is obtained by setting $\underline{d}^\sigma = 0$ in bnet G_{im} . Bnet $G_{im}(t_1)$ is obtained by setting $\tilde{\underline{d}}^\sigma = \underline{d}^\sigma$ in bnet G_{im} .

$$P(x^\sigma) = P_{\underline{x}}(x^\sigma) \quad (10.6)$$

$$P(d^\sigma|x^\sigma) = \begin{cases} P_{\underline{d}|\underline{x}}(d^\sigma|x^\sigma)\delta(d^\sigma, 0) & \text{for graph } G(t_0) \\ P_{\underline{d}|\underline{x}}(d^\sigma|x^\sigma)\delta(d^\sigma, \tilde{d}^\sigma) & \text{for graph } G(t_1) \end{cases} \quad (10.7)$$

$$P(y^\sigma|\tilde{d}^\sigma, x^\sigma) = P_{\underline{y}|\tilde{\underline{d}}, \underline{x}}(y^\sigma|\tilde{d}^\sigma, x^\sigma) \quad (10.8)$$

$$P((\tilde{d}^\sigma)') = \delta((\tilde{d}^\sigma)', \tilde{d}^\sigma) \quad (10.9)$$

Henceforth, for simplicity, we will omit the confounder state x from the indices of \mathcal{Y} ; i.e., we will write $\mathcal{Y}_{d|\tilde{d}}(t)$ instead of $\mathcal{Y}_{d|\tilde{d},x}(t)$. The fact that we will not explicitly mention x does not mean that it doesn't exist or that it doesn't affect our analysis. John Snow does not seem to have considered any confounders in his cholera study, or else he tried to collect data restricted to a single stratum x . If there are confounders, they cannot be neglected. As discussed in Chapter 38 under the subject of strata-matching in PO, one must condition \mathcal{Y} on a single x stratum and, later on, one must average over all the possible x strata.

Let $\mathcal{MY}_{d|\tilde{d}}(t)$ denote the **measured** $\mathcal{Y}_{d|\tilde{d}}(t)$. We define this quantity as

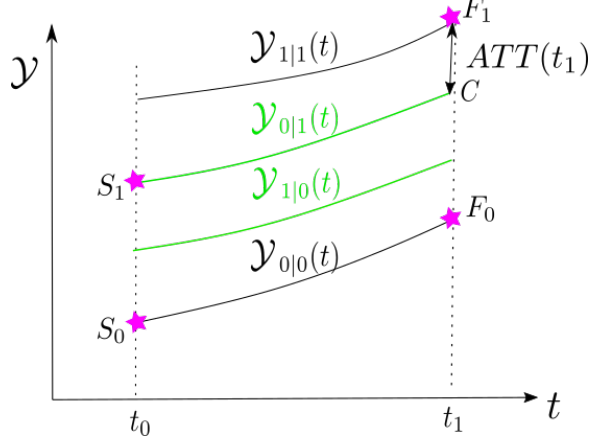


Figure 10.3: Four different time-dependent expected values $\mathcal{Y}_{d|\tilde{d}}(t)$ of y^σ . Bnets $G(t_0)$ and $G(t_1)$ are defined in Fig.10.1. The \mathcal{Y} coordinates of the 2 magenta stars at time $t = t_0$ (resp., $t = t_1$) can be calculated using bnet $G(t_0)$ (resp., $G(t_1)$).

$$\mathcal{MY}_{d|\tilde{d}}(t) = \begin{cases} \mathcal{Y}_{0|\tilde{d}}(t)\mathbb{1}(d=0) & \text{if } t = t_0 \\ \mathcal{Y}_{\tilde{d}|\tilde{d}}(t)\mathbb{1}(d=\tilde{d}) & \text{if } t = t_1 \end{cases} \quad (10.10)$$

$$= \mathcal{Y}_{0|\tilde{d}}(t)\mathbb{1}(d=0, t=t_0) + \mathcal{Y}_{\tilde{d}|\tilde{d}}(t)\mathbb{1}(d=\tilde{d}, t=t_1) \quad (10.11)$$

Now we claim that the DID δ calculated in the previous section for John Snow's data, can be expressed in PO formalism as follows:

$$\delta = \Delta_{\tilde{d}}\Delta_t \sum_d \mathcal{MY}_{d|\tilde{d}}(t) . \quad (10.12)$$

Fig.10.3 depicts the four functions $\mathcal{Y}_{d|\tilde{d}}(t)$ for t in the interval $[t_0, t_1]$ and for $d, \tilde{d} \in \{0, 1\}$. The \mathcal{Y} coordinates of the four magenta stars in Fig.10.3 can be calculated using bnets $G(t_0)$ and $G(t_1)$.

Define the **parallel trends** (PT) by

$$PT = \Delta_{\tilde{d}}\Delta_t \mathcal{Y}_{0|\tilde{d}}(t) . \quad (10.13)$$

We will say the **parallel trends assumption (PTA)** holds if $PT = 0$.

Next we prove that the DID δ equals the sum of an ATT^1 and PT.

¹ATT stands for the average treatment effect of the treated. ATT is defined in Chapter 38

$$\delta = \Delta_{\tilde{d}} \Delta_t \sum_d \mathcal{M} \mathcal{Y}_{d|\tilde{d}}(t) \quad (10.14)$$

$$= \sum_d [\Delta_t \mathcal{M} \mathcal{Y}_{d|1}(t) - \Delta_t \mathcal{M} \mathcal{Y}_{d|0}(t)] \quad (10.15)$$

$$= \sum_d [\mathcal{M} \mathcal{Y}_{d|1}(t_1) - \mathcal{M} \mathcal{Y}_{d|1}(t_0)] - \sum_d [\Delta_t \mathcal{M} \mathcal{Y}_{d|0}(t_1) - \Delta_t \mathcal{M} \mathcal{Y}_{d|0}(t_0)] \quad (10.16)$$

$$= \mathcal{Y}_{1|1}(t_1) - \mathcal{Y}_{0|1}(t_0) - \{\mathcal{Y}_{0|0}(t_1) - \mathcal{Y}_{0|0}(t_0)\} \quad (10.17)$$

$$= \mathcal{Y}_{1|1}(t_1) - \mathcal{Y}_{0|1}(t_0) - \{\mathcal{Y}_{0|0}(t_1) - \mathcal{Y}_{0|0}(t_0)\} + \underbrace{\{\mathcal{Y}_{0|1}(t_1) - \mathcal{Y}_{0|1}(t_1)\}}_{\text{zero}} \quad (10.18)$$

$$= \underbrace{\mathcal{Y}_{1|1}(t_1) - \mathcal{Y}_{0|1}(t_1)}_{ATT(t_1)} - \mathcal{Y}_{0|1}(t_0) - \{\mathcal{Y}_{0|0}(t_1) - \mathcal{Y}_{0|0}(t_0)\} + \mathcal{Y}_{0|1}(t_1) \quad (10.19)$$

$$= ATT(t_1) - \Delta_t \mathcal{Y}_{0|0}(t) + \Delta_t \mathcal{Y}_{0|1}(t) \quad (10.20)$$

$$= ATT(t_1) + \underbrace{\Delta_{\tilde{d}} \Delta_t \mathcal{Y}_{0|\tilde{d}}(t)}_{\text{zero if PTA holds}} \quad (10.21)$$

10.3 Linear Regression

In this section, we show how to apply linear regression (LR) to the PO analysis of DID.

As before, let y^σ be the treatment outcome for individual σ , who receives a treatment dose \tilde{d}^σ at times $t \in \{t_0, t_1\}$. $y^\sigma(\tilde{d}^\sigma; t)$ can be fitted as follows. Here ϵ^σ is the residual for individual σ and $b_0, m_0, b_1, m_1 \in \mathbb{R}$ are the fit parameters.

$$y^\sigma = [b_0 + m_0 t](1 - \tilde{d}^\sigma) + [b_1 + m_1 t]\tilde{d}^\sigma + \epsilon^\sigma. \quad (10.22)$$

Note that Eq.(10.22) yields a straight line in the $y^\sigma - t$ plane for $d^\sigma = 0$, and another straight line for $d^\sigma = 1$. 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.(10.22), we get

$$\mathcal{Y}_{d|\tilde{d}}(t) = [b_0 + m_0 t](1 - \tilde{d}) + [b_1 + m_1 t]\tilde{d}. \quad (10.23)$$

with $d = 0$ for $t = t_0$ and $d = \tilde{d}$ for $t = t_1$.

Let $T = t_1 - t_0$. Since $\Delta_t t = T$ and $\Delta_d d = 1$, one gets

$$\delta = \Delta_d \Delta_t \mathcal{M} \mathcal{Y}_{d|\tilde{d}}(t) = \Delta_d \Delta_t y^\sigma = (m_1 - m_0)T. \quad (10.24)$$

Figs.10.3 and 10.4 define points S_0, S_1, F_0, F_1, I, C . The \mathcal{Y} coordinates of points S_0, S_1, F_0, F_1 are given by Table 10.2. The \mathcal{Y} coordinates of points C, I are given by Eqs.10.25.

$$\mathcal{Y}(C) = \mathcal{Y}_{0|1}(t_1) \quad (10.25a)$$

Chapter 21

Instrumental Inequality and beyond

This chapter is based on Refs. [4] and [19].

Instrumental Variables (IVs) are discussed in Chapter 22. 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} .

21.1 I-inequality

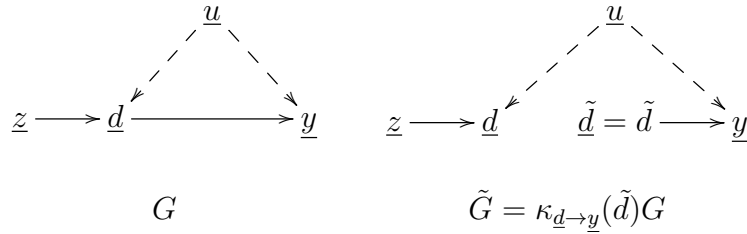


Figure 21.1: In bnet G , an IV \underline{z} acts on a treatment $\underline{d} \rightarrow \underline{y}$. Bnet \tilde{G} is obtained by applying an imagine operator to arrow $\underline{d} \rightarrow \underline{y}$ of bnet G .

Claim 18 *The TPMs for the bnet G in Fig.21.1 satisfy*

$$\max_d \sum_y \max_z P(d, y|z) \leq 1 \quad (21.1)$$

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

$$P(d, y|z) = \sum_u P(u)P(y|u, d)P(d|u, z) , \quad (21.2)$$

and \tilde{G} satisfies

$$P(d, y|z, \tilde{d}) = \sum_u P(u)P(y|u, \tilde{d})P(d|u, z) . \quad (21.3)$$

Note that Eqs.(21.2) and (21.3) imply that

$$P(d, y|z, d) = P(d, y|z) \quad (21.4)$$

and that

$$\boxed{P(\tilde{d}, y|z, \tilde{d}) \leq \sum_d P(d, y|z, \tilde{d}) = P(y|\tilde{d})} . \quad (21.5)$$

Thus,

$$\max_{\tilde{d}} \sum_y \max_z P(\tilde{d}, y|z, \tilde{d}) \leq \max_{\tilde{d}} \sum_y \max_z P(y|\tilde{d}) \quad (21.6)$$

$$\leq \max_{\tilde{d}} \sum_y P(y|\tilde{d}) \quad (21.7)$$

$$\leq \max_{\tilde{d}} 1 \quad (21.8)$$

$$\leq 1 \quad (21.9)$$

QED

As pointed out in Ref.[4] from which I learned the above proof, the above proof is highly generalizable.

Fig.21.2 gives a graphical representation of the boxed Eq.(21.5) 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: $\sum_d M_{d,\tilde{d}} \geq M_{\tilde{d},\tilde{d}}$.

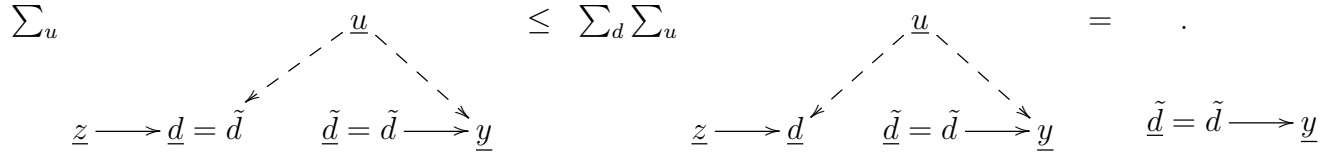


Figure 21.2: Graphical representation of the boxed equation Eq.(21.5).

$$P(d = 1, y|z) = \begin{array}{c} z = 0 \quad z = 1 \\ y = 0 \quad \begin{array}{|c|c|} \hline a & b \\ \hline \end{array} \\ y = 1 \quad \begin{array}{|c|c|} \hline c & d \\ \hline \end{array} \end{array}$$

$$a + d \leq 1$$

$$b + c \leq 1$$

Figure 21.3: I-inequality for binary $\underline{z}, \underline{d}, \underline{y}$. The same picture except with $d = 0$ is also true.

21.1.1 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.

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.

$$\sum_{y=0}^1 \sum_{z=0}^1 \mathbb{1}(y = z) P(d, y|z) , \quad (21.10a)$$

$$\sum_{y=0}^1 \sum_{z=0}^1 \mathbb{1}(y \neq z) P(d, y|z) . \quad (21.10b)$$

One gets an additional 2 inequalities by setting $d = 0$ in Eqs.(21.10). These 4 inequalities are illustrated in Fig.21.3.

What do they mean? That at fixed \underline{d} , the correlation between \underline{z} and \underline{y} is limited.

21.2 Bounds on Effect of IV on treatment outcome \underline{y}

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 $\underline{d} \in \{0, 1\}$.

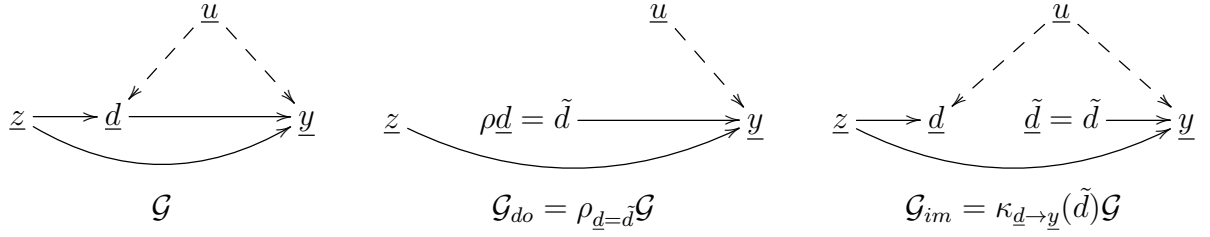


Figure 21.4: Bnet \mathcal{G} is obtained from the bnet G in Fig.21.1 by adding to G an arrow from the IV \underline{z} to the treatment outcome \underline{y} . Bnet \mathcal{G}_{do} is obtained by applying a do operator to node \underline{d} of \mathcal{G} . Bnet \mathcal{G}_{im} is obtained by applying an imagine operator to arrow $\underline{d} \rightarrow \underline{y}$ of \mathcal{G} .

Below, we will use the following 3 shorthand notations:

$$P_{y|z}(d) = P(d, y|z) , \quad (21.11)$$

$$P_{|z}(d) = \sum_y P(d, y|z) , \quad (21.12)$$

and

$$\pi_{|z}(d) = 1 - P_{|z}(d) . \quad (21.13)$$

For the bnet \mathcal{G}_{do} in Fig.21.4, define the IV effect at fixed $\rho\underline{d} = \tilde{d}$ by

$$IVE(\tilde{d}) = P(y = 1|z = 1, \rho\underline{d} = \tilde{d}) - P(y = 1|z = 0, \rho\underline{d} = \tilde{d}) . \quad (21.14)$$

Claim 19 *The TPMs for the bnet \mathcal{G}_{do} in Fig.21.4 satisfy*

$$\pi_{|0}(d) \leq [IVE(d) - \{P_{1|1}(d) - P_{1|0}(d)\}] \leq \pi_{|1}(d) \quad (21.15)$$

proof:

$$P(y|z, \rho\underline{d} = \tilde{d}) = \sum_u P(u)P(y|u, z, \tilde{d}) \quad (21.16)$$

$$= \sum_u P(u) \sum_d P(d, y|u, z, \tilde{d}) \quad (21.17)$$

$$\geq \sum_u P(u)P(\tilde{d}, y|u, z, \tilde{d}) \quad (21.18)$$

$$= \sum_u P(u)P(\tilde{d}, y|u, z) \quad (21.19)$$

$$= P_{y|z}(\tilde{d}) \quad (21.20)$$

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 ≤ 1 :

$$\sum_{d \neq \tilde{d}} P(d, y|z, \tilde{d}) + \underbrace{\sum_{y'} P(\tilde{d}, y'|z, \tilde{d})}_{P_{|z}(\tilde{d})} \leq 1 . \quad (21.21)$$

Using the definitions of $P_{|z}$ and $\pi_{|z}$, we can rewrite the last equation as

$$\sum_{d \neq \tilde{d}} P(d, y|z, \tilde{d}) \leq \pi_{|z}(\tilde{d}) . \quad (21.22)$$

Next note that

$$P(y|z, \rho \underline{d} = \tilde{d}) = \sum_u P(u) P(y|u, z, \tilde{d}) \quad (21.23)$$

$$= \sum_u P(u) \sum_d P(d, y|u, z, \tilde{d}) \quad (21.24)$$

$$= P(\tilde{d}, y|z, \tilde{d}) + \sum_{d \neq \tilde{d}} P(d, y|z, \tilde{d}) \quad (21.25)$$

$$= P_{y|z}(\tilde{d}) + \sum_{d \neq \tilde{d}} P(d, y|z, \tilde{d}) \quad (21.26)$$

$$\leq P_{y|z}(\tilde{d}) + \pi_{|z}(\tilde{d}) . \quad (21.27)$$

Hence,

$$P_{y|z}(\tilde{d}) \leq P(y|z, \rho \underline{d} = \tilde{d}) \leq P_{y|z}(\tilde{d}) + \pi_{|z} \quad (21.28)$$

$$P_{1|1}(\tilde{d}) \leq P(y = 1|z = 1, \rho \underline{d} = \tilde{d}) \leq P_{1|1}(\tilde{d}) + \pi_{|1} \quad (21.29)$$

$$-P_{1|0}(\tilde{d}) - \pi_{|0} \leq -P(y = 1|z = 0, \rho \underline{d} = \tilde{d}) \leq -P_{1|0}(\tilde{d}) \quad (21.30)$$

QED

Chapter 22

Instrumental Variables

This chapter is based on Refs.[3] and [50].

The theory of potential outcomes (PO) discussed in Chapter 38 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 13).

Most of the discussion in this chapter is limited to LDEN (linear deterministic bnets with external noise). These are discussed in Chapter 26. However, as will become obvious to the reader, IVs are also applicable and useful in general bnet modeling.

22.1 δ with unmeasured confounder

In this section, we explain using LDENs why unmeasured confounders prejudice PO calculations.

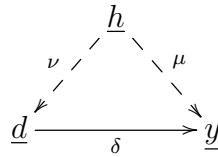


Figure 22.1: An LDEN bnet. The direct path $\underline{d} \rightarrow \underline{y}$ is confounded by a hidden variable \underline{h} .

Consider the LDEN bnet of Fig.22.1, For some $\delta, \mu \in \mathbb{R}$, we have

$$\underline{y} = \delta \underline{d} + \underbrace{\mu \underline{h} + \underline{u}_y}_{\underline{n}_y} . \quad (22.1)$$

If $\langle \underline{n}_y, \underline{d} \rangle = 0$, then

$$\langle \underline{y}, \underline{d} \rangle = \delta_0 \langle \underline{d}, \underline{d} \rangle , \quad (22.2)$$

whereas if $\langle \underline{n}_y, \underline{d} \rangle \neq 0$, then

$$\langle \underline{y}, \underline{d} \rangle = \delta_1 \langle \underline{d}, \underline{d} \rangle + \langle \underline{n}_y, \underline{d} \rangle . \quad (22.3)$$

Therefore,

$$\delta_0 = \frac{\langle \underline{y}, \underline{d} \rangle}{\langle \underline{d}, \underline{d} \rangle} , \quad (22.4)$$

$$\delta_1 = \underbrace{\frac{\langle \underline{y}, \underline{d} \rangle}{\langle \underline{d}, \underline{d} \rangle}}_{\delta_0} - \frac{\langle \underline{n}_y, \underline{d} \rangle}{\langle \underline{d}, \underline{d} \rangle} . \quad (22.5)$$

If we assume no confounders and there is one, this gives the difference between the estimate δ_1 of δ for the truth, versus the naive estimate δ_0 .

If the confounder \underline{h} had been measured, then we would calculate the covariances at fixed \underline{n}_y , and the conditional covariance $\langle \underline{n}_y, \underline{d} \rangle_{|\underline{n}_y} = 0$

22.2 δ (with unmeasured confounder) can be inferred via IV

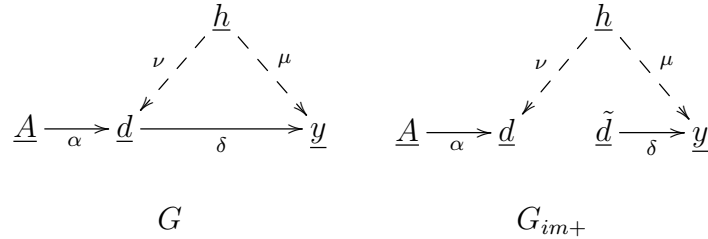


Figure 22.2: Two LDEN bnets. The direct path $\underline{d} \rightarrow \underline{y}$ is confounded by a hidden variable \underline{h} , but by using the IV \underline{A} , we are still able to identify (i.e. calculate) δ .

Now consider the two LDEN bnets shown in Fig.22.2. Note that there are no arrows $\underline{A} \rightarrow \underline{y}$ or $\underline{A} \rightarrow \underline{h}$. Note that node \underline{d} is a collider in the path $\underline{A} - \underline{d} - \underline{h} - \underline{y}$, 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.

$$\underline{d} \perp_G \underline{y} = \text{false}, \quad \underline{A} \perp_G \underline{y} = \text{false} . \quad (22.6)$$

$$\underline{d} \perp_{G_{im+}} \underline{y} = \text{false}, \quad \underline{A} \perp_{G_{im+}} \underline{y} = \text{true} . \quad (22.7)$$

The following is true for G :

$$\underline{y} = \delta \underline{d} + \underbrace{\mu \underline{h} + \underline{u}_y}_{\underline{n}_y} \quad (22.8)$$

$$\underline{d} = \alpha \underline{A} + \underbrace{\nu \underline{h} + \underline{u}_d}_{\underline{n}_d} . \quad (22.9)$$

Since $\langle \underline{n}_y, \underline{A} \rangle = \langle \underline{n}_d, \underline{A} \rangle = 0$ is true in G , we have

$$\langle \underline{y}, \underline{A} \rangle = \delta \langle \underline{d}, \underline{A} \rangle \quad (22.10)$$

and

$$\langle \underline{d}, \underline{A} \rangle = \alpha \langle \underline{A}, \underline{A} \rangle . \quad (22.11)$$

Note that $\langle \underline{y}, \underline{A} \rangle = \delta = 0$ for G_{im+} but not for G , so we are speaking about G from here on. It follows that

$$\alpha = \frac{\langle \underline{d}, \underline{A} \rangle}{\langle \underline{A}, \underline{A} \rangle} \quad (22.12)$$

and

$$\delta = \frac{\langle \underline{y}, \underline{A} \rangle}{\langle \underline{d}, \underline{A} \rangle} \quad (22.13)$$

$$= \frac{\langle \underline{y}, \underline{A} \rangle}{\langle \underline{A}, \underline{A} \rangle} \frac{\langle \underline{A}, \underline{A} \rangle}{\langle \underline{d}, \underline{A} \rangle} \quad (22.14)$$

$$= \frac{\langle \underline{y}, \underline{A} \rangle}{\langle \underline{A}, \underline{A} \rangle} \frac{1}{\alpha} \quad (22.15)$$

$$= \frac{\langle \underline{y}, \alpha \underline{A} \rangle}{\langle \alpha \underline{A}, \alpha \underline{A} \rangle} . \quad (22.16)$$

22.3 More general bnets with IVs

Figs.22.3 and 22.4 are examples of other bnets for which the effect δ is identifiable thanks to the IV \underline{A} .

22.4 Instrumental Inequality

Pearl's instrumental inequality and related inequalities are discussed in Chapter 21.

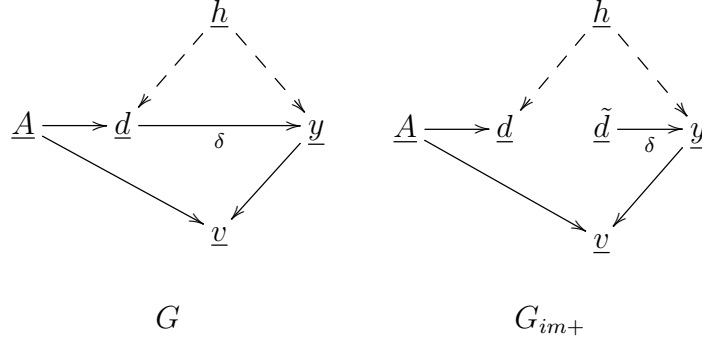


Figure 22.3: The 2 paths in G_{im+} from IV variable \underline{A} to \underline{y} are blocked by colliders \underline{v} and \underline{d} . Thus, $\underline{d} \perp_{G_{im+}} \underline{y} = \text{false}$, $\underline{A} \perp_{G_{im+}} \underline{y} = \text{true}$

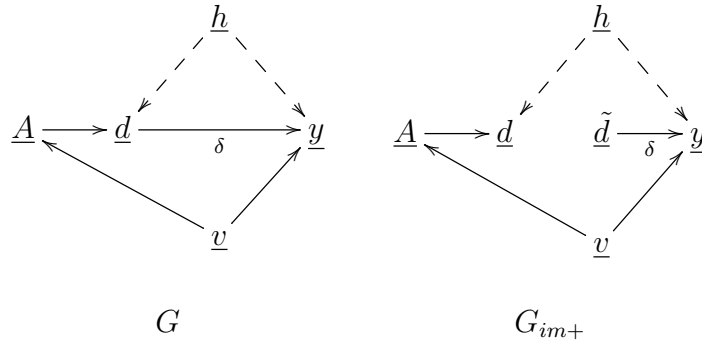


Figure 22.4: There are 2 paths in G_{im+} from IV variable \underline{A} to \underline{y} . One is blocked by the collider \underline{d} and the other can be blocked by conditioning on \underline{v} . Thus, $\underline{d} \perp_{G_{im+}} \underline{y} | \underline{v} = \text{false}$, $\underline{A} \perp_{G_{im+}} \underline{y} | \underline{v} = \text{true}$

Chapter 38

Potential Outcomes

This chapter is based on Ref.[3], 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 refuses to 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 that we discuss in Chapter 13 is especially useful in this regard.

In this chapter, we stress the connection of PO theory to bnets, and, in particular, to the do and imagine operators defined in Chapter 8. Hence, before reading this chapter, the reader is expected to have at least skimmed Chapter 8, so that he/she understands the definition of do and imagine operators.

σ	\underline{d}^σ	y^σ	$(1 - \underline{d}^\sigma)y^\sigma$	$\underline{d}^\sigma y^\sigma$
Andy	1	10	.	10
Ben	1	5	.	5
Chad	1	16	.	16
Daniel	1	3	.	3
Edith	0	5	5	.
Frank	0	7	7	.
George	0	8	8	.
Hank	0	10	10	.

Table 38.1: Dataset describing whether individual σ took a treatment dose ($d^\sigma = 1$) or didn’t ($d^\sigma = 0$). The treatment outcome is measured by the real number y^σ .

Suppose a **population of individuals** $\sigma = 0, 1, 2, \dots, nsam - 1$ is given ($d^\sigma = 1$) or not given ($d^\sigma = 0$) a **treatment drug dose** d^σ , and that the **treatment outcome (i.e., response)** is measured by a real number y^σ . Table 38.1 gives a possible dataset for this scenario. As you can see from that table, each individual either takes a drug dose or doesn’t, but not both. PO theory can be viewed as a **missing data (MD) problem**. MD problems are discussed in Chapter 31. However, the PO MD problem is much more specialized than the generic MD problems discussed

in Chapter 31. 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 38.1 nx extra columns giving the value of the feature vector x^σ for each individual. Members of a population with the same x^σ are referred to as a **subpopulation or stratum (ie., layer)**.

In a **randomized clinical trial (RCT)**, the effect of the variable x^σ on the value of d^σ is eliminated by randomizing the population and therefore making the effect of x^σ average out to zero. However, there are many situations in which carrying out an RCT is not possible. PO theory is a way of predicting the result of an RCT in situations where doing a real RCT is not physically possible.

In this chapter, x^σ 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^σ 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 22 for a discussion of **instrumental variables**.

38.1 G and G_{den} , bnets, the starting point bnets

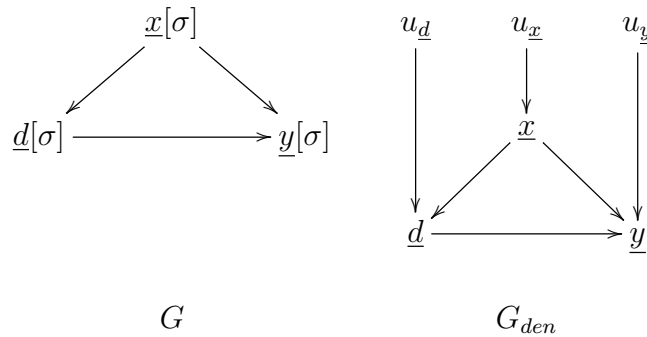


Figure 38.1: Bnets G and G_{den} are our starting point in discussing PO theory. G is for a single individual σ of the population. Bnet G_{den} is the DEN counterpart to G . DEN (Deterministic with External Noise) bnets are discussed in Chapter 26.

In this chapter, we will abbreviate $\underline{X}[\sigma] = \underline{X}^\sigma$ for $X \in \{d, x, y\}$ and for $\sigma = \{0, 1, 2, \dots, nsam - 1\}$.

For each individual (aka unit, sample) $\sigma = 0, 1, 2, \dots, nsam - 1$, let:

$\underline{d}^\sigma \in \{0, 1\}$: treatment discrete drug dose, 1 if treated and 0 if untreated

$\underline{y}^\sigma \in \mathbb{R}$: treatment potential outcome

\underline{x}^σ : column vector of treatment confounders (aka covariates, because they are often used as covariates (i.e., independent variables) in linear regression.)

Consider bnets G and G_{den} in Fig.38.1. G reflects the language used in Ref.[3] 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.

$$\underline{X}^\sigma \leftrightarrow \underline{X}(\underline{u}) \text{ for } X \in \{d, x, y\}.$$

$$P(\sigma) = \frac{1}{n_{sam}} \leftrightarrow P(u)$$

$$\sum_\sigma P(\sigma)(\cdot) \leftrightarrow \sum_u P(u)(\cdot)$$

The TPMs, printed in blue, for the bnet G in Fig.38.1, are as follows:

$$P(x^\sigma) = P_{\underline{x}}(x^\sigma) \quad (38.1)$$

$$P(d^\sigma | x^\sigma) = P_{\underline{d}|\underline{x}}(d^\sigma | x^\sigma) \quad (38.2)$$

$$P(y^\sigma | x^\sigma, d^\sigma) = P_{\underline{y}|\underline{x},\underline{d}}(y^\sigma | x^\sigma, d^\sigma) \quad (38.3)$$

Now let:

$\underline{d} \in \{0, 1\}$: treatment discrete drug dose, 1 if treated and 0 if untreated

$\underline{y} \in \mathbb{R}$: treatment potential outcome

\underline{x} : column vector of treatment confounders (aka covariates)

$\underline{u} = (\underline{u}_d, \underline{u}_x, \underline{u}_y)$: external noise

The TPMs, printed in blue, for the bnet G_{den} in Fig.38.1, are as follows:

$$P(x | \underline{u}_x) = \mathbb{1}(x = \underline{u}_x) \quad (38.4)$$

$$P(d | x, \underline{u}_d) = \mathbb{1}(d = \underline{f}_d(x, \underline{u}_d)) \quad (38.5)$$

$$P(y | d, x, \underline{u}_y) = \mathbb{1}(y = \underline{f}_y(d, x, \underline{u}_y)) \quad (38.6)$$

If we linearize \underline{f}_y in Eq.(38.6), we get

$$\underline{y} = \delta \underline{d} + \beta \underline{x} + \underline{u}_y, \quad (38.7)$$

where $\delta, \beta \in \mathbb{R}$. Assuming that $\underline{x}, \underline{y} \in \mathbb{R}$ and $\underline{d} \in \{0, 1\}$, Eq.(38.7) can be plotted. The resulting plot is given in Fig.38.2. 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 in the experiment experiences either $y(1)$ or $y(0)$, but not both.

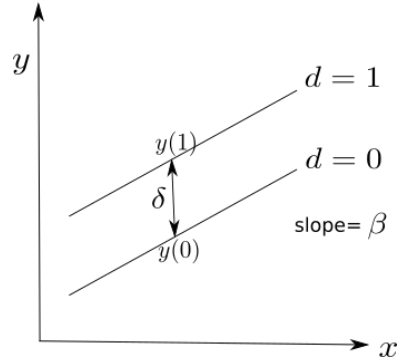


Figure 38.2: Plot of Eq.(38.7)

38.2 G_{do+} bnet

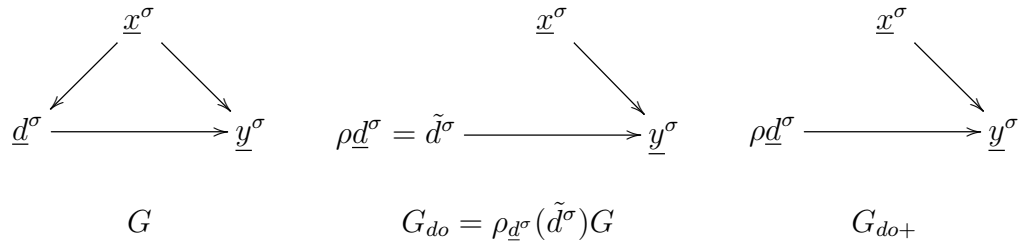


Figure 38.3: Bnet $G_{do} = \rho_{\underline{d}^\sigma}(\tilde{d}^\sigma)G$ is obtained by applying the do operator to node \underline{d}^σ of bnet G . Bnet G_{do+} is obtained by adding a prior probability distribution $P(\tilde{d}^\sigma)$ to node $\rho_{\underline{d}^\sigma}$ of bnet G_{do} .

Fig.38.3 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}^σ has been stripped of all outside influences and fixed to a specific state \tilde{d}^σ . 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 .

$$P(x^\sigma) = P_{\underline{x}}(x^\sigma) \quad (38.8)$$

$$P_{\rho_{\underline{d}}}(d) = \sum_x P_{\underline{d}|\underline{x}}(d|x)P_{\underline{x}}(x) \quad (38.9)$$

$$P(\tilde{d}^\sigma) = \begin{cases} \delta(\tilde{d}^\sigma, (\tilde{d}^\sigma)') & \text{for } G_{do} \\ P_{\rho\tilde{d}}(\tilde{d}^\sigma) & \text{for } G_{do+} \end{cases} \quad (38.10)$$

$$P(y^\sigma | x^\sigma, \tilde{d}^\sigma) = P_{\underline{y}|\underline{x},\underline{\tilde{d}}}(y^\sigma | x^\sigma, \tilde{d}^\sigma) \quad (38.11)$$

It is convenient to define the following expected values of \underline{y}^σ in terms of the TPMs of bnet G_{do+} :

$$\mathcal{Y}_{|\tilde{d},x} = E_{\sigma|\tilde{d},x}[\underline{y}^\sigma(\tilde{d})] \rightarrow E_{y|\tilde{d},x}[\underline{y}(\tilde{d})] = \sum_y y P(y|\tilde{d}, x) \quad (38.12)$$

$$\mathcal{Y}_{|\tilde{d}} = E_{\sigma|\tilde{d}}[\underline{y}^\sigma(\tilde{d})] \rightarrow E_{y|\tilde{d}}[\underline{y}(\tilde{d})] = \sum_x \mathcal{Y}_{|\tilde{d},x} P(x) \quad (38.13)$$

$$\mathcal{Y}_{|x} = E_{\sigma|x}[\underline{y}^\sigma(\tilde{d})] \rightarrow E_{y|x}[\underline{y}(\tilde{d})] = \sum_{\tilde{d}} \mathcal{Y}_{|\tilde{d},x} P(\tilde{d}) \quad (38.14)$$

$$\mathcal{Y} = E_\sigma[\underline{y}^\sigma] \rightarrow E[\underline{y}] = \sum_{\tilde{d},x} \mathcal{Y}_{|\tilde{d},x} P(\tilde{d}) P(x) \quad (38.15)$$

38.3 G_{im+} bnet

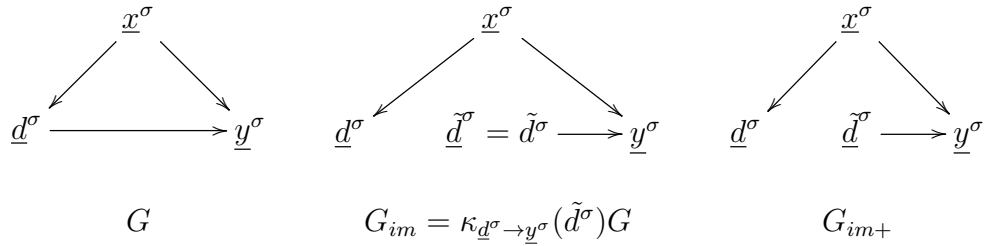


Figure 38.4: Bnet $G_{im} = \kappa_{\underline{d}^\sigma \rightarrow \underline{y}^\sigma}(\tilde{d}^\sigma)G$ is obtained by applying the imagine operator to arrow $\underline{d}^\sigma \rightarrow \underline{y}^\sigma$ of bnet G . Bnet G_{im+} is obtained by adding a prior probability distribution $P(\tilde{d}^\sigma)$ to node $\underline{\tilde{d}}^\sigma$ of bnet G_{im} .

Fig.38.4 shows how bnet G_{im} is obtained by applying an imagine operator to bnet G , and how bnet G_{im+} is obtained from bnet G_{im} by adding a prior probability distribution to one of the nodes of G_{im} . $\underline{d} \in \{0, 1\}$ represents the dose that a patient is told to take by a doctor, and $\tilde{d} \in \{0, 1\}$ represents the dose he actually takes. If $\underline{d} = \tilde{d}$, the patient is compliant, and if $\underline{d} \neq \tilde{d}$, he is non-compliant.

It is convenient to define $\underline{y}^\sigma(\tilde{d}^\sigma)$ so that

$$\underline{y}^\sigma(\tilde{d}^\sigma) = \underline{y}_{G_{im}}^\sigma \quad (38.16)$$

and

$$\underline{y}^\sigma = \underline{y}^\sigma(\tilde{d}^\sigma) = \underline{y}^\sigma(1)\tilde{d}^\sigma + \underline{y}^\sigma(0)(1 - \tilde{d}^\sigma) . \quad (38.17)$$

The TPMs, printed in blue, for the nodes of bnets G_{im} and G_{im+} , are as follows. Note that the TPMs for bnets G_{im} and G_{im+} are defined in terms of the TPMs of bnet G . Note that the prior $P(\tilde{d})$ is not arbitrary; it's calculated from the TPMs of bnet G .

$$P(x^\sigma) = P_{\underline{x}}(x^\sigma) \quad (38.18)$$

$$P(d^\sigma|x^\sigma) = P_{\underline{d}|\underline{x}}(d^\sigma|x^\sigma) \quad (38.19)$$

$$\pi_{\tilde{d}} = P(\tilde{d}) = \sum_x P_{\underline{d}|\underline{x}}(\tilde{d}|x) P_{\underline{x}}(x) \quad (38.20)$$

$$P(\tilde{d}^\sigma) = \begin{cases} \delta(\tilde{d}^\sigma, (\tilde{d}^\sigma)') & \text{for } G_{im} \\ \pi_{\tilde{d}^\sigma} & \text{for } G_{im+} \end{cases} \quad (38.21)$$

$$P(y^\sigma(\tilde{d}^\sigma)|x^\sigma, \tilde{d}^\sigma) = P_{\underline{y}|\underline{x}, \underline{d}}(y^\sigma(\tilde{d}^\sigma)|x^\sigma, \tilde{d}^\sigma) \quad (38.22)$$

It is convenient to define the following expected values of \underline{y}^σ in terms of the TPMs of bnet G_{im+} :

$$\mathcal{Y}_{d|\tilde{d},x} = E_{\sigma|d,\tilde{d},x}[\underline{y}^\sigma(\tilde{d})] \rightarrow E_{y|d,\tilde{d},x}[\underline{y}(\tilde{d})] = \sum_y y P(y|\tilde{d},x) P(d|x) \quad (38.23)$$

$$\mathcal{Y}_{d|\tilde{d}} = E_{\sigma|d,\tilde{d}}[\underline{y}^\sigma(\tilde{d})] \rightarrow E_{y|d,\tilde{d}}[\underline{y}(\tilde{d})] = \sum_x \mathcal{Y}_{d|\tilde{d},x} P(x) \quad (38.24)$$

$$\mathcal{Y}_{d|x} = E_{\sigma|d,x}[\underline{y}^\sigma(\tilde{d})] \rightarrow E_{y|d,x}[\underline{y}(\tilde{d})] = \sum_{\tilde{d}} \mathcal{Y}_{d|\tilde{d},x} P(\tilde{d}) \quad (38.25)$$

$$\mathcal{Y}_d = E_{\sigma|d}[\underline{y}^\sigma(\tilde{d})] \rightarrow E_{y|d}[\underline{y}(\tilde{d})] = \sum_{\tilde{d},x} \mathcal{Y}_{d|\tilde{d},x} P(\tilde{d}) P(x) \quad (38.26)$$

$\mathcal{Y}_{0|0}, \mathcal{Y}_{1|1}$ 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).

38.4 Translation Dictionary

In standard PO notation	In our notation (for G_{im+} , unless otherwise specified)
i , individual (i.e., unit, sample) index	σ
$D_i = d_i$, treatment dose	$\underline{d}^\sigma = d^\sigma$
$Y_i = y_i$, treatment outcome	$\underline{y}^\sigma = y^\sigma$
$X_i = x_i$, treatment confounders	$\underline{x}^\sigma = x^\sigma$
$Y_i(\tilde{d})$	$\underline{y}^\sigma = \underline{y}^\sigma(\tilde{d})$ for G_{im}
$E[Y_i(d)]$	$E_\sigma[\underline{y}^\sigma(d)] = \mathcal{Y}_d$
$E[Y_i D_i = \tilde{d}]$	$E_{\sigma \tilde{d}}[\underline{y}^\sigma] = \mathcal{Y}_{ \tilde{d}}$
$E[Y_i(d) D_i = \tilde{d}]$	$E_{\sigma d,\tilde{d}}[\underline{y}^\sigma] = \mathcal{Y}_{d \tilde{d}}$
$E[Y_i(d) D_i = \tilde{d}, X = x]$	$E_{\sigma d,\tilde{d},x}[\underline{y}^\sigma] = \mathcal{Y}_{d \tilde{d},x}$

Table 38.2: Dictionary for translating from standard PO notation of Ref.[3] to our notation.

Table 38.2 gives a dictionary for translating from the standard PO notation of Ref.[3] to our notation. $d, \tilde{d} \in \{0, 1\}$. I find the standard PO notation confusing because it often uses D_i to represent two different nodes, \underline{d}^σ and \tilde{d}^σ in G_{im+} . This confusion becomes particularly distressing when we are told in PO notation that

$$Y_i = D_i Y_i(0) + (1 - D_i) Y_i(1) . \quad (38.27)$$

This could mean that

$$\underline{y}^\sigma = \tilde{d}^\sigma y^\sigma(1) + (1 - \tilde{d}^\sigma) \underline{y}^\sigma(0) \quad (38.28)$$

which is always true, or it could mean

$$\underline{y}^\sigma = \underline{d}^\sigma y^\sigma(1) + (1 - \underline{d}^\sigma) \underline{y}^\sigma(0) \quad (38.29)$$

which is not necessarily true.

38.5 $\mathcal{Y}_{d|\tilde{d}}$ differences (aka treatment effects)

Note the \mathcal{Y}_d and $\mathcal{Y}_{|\tilde{d}}$ are not the same thing.

$$\mathcal{Y}_{|\tilde{d}} = \sum_d \mathcal{Y}_{d|\tilde{d}} = \mathcal{Y}_{0|\tilde{d}} + \mathcal{Y}_{1|\tilde{d}} \quad (38.30)$$

whereas

$$\mathcal{Y}_d = \sum_{\tilde{d}} \mathcal{Y}_{d|\tilde{d}} P(\tilde{d}) = \mathcal{Y}_{d|0} \pi_0 + \mathcal{Y}_{d|1} \pi_1 . \quad (38.31)$$

$\mathcal{Y}_{|\tilde{d}}$ is connected to the do operator as follows.

$$P(\underline{y} = y | \rho \underline{d} = \tilde{d}) = \sum_x P(y | \tilde{d}, x) P(x) \quad (38.32)$$

so

$$\mathcal{Y}_{|\tilde{d}} = \sum_y y P(\underline{y} = y | \rho \underline{d} = \tilde{d}) . \quad (38.33)$$

In particular, when \underline{y} is binary (i.e., $\underline{y} \in \{0, 1\}$), Eq.(38.33) becomes

$$\mathcal{Y}_{|\tilde{d}} = P(\underline{y} = 1 | \rho \underline{d} = \tilde{d}) . \quad (38.34)$$

It is convenient to define the following effects. Note that we use the word “**effect**” to refer to a difference of two $\mathcal{Y}_{d|\tilde{d}}$.

- average controlled effect (ACE), used when doing an RCT.

$$\textcolor{red}{ACE} = \mathcal{Y}_{|1} - \mathcal{Y}_{|0} \quad (38.35)$$

- average treatment effect¹ (ATE).

$$\textcolor{red}{ATE} = \mathcal{Y}_1 - \mathcal{Y}_0 = \delta \quad (38.36)$$

- average treatment effect of the treated (ATT)

$$\textcolor{red}{ATT} = \mathcal{Y}_{1|1} - \mathcal{Y}_{0|1} \quad (38.37)$$

- average treatment effect of the untreated (ATU)

$$\textcolor{red}{ATU} = \mathcal{Y}_{1|0} - \mathcal{Y}_{0|0} \quad (38.38)$$

- simple difference in outcomes (SDO)

$$\textcolor{red}{SDO} = \mathcal{Y}_{1|1} - \mathcal{Y}_{0|0} \quad (38.39)$$

- selection bias (SB)

$$\textcolor{red}{SB} = \mathcal{Y}_{0|1} - \mathcal{Y}_{0|0} \quad (38.40)$$

¹ Note that effects in which \tilde{d} varies are called “controlled”, whereas those in which d varies instead, are called simply “treatments”. y is averaged over in both cases.

Note that some of these effects are linearly related

$$\underbrace{\mathcal{Y}_{1|1} - \mathcal{Y}_{0|0}}_{SDO} = \underbrace{(\mathcal{Y}_{1|1} - \mathcal{Y}_{0|1})}_{ATT} + \underbrace{\mathcal{Y}_{0|1} - \mathcal{Y}_{0|0}}_{SB} \quad (38.41)$$

$$\underbrace{\mathcal{Y}_1 - \mathcal{Y}_0}_{ATE} = \underbrace{(\mathcal{Y}_{1|1} - \mathcal{Y}_{0|1})}_{ATT} \pi_1 + \underbrace{(\mathcal{Y}_{1|0} - \mathcal{Y}_{0|0})}_{ATU} \pi_0 \quad (38.42)$$

$$\underbrace{\mathcal{Y}_{1|1} - \mathcal{Y}_{0|0}}_{SDO} = \underbrace{(\mathcal{Y}_{1|1} - \mathcal{Y}_{0|1})\pi_1 + (\mathcal{Y}_{1|0} - \mathcal{Y}_{0|0})\pi_0}_{ATE} \quad (38.43)$$

$$+ \underbrace{\mathcal{Y}_{0|1} - \mathcal{Y}_{0|0}}_{SB} \quad (38.44)$$

$$+ \underbrace{(\mathcal{Y}_{1|1} - \mathcal{Y}_{0|1})}_{ATT} \pi_0 \quad (38.45)$$

$$- \underbrace{(\mathcal{Y}_{1|0} - \mathcal{Y}_{0|0})}_{ATU} \pi_0 \quad (38.46)$$

38.6 Ignorability

Confounders are said to be **ignorable** (i.e., there is independence from confounders) if

$$\underline{y}^\sigma(\underline{\tilde{d}}^\sigma) \perp_P \underline{d}^\sigma . \quad (38.47)$$

This is satisfied by G_{do} . To prove so, check that

$$\underline{y}^\sigma(\underline{\tilde{d}}^\sigma) \perp_{G_{do}} \underline{d}^\sigma \quad (38.48)$$

and then invoke the d-separation theorem (see Chapter 13). When confounders are ignorable, we have

$$\mathcal{Y}_{d|\tilde{d}} = \mathcal{Y}_{d|y(\tilde{d})} = \mathcal{Y}_d , \quad (38.49)$$

or, equivalently,

$$\mathcal{Y}_{d|\tilde{d}=0} = \mathcal{Y}_{d|\tilde{d}=1} . \quad (38.50)$$

Therefore,

$$ATE = ATT = ATU = SDO \quad (38.51a)$$

and

$$SB = 0 . \quad (38.51b)$$

Let $\mathcal{E} \in \{ACE, ATE, ATT, ATU, SDO, SB\}$. \mathcal{E} can be defined for a fixed stratum x by replacing $\mathcal{Y}_{d|\tilde{d}}$ with $\mathcal{Y}_{d|\tilde{d},x}$. We will denote such an extension by \mathcal{E}_x , or, sometimes, simply by \mathcal{E} .

Confounders are said to be **conditionally ignorable** (i.e., there is conditional independence from confounders) if

$$\underline{y}^\sigma(\underline{\tilde{d}}^\sigma) \perp_P \underline{d}^\sigma | \underline{x}^\sigma . \quad (38.52)$$

This is satisfied by G_{im} . To prove this, check that

$$\underline{y}^\sigma(\underline{\tilde{d}}^\sigma) \perp_{G_{im}} \underline{d}^\sigma | \underline{x}^\sigma \quad (38.53)$$

and then invoke the d-separation theorem (see Chapter 13). When confounders are conditionally ignorable, we have

$$\mathcal{Y}_{d|\tilde{d},x} = \mathcal{Y}_{d|y(\tilde{d}),x} = \mathcal{Y}_{d|x} , \quad (38.54)$$

or, equivalently,

$$\mathcal{Y}_{d|\tilde{d}=0,x} = \mathcal{Y}_{d|\tilde{d}=1,x} . \quad (38.55)$$

If conditional ignorability holds, then Eqs.(38.51) are valid at fixed x .

38.7 Hypothesis testing for sharp null

In this section, we assume no x dependence, or else we assume that the whole discussion refers to a single stratum x . Hence, we will omit the x subscript in this section.

Assume $\underline{d}^\sigma = \underline{\tilde{d}}^\sigma$. In this section, we will discuss hypothesis testing between the following two opposite hypotheses:

$$\begin{aligned} H_0 : \underline{y}^\sigma(1) &= \underline{y}^\sigma(0) \quad \forall \sigma \\ H_1 &= \neg H_0 \end{aligned} . \quad (38.56)$$

H_0 is called the **sharp null hypothesis**.

Table 38.1 becomes Table 38.3 if we fill the blank cells according to the sharp null hypothesis H_0 . And Table 38.3 becomes Table 38.4 by permuting the entries of column \underline{d}^σ .

Define

$$N_1 = \sum_{\sigma} d^\sigma, \quad \pi_1 = \frac{N_1}{nsam} , \quad (38.57)$$

$$N_0 = \sum_{\sigma} (1 - d^\sigma) = nsam - N_1, \quad \pi_0 = \frac{N_0}{nsam} , \quad (38.58)$$

$$\vec{d} = (d^\sigma)_{\sigma=01,2,\dots,nsam-1} , \quad (38.59)$$

σ	\underline{d}^σ	\underline{y}^σ	$(1 - \underline{d}^\sigma)\underline{y}^\sigma$	$\underline{d}^\sigma \underline{y}^\sigma$
Andy	1	10	10	10
Ben	1	5	5	5
Chad	1	16	16	16
Daniel	1	3	3	3
Edith	0	5	5	5
Frank	0	7	7	7
George	0	8	8	8
Hank	0	10	10	10

Table 38.3: Table 38.1 with blank cells filled according to the sharp null hypothesis H_0 . Note that $\vec{d}_0 = (1, 1, 1, 1, 0, 0, 0, 0)$. If $\xi(\vec{d})$ is defined by Eq.(38.60), then $\xi = |34 - 30|/4 = 1$

σ	\underline{d}^σ	\underline{y}^σ	$(1 - \underline{d}^\sigma)\underline{y}^\sigma$	$\underline{d}^\sigma \underline{y}^\sigma$
Andy	1	10	10	10
Ben	0	5	5	5
Chad	1	16	16	16
Daniel	1	3	3	3
Edith	0	5	5	5
Frank	1	7	7	7
George	0	8	8	8
Hank	0	10	10	10

Table 38.4: Table 38.3 after permuting the entries of column \underline{d}^σ . Note that $\vec{d}_1 = (1, 0, 1, 1, 0, 1, 0, 0)$. If $\xi(\vec{d})$ is defined by Eq.(38.60), then $\xi = |36 - 28|/4 = 2$

and

$$\xi(\vec{d}) = \left| \frac{\sum_{\sigma} d^\sigma y^\sigma}{N_1} - \frac{\sum_{\sigma} (1 - d^\sigma) y^\sigma}{N_0} \right| \rightarrow |\mathcal{Y}_1 - \mathcal{Y}_0|. \quad (38.60)$$

$\xi(\vec{d})$ is the statistic that we will use to test the sharp null hypothesis H_0 . There are other possible functions $\xi(\vec{d})$ that are commonly used to test H_0 ; for example, the Kolgomorov-Smirmov statistic (see Ref.[3])

According to Tables 38.3 and 38.4, $\xi(\vec{d}) = 1$ for the true (i.e., H_0 -satisfying) vector $\vec{d} = \vec{d}_0$, and $\xi(\vec{d}) = 2$ for one possible H_1 -satisfying vector $\vec{d} = \vec{d}_1$. Let \mathcal{D} be the set of all permutations of \vec{d}_0 , and define $F : \mathbb{R} \rightarrow [0, 1]$ by

$$F(\xi) = \frac{1}{|\mathcal{D}|} \sum_{\vec{d} \in \mathcal{D}} \mathbb{1}(\xi(\vec{d}) \leq \xi) \quad (38.61)$$

$$= E_{\vec{d}}[\mathbb{1}(\xi(\vec{d}) \leq \xi)] \quad \text{where } P(\vec{d}) = \frac{1}{|\mathcal{D}|} \quad (38.62)$$

The function $F(\xi)$ is monotonically increasing from $F(-\infty) = 0$ to $F(+\infty) = 1$ so it can be interpreted to be a cumulative distribution for ξ . Then one can define a p value for the sharp null hypothesis by

$$p = 1 - F(\xi(\vec{d}_0)) . \quad (38.63)$$

$p \in [0, 1]$ measures the likelihood that H_0 is true. The smaller it is, the less likely H_0 is.

Often, $|\mathcal{D}|$ = the number of permutations of \vec{d}_0 , is too large to average over all the elements of \mathcal{D} . In that case, one can use random sampling methods. For example, one can choose a \vec{d} at random from \mathcal{D} , and calculate a step function $F_i(\xi)$ from that. Do this ni times. Then average all the ni step functions to obtain an estimate of $F(\xi)$.

38.8 Matching Strata

For a situation described by the bnet G_{im+} , we can match *similar* individuals to fill the blank cells of Table 38.1. By “similar”, we mean that they have the same or almost the same value of \underline{x}^σ .

38.8.1 1-1 strata-match

In 1-1 strata-match, we match each individual with $d^\sigma = 1$ with exactly one individual with $d^\sigma = 0$.

Recall that

$$SDO = \mathcal{Y}_{1|1,x} - \mathcal{Y}_{0|0,x} \quad (38.64a)$$

$$ATT = \mathcal{Y}_{1|1,x} - \mathcal{Y}_{0|1,x} \quad (38.64b)$$

$$ATU = \mathcal{Y}_{1|0,x} - \mathcal{Y}_{0|0,x} \quad (38.64c)$$

$$ATE = ATT\pi_1 + ATU\pi_0 \quad (38.64d)$$

Note that π_0, π_1 do not depend on x . This can be justified by looking at the bnet G_{im+} , for which $\pi_{\tilde{d}} = P(\tilde{d})$ is the prior of node \tilde{d} .

Eqs.(38.64) can be estimated from the data via the following estimators. In these estimators, $s(\sigma)$ is the single match for individual σ .

$$\widehat{SDO} = \frac{1}{N_1} \sum_{\sigma} d^{\sigma} y^{\sigma} - \frac{1}{N_0} \sum_{\sigma} (1 - d^{\sigma}) y^{\sigma} \quad (38.65)$$

$$\widehat{ATT} = \frac{1}{N_1} \sum_{\sigma} d^{\sigma} y^{\sigma} - \frac{1}{N_1} \sum_{\sigma} d_{\sigma} y^{s(\sigma)} \quad (38.66)$$

$$= \frac{1}{N_1} \sum_{\sigma} d^{\sigma} (y^{\sigma} - y^{s(\sigma)}) \quad (38.67)$$

$$\widehat{ATU} = \frac{1}{N_0} \sum_{\sigma} (1 - d^{\sigma})(y^{s(\sigma)} - y^{\sigma}) \quad (38.68)$$

$$\widehat{ATE} = \widehat{ATT}\pi_1 + \widehat{ATU}\pi_0 \quad (38.69)$$

$$= \frac{1}{nsam} [\widehat{ATT}N_1 + \widehat{ATU}N_0] \quad (38.70)$$

$$= \frac{1}{nsam} \left[\sum_{\sigma} d^{\sigma}(y^{\sigma} - y^{s(\sigma)}) + \sum_{\sigma} (1 - d^{\sigma})(y^{s(\sigma)} - y^{\sigma}) \right] \quad (38.71)$$

$$= \frac{1}{nsam} \sum_{\sigma} (2d^{\sigma} - 1)(y^{\sigma} - y^{s(\sigma)}) \quad (38.72)$$

38.8.2 Exact and approximate strata-match

It is very often the case that one can't find for a given individual σ another individual that has exactly the same value of x^{σ} . 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 σ with another individual s such that x^s and x^{σ} are very close in some metric.

More precisely, for some arbitrary parameter $\epsilon > 0$, and an individual σ with $d^{\sigma} = 1$, define the **strata-matching set** $\mathcal{M}_{\epsilon}(\sigma)$ by²

$$\mathcal{M}_{\epsilon}(\sigma) = \{s : d^{\sigma} = 1, d^s = 0, \text{dist}(x^{\sigma}, x^s) \leq \epsilon\} , \quad (38.73)$$

where

$$\text{dist}(x^{\sigma}, x^s) = [x^{\sigma}]^T [\Sigma]^{-1} x^s , \quad (38.74)$$

where $\Sigma = \langle \underline{x}^{\sigma}, [\underline{x}^s]^T \rangle$. This metric $\text{dist}(x^{\sigma}, x^s)$ is called the **Mahalanobis distance**. We will call the case $\epsilon = 0$ an **exact strata-match**, and the case $\epsilon \neq 0$ an **approximate strata-match**. To do an approximate strata-match, replace $y^{s(\sigma)}$ by $\langle y \rangle^{\sigma}$ in the estimators given above for a 1-1 strata-match. $\langle y \rangle^{\sigma}$ is defined by

$$\langle y \rangle^{\sigma} = \frac{1}{|\mathcal{M}_{\epsilon}(\sigma)|} \sum_{s \in \mathcal{M}_{\epsilon}(\sigma)} y^s . \quad (38.75)$$

Ref.[3] calculates the mean and variance of estimator \widehat{ATT} . The mean is biased, but one can define a new bias-corrected estimator.

² One can use an ϵ that depends on σ . Let $\epsilon(\sigma, 5)$ be the radius necessary so that $\mathcal{M}_{\epsilon(\sigma, 5)}(\sigma)$ contains exactly 5 elements s . Thus, $\mathcal{M}_{\epsilon(\sigma, 5)}(\sigma)$ contains the s of the 5 points x^s that are the nearest neighbors of x^{σ} in the $\text{dist}()$ metric.

38.8.3 Positivity

Positivity is defined as the requirement that for all layers x ,

$$0 < P(d^\sigma = 1|x^\sigma = x) < 1 \quad (38.76)$$

or, equivalently,

$$P(d^\sigma = 1|x^\sigma = x) > 0 \quad \text{and} \quad P(d^\sigma = 0|x^\sigma = x) > 0 . \quad (38.77)$$

In other words, for each layer x , there is a non-zero probability of being both treated and untreated.

If positivity is violated, then for some layer x , $\mathcal{Y}_{0|\tilde{d},x}$ or $\mathcal{Y}_{1|\tilde{d},x}$ is zero, so we can't calculate effect estimators such as \widehat{ATE} . If \widehat{ATE} can be calculated, one says it is identifiable (i.e., calculable). Positivity is a requirement for identifiability of \widehat{ATE} .

When $P(d^\sigma|x^\sigma = x)$ becomes 0 or 1 for some x , the arrow $\underline{x} \rightarrow \underline{d}$ becomes deterministic for some x . This situation is the very antithesis of RCTs, wherein the influence exerted by \underline{x}^σ on \underline{d}^σ is uniformly random and therefore ignorable. Hence, it is perhaps not too surprisingly that a violation of positivity makes \widehat{ATE} non-identifiable.

38.9 Propensity Score

It is often the case that the discrete vector \underline{x}^σ has too many possible values to make matching possible. In such cases, it is convenient to map the space of vectors \underline{x}^σ to the real line. One very convenient choice for that map is the **propensity score**, which is defined as

$$g(x^\sigma) = P(d^\sigma = 1|x^\sigma) . \quad (38.78)$$

The propensity score is usually approximated by a sigmoid function using logistic regression³

$$g(x^\sigma) = \text{sig}(\alpha + \beta x^\sigma) \quad (38.79)$$

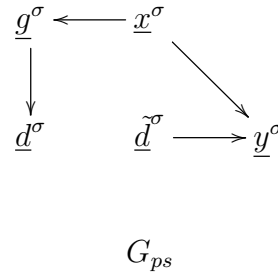


Figure 38.5: Bnet G_{ps} used when doing propensity scoring.

³ The sigmoid function is defined in Chapter Notational Conventions and Preliminaries to be $\text{sig}(x) = 1/(1 - e^{-x})$.

To use the propensity score, one replaces the bnct G_{im+} by the bnct G_{ps} shown in Fig.38.5. The TPMs, printed in blue, for the 2 nodes of G_{ps} that differ from the nodes of G_{im+} , are as follows:

$$P(g^\sigma|x^\sigma) = \delta(g^\sigma, g(x^\sigma)) \quad (38.80)$$

$$P(d^\sigma|g^\sigma) = g^\sigma d^\sigma + (1 - g^\sigma)(1 - d^\sigma) \quad (38.81)$$

Note that these TPMs are self-consistent because

$$P(d|x) = \sum_g P(d|g)P(g|x) \quad (38.82)$$

$$= g(x)d + [1 - g(x)](1 - d) \quad (38.83)$$

$$= P(d = 1|x)d + [1 - P(d = 1|x)](1 - d) \quad (38.84)$$

$$= P(d|x) \quad (38.85)$$

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

$$\boxed{P(d|g) = gd + (1 - g)(1 - d)} \quad (38.86)$$

and

$$\boxed{P(g) = \sum_x \overbrace{\delta(g, g(x))}^{P(g|x)} P(x)} \quad (38.87)$$

Next, note that

$$P(y|d, g) = \sum_x P(y|d, x)P(x|g) \quad (38.88)$$

so we need to find $P(x|g)$. Since

$$P(x|g) = \frac{P(g|x)P(x)}{P(g)} \quad (38.89)$$

$$= \frac{\delta(g, g(x))P(x)}{P(g)} \quad (38.90)$$

we finally get

$$\boxed{P(y|d, g) = \sum_x P(y|d, x) \frac{\delta(g, g(x))P(x)}{P(g)}}. \quad (38.91)$$

Chapter 41

Regression Discontinuity Design

This chapter is based on Ref.[3].

This chapter assumes that the reader has read Chapter 38 on Potential Outcomes.

In Regression Discontinuity Design (RDD), one switches the treatment dose \underline{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 ξ is a threshold value for \underline{x} . One measures the jump δ in the treatment outcome \underline{y} as \underline{x} passes through $\underline{x} = \xi$. Then one makes the very reasonable assumption that δ equals¹ $\mathcal{Y}_{1|\underline{x}=\xi} - \mathcal{Y}_{0|\underline{x}=\xi} = ATE|_{\underline{x}=\xi}$ for an imaginary experiment in which the confounder \underline{x} acts as a normal confounder that doesn't switch the treatment dose \underline{d} .

For example, d^σ might be whether an individual is admitted to Harvard Univ., y^σ might be how much money the individual earns for the first 20 years after graduating from Harvard, and x^σ might be his SAT scores. We assume Harvard only admits students with an SAT score higher than ξ .

41.1 PO analysis

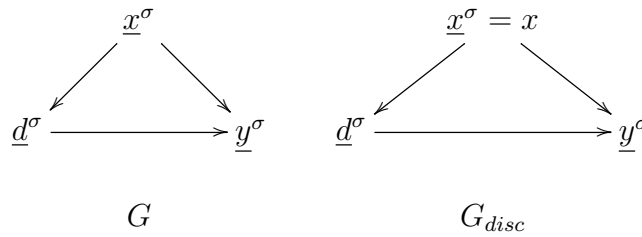


Figure 41.1: 2 bnets used in the PO analysis of RDD. The TPMs for G_{disc} are defined in terms of the TPMs for G . The TPM $P(d^\sigma|x^\sigma)$ for G_{disc} is discontinuous in x^σ .

The TPMs, printed in blue, for the bnet G_{disc} shown in Fig.41.1, are as follows. Note that

¹ ATE, which stands for “average treatment effect”, is defined in Chapter 38.

the TPMs for the bnet G_{disc} are defined in terms of the TPMs for the bnet G .

$$P(x^\sigma) = \delta(x^\sigma, x) \quad (41.1)$$

$$P(y^\sigma | d^\sigma, x^\sigma = x) = P_{\underline{y}|\underline{d},x}(y^\sigma | d^\sigma, x) \quad (41.2)$$

$$P(d^\sigma | x^\sigma = x) = \begin{cases} P_{\underline{d}|\underline{x}}(d^\sigma | x^\sigma = x) & \text{for } x > \xi \\ \delta(d^\sigma, 0) & \text{for } x < \xi \end{cases} \quad (41.3)$$

Define

$$E_{\sigma|d,x}[y^\sigma] = E_{y|d,x}[\underline{y}(d, x)] = \mathcal{Y}_{d|x} \quad (41.4)$$

and

$$\xi \pm = \xi \pm \epsilon \quad (41.5)$$

for some infinitesimal $\epsilon > 0$.

See Fig.41.2. In RDD, we assume that if we define the following 2 δ 's, one for bnet G and the other for bnet G_{disc} , then the two δ 's are equal, and they equal a conditional ATE.

$$\delta_{G_{disc}} = \mathcal{Y}_{1|x=\xi+} - \mathcal{Y}_{0|x=\xi-} \quad (41.6)$$

$$\delta_G = \mathcal{Y}_{1|x=\xi} - \mathcal{Y}_{0|x=\xi} \quad (41.7)$$

$$\delta_G = \delta_{G_{disc}} = \delta \quad (41.8)$$

$$\delta = ATE_{|x=\xi} \quad (41.9)$$

41.2 Linear Regression

In this section, we show how to apply linear regression (LR) to the PO analysis of RDD.

y^σ can be fitted as a function of $x \in \mathbb{R}$, for $d^\sigma \in \{0, 1\}$, as follows. Here ϵ^σ is the residual for individual σ and $b_0, m_0, b_1, m_1 \in \mathbb{R}$ are the fit parameters.

$$y^\sigma = [b_0 + m_0(x - \xi)](1 - d^\sigma) + [b_1 + m_1(x - \xi)]d^\sigma + \epsilon^\sigma. \quad (41.10)$$

Note that Eq.(41.10) yields a straight line in the $y^\sigma - x$ plane for $d^\sigma = 0$, and another straight line for $d^\sigma = 1$. These 2 lines are colored magenta in Fig.41.2. We are using the standard symbols b to denote the y-intercept, and m to denote the slope of a straight line.

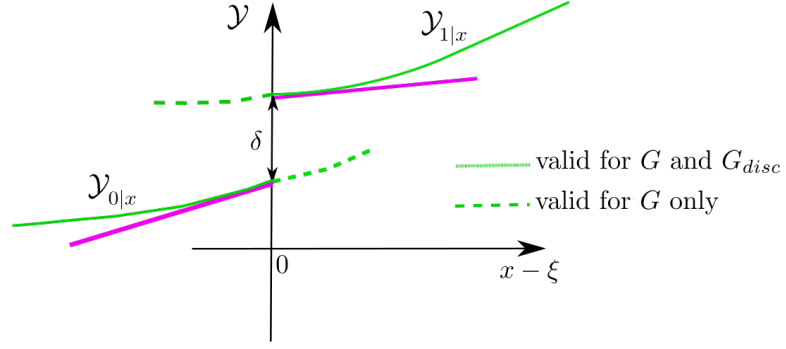


Figure 41.2: The jump δ between $\mathcal{Y}_{1|x}$ and $\mathcal{Y}_{0|x}$ is the same for G and G_{disc} .

Taking the expected value of Eq.(41.10), we get

$$\mathcal{Y}_{d|x} = [b_0 + m_0(x - \xi)](1 - d) + [b_1 + m_1(x - \xi)]d. \quad (41.11)$$

Hence,

$$\mathcal{Y}_{1|x=\xi+} = b_1, \quad \mathcal{Y}_{0|x=\xi-} = b_0 \quad (41.12)$$

$$\delta = b_1 - b_0 \quad (41.13)$$

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