

Causality

Lecture Notes

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Jonas Peters

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Preface

Zurich and Tübingen, May 2015

Script. This script has been written for the lecture “Causality” given by Marloes Maathuis, Nicolai Meinshausen and myself at ETH Zurich in spring semester 2015.

The key idea is to provide a short introduction into the field of causality. This means that I am omitting many important results. Please send an email (see below) if you think that this is the case.

Causal concepts are developed from structural equation models and particular stress is laid on the idea of invariance.

This script is meant as additional material to the lecture, especially Example 3.1.7 and Sections 2.4 and 3.3 slightly differ from what has been discussed in the lecture. Therefore, please also look at your lecture notes when preparing for the exam. The script may contain many typos, mistakes and missing references. I am thankful for any correction. Please send it to jonas.peters@tuebingen.mpg.de.

Disclaimer. Although I put some effort into the presentation of material (e.g. looking for examples, improving existing proofs etc.), I do not claim that this script contains novel results that are unknown in the literature.

Thanks. First, I want to thank Marloes Maathuis and Nicolai Meinshausen with whom I hold the first causality lecture in spring semester 2015 at ETH Zurich during which this script was written.

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Jonas Peters

Chapter 1

Introduction

1.1 Motivation

In statistics, we often deal with properties of a joint distribution $\mathbb{P}^{\mathbf{X}}$ of some p -dimensional random vector \mathbf{X} . In many situations, however, we are interested in another distribution $\tilde{\mathbb{P}}^{\mathbf{X}}$ that differs from the observed distribution, $\tilde{\mathbb{P}}^{\mathbf{X}} \neq \mathbb{P}^{\mathbf{X}}$. We are trying to support this claim by the following three illustrative examples.

Example 1.1.1 [Chocolate - Nobel Prizes] Messerli [2012] reports that there is a significant correlation between a country’s chocolate consumption (per capita) and the number of Nobel prizes awarded to its citizens (also per capita), see Figure 1.1. These correlations are properties of some observational distribution $\mathbb{P}^{\mathbf{X}}$. We must be careful with drawing conclusions like “Eating chocolate produces Nobel prize.” or “Geniuses are more likely to eat lots of chocolate”, see Figure 1.2 because these statements are “causal”. We will see later (Definition 2.2.1) that they concern different distributions $\tilde{\mathbb{P}}^{\mathbf{X}}$: The first statement suggests, for example, that in a distribution, where each country dictates its citizen to eat a randomly chosen amount of chocolate (same for all citizens), there is still a dependence between chocolate consumption and Nobel prizes: more chocolate means more Nobel prizes. Taking our background knowledge into account, however, we do not expect this to happen. We might rather think that the correlation stems from some hidden variables like economic strength of a country, for example.

In this sense, the famous sentence “Correlation does not imply causation” can also be understood as: properties in $\mathbb{P}^{\mathbf{X}}$ do not necessarily tell you anything about properties in $\tilde{\mathbb{P}}^{\mathbf{X}}$. We will see in Section 2.2 how causal language helps us to formulate relations between those distributions.

This data set comes with many difficulties: the variables are averaged quantities, for example, and the observations for different countries are not independent (e.g. there are not arbitrary many Nobel prizes). We nevertheless hope that the reader can still filter out the relevant causal deliberations.

Example 1.1.2 [Myopia] Only very few people infer a direct causal relationship between

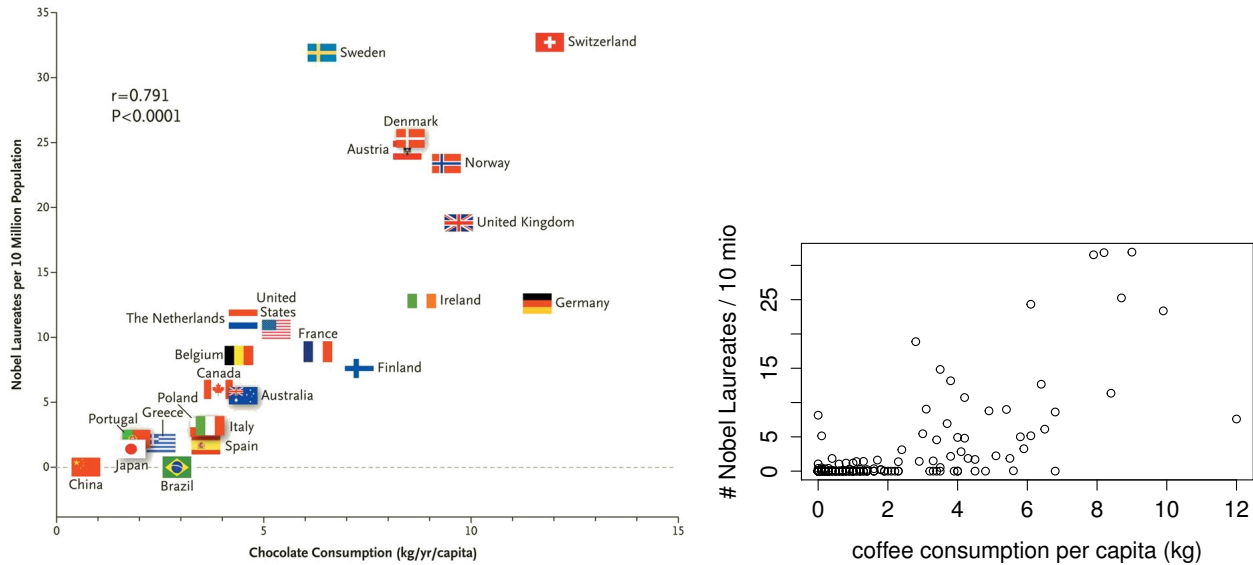
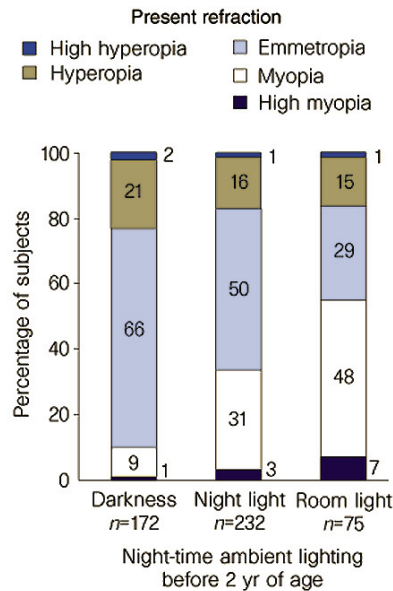


Figure 1.1: The left figure is slightly modified from [Messerli, 2012], it shows a significant correlation between a country's consumption of chocolate and the number of Nobel prizes (averaged per person). The right figure shows a similar result for coffee consumption; the data are based on [Wikipedia, 2013b,a].



Figure 1.2: Two online articles (downloaded from confectionarynews.com and forbes.com on Jan 29th 2013) drawing causal conclusions from the observed correlation between chocolate consumption and Nobel prizes, see Figure 1.1.



Patente

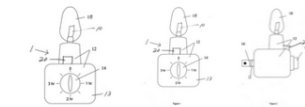
Night light with sleep timer

US 20050007889 A1

ZUSAMMENFASSUNG

A timer a light and an optional music source is located on or in a housing of a nightlight assembly. When this assembly is plugged into a source of electric power, the timer is set to a selected time for the light and optional music to remain on. After this selected time has elapsed, the light and music automatically turns off, allowing for sleep in appropriate darkness and silence.

BILDER (3)



BESCHREIBUNG

I FIELD OF THE INVENTION

This invention relates to a nightlight with a sleep timer.

II BACKGROUND OF THE INVENTION

Many young children prefer the comfort of a nightlight when they go to bed, but their caregivers would prefer them to sleep in darkness. A University of Pennsylvania study, Quinn, G. E., Shin, C. H., Maguire, M. G. and Stone, R. A. Myopia and ambient lighting at night. Nature, 399: 113-114, 1999 (May 13, 1999), has shown that children who sleep with a light on may have a higher risk of developing nearsightedness as they get older.

| | |
|-------------------------------|-----------------------------|
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| Publikationstyp | Anmeldung |
| Anmeldenummer | US 10/614,245 |
| Veröffentlichungsdatum | 13. Jan. 2005 |
| Eingetragen | 8. Juli 2003 |
| Prioritätsdatum | 8. Juli 2003 |
| Erfinder | Karin Peterson |
| Ursprünglich Bevollmächtigter | Peterson Karin Lyn |
| Zitat exportieren | BIBTeX, EndNote, F |
| Klassifizierungen (4) | |
| Externe Links: | USPTO, USPTO-Zuordnung, Esp |

ANSPRÜCHE (16)

1. An night light assembly comprising:

a night light mounted on a housing;

a timer located on said housing adjacent said n

means for setting the time that said night light w

means for connecting said light to a source of e

whereby when the assembly is plugged into a s
said timer may be set to a selected time for the l
after this selected time has elapsed, said light s

Figure 1.3: The plot on the left shows a (significant) dependence between lighting conditions in a child's bedroom and the development of myopia (shortsightedness). The right figure shows a patent for a night light with timer indicating that enforcing dark rooms decreases the risk of myopia.

Nobel prize winners and chocolate consumption when looking at Figure 1.1. Most people realize that the dependence must be due to "some latent factors". There is an increased risk of false inference when less background knowledge is available. Figure 1.3 (left) shows an example, where people have falsely drawn causal conclusions from observational data. The data set shows a dependence between the usage of a night light in a child's room and the occurrence of myopia [Quinn et al., 1999]. While the authors are cautious enough to say that the study "does not establish a causal link", they add that "the strength of the association [...] does suggest that the absence of a daily period of darkness during childhood is a potential precipitating factor in the development of myopia. Later Gwiazda et al. [2000], Zadnik et al. [2000] found that the correlation is due to whether the child's parents have myopia. If they have, they are more likely to put a night light in their child's room and at the same time, the child has an increased risk of inheriting the disease from its parents. In the meantime, there was a patent filed, see Figure 1.3 (right).

Example 1.1.3 [Kidney Stones] Table 1.1 shows a famous data set from kidney stone recovery [Charig et al., 1986]. Out of 700 patients, one half has been treated with open surgery (78% recovery rate) the other with have with percutaneous nephrolithotomy (treatment B, with 83% success), a surgical procedure to remove kidney stones by a

Table 1.1: A classic example of Simpson’s paradox. The table reports the success rates of two treatments for kidney stones [Charig et al., 1986, tables I and II] and [Bottou et al., 2013]. Although the overall success rate of treatment B seems better, treatment B performs worse than treatment A on both patients with small kidney stones and patients with large kidney stones, see Examples 3.1.1 and 3.1.7.

| | Overall | Patients with small stones | Patients with large stones |
|--|----------------------|-------------------------------|-------------------------------|
| Treatment A: Open surgery | 78% (273/350) | 93% (81/87) | 73% (192/263) |
| Treatment B: Percutaneous nephrolithotomy | 83% (289/350) | 87% (234/270) | 69% (55/80) |

small puncture wound. If we do not know anything else than the overall recovery rates, many people would prefer treatment B if they had to decide. Observing the data in more detail, however, we realize that the open surgery performs better on both small and large kidney stones. How do we deal with this inversion of conclusion? The answer is to concentrate on the precise question we are interested in. This is not whether treatment A or treatment B was more successful in this particular study but how the treatments compare when we force all patients to take treatment A or B, respectively; alternatively, we can compare them only on large stones or small stones, of course. Again, these questions concern some distribution $\tilde{\mathbb{P}}^{\mathbf{X}}$ different from the observational distribution $\mathbb{P}^{\mathbf{X}}$. We will see in Example 3.1.1 why we should prefer treatment A over treatment B. This data set is a famous example for Simpson’s paradox [Simpson, 1951], see Example 3.1.7. In fact, it is much less a paradox than the result of the influence of a confounder (i.e. hidden common cause).

If you perform a significance test on the data (e.g. using a proportion test or χ^2 independence test) it turns out that the difference in methods is not significant on a 5% significance level. Note, however, this is not the point of this example. By multiplying each entry in Table 1.1 by a factor of ten, the results would become statistically significant.

Example 1.1.4 [Genetic Data] Causal questions also appear in biological data sets, where we try to predict the effect of interventions (e.g. gene knock-outs). Kemmeren et al. [2014] measures genome-wide mRNA expression levels in yeast, we therefore have data for $p = 6170$ genes. There are $n_{obs} = 160$ “observational” samples of wild-types and $n_{int} = 1479$ data points for the “interventional” setting where each of them corresponds to a strain for which a single gene $k \in K := \{k_1, \dots, k_{1479}\} \subset \{1, \dots, 6170\}$ has been deleted. The data may therefore be interpreted as coming from an observational distribution $\mathbb{P}^{\mathbf{X}}$ and then from 1479 other distributions $\mathbb{P}_1^{\mathbf{X}}, \dots, \mathbb{P}_{1479}^{\mathbf{X}}$. And we are interested in yet other distributions $\tilde{\mathbb{P}}^{\mathbf{X}}$ that tell us how the system reacts after deleting other genes or any combination of genes. Figure 1.4 shows a small subset of the data.



Figure 1.4: The plot on the left shows the observational data (log expression level) for two of the 6170 genes. The middle plot shows 1478 out of the 1479 interventional data points for the same two genes; only the data point that corresponds to a deletion of gene 5954 is omitted. It is shown as the red point in the right plot. Because gene 4710 shows reduced activity after we have intervened on gene 5954, we can infer that 5954 has a (possibly indirect) causal influence on gene 4710. This way, we can use (part of the data) as ground truth for evaluating causal inference methods, that try to infer causal statements either from observational data or from a combination of observational and interventional data. The black lines indicate that the expression levels of both genes are correlated.

Example 1.1.4 is taken from [Peters et al., 2015].

Example 1.1.5 [Advertising placement]

The system Figure 1.5 shows a (heavily) simplified version of an advertisement system that is implemented on a search website. In a nutshell, advertisers can bid on a combination of advertisements and search queries hoping that their ad will be placed in a good location: either on the top of the “sidebar” or even above the search results, i.e. in the “mainline”. Only if the user clicks on one of the ads, the advertiser pays money to the publisher according to some (rather involved) pricing system. When the user enters the site, he has some intention (e.g. to buy some organic fruits) and puts a query into the search mask. While the intention usually remains hidden, the publisher does have access to some user data as search query, time of the year or location. Based on this information he chooses the number and kind of ads that are chosen. In particular, we are concentrating now on a parameter that is called the main line reserve which determines the number of ads shown in the mainline.

Making money In practice, the publisher can control the edge “user data \rightarrow main line reserve”, that is he can decide which conditional $p(\text{main line reserve} | \text{user data})$ to use. Assume that the publisher lets the system run for a while and observes data

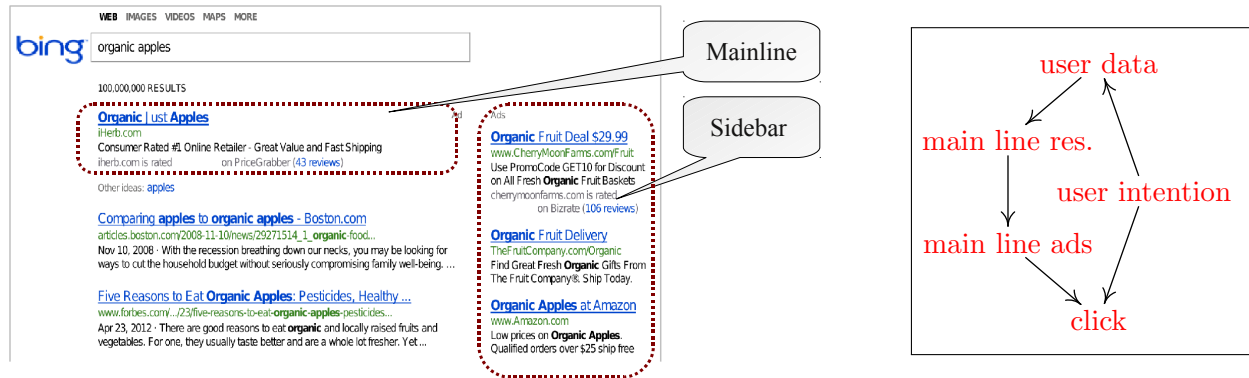


Figure 1.5: Search results (left) and simplified version of an advertisement system (right)

from this system. He would then like to know whether he could perform even better. That is, would a different parameter setting $p(\text{main line reserve} | \text{user data})$ lead to a higher expected number of clicks? Again, we are interested in the system's behavior under a different distribution $\hat{\mathbb{P}}^{\mathbf{X}} \neq \mathbb{P}^{\mathbf{X}}$.

Disclaimer In practice the system is more complicated since one may want to take into account the bids of the advertiser. Also, the publisher has to take care of some long-term goals: showing too many or misleading ads, may lead to more clicks but may also annoy users which then decide to use another search website or install an adblock system (which, by the way, is available for free and very easy to install).

1.2 Some bits of probability and statistics

Throughout the lecture we use the following notation.

- $(\Omega, \mathcal{F}, \mathbb{P})$: probability space, where Ω , \mathcal{F} and \mathbb{P} are set, σ -algebra and probability measure, respectively.
- We use capital letters for real-valued random variables. E.g., $X : (\Omega, \mathcal{F}) \rightarrow (\mathbb{R}, \mathcal{B}_{\mathbb{R}})$ is a measurable function, with respect to the Borel σ -algebra.
- We usually denote vectors with bold letters.
- $\mathbb{P}^{\mathbf{X}}$ is the distribution of the p -dimensional random vector \mathbf{X} , i.e. a probability measure on $(\mathbb{R}^p, \mathcal{B}_{\mathbb{R}^p})$.
- We write $x \mapsto p_X(x)$ or simply $x \mapsto p(x)$ for the Radon-Nikodym derivative of $\mathbb{P}^{\mathbf{X}}$ either with respect to the Lebesgue or the counting measure. We (sometimes implicitly) assume its existence or continuity.
- We call X **independent** of Y and write $X \perp\!\!\!\perp Y$ if and only if

$$p(x, y) = p(x)p(y) \quad (1.1)$$

for all x, y . Otherwise, X and Y are **dependent** and we write $X \not\perp\!\!\!\perp Y$.

- We call X_1, \dots, X_p **jointly (or mutually) independent** if and only if

$$p(x_1, \dots, x_p) = p(x_1) \cdot \dots \cdot p(x_p) \quad (1.2)$$

for all x_1, \dots, x_p .

- We call X **independent of Y conditional on Z** and write $X \perp\!\!\!\perp Y \mid Z$ if and only if

$$p(x, y \mid z) = p(x \mid z)p(y \mid z) \quad (1.3)$$

for all x, y, z such that $p(z) > 0$. Otherwise, X and Y are dependent conditional on Z and we write $X \not\perp\!\!\!\perp Y \mid Z$.

- The **variance** of a random variable X is defined as

$$\text{var}X := \mathbf{E}(X - \mathbf{E}X)^2 = \mathbf{E}X^2 - (\mathbf{E}X)^2$$

if $\mathbf{E}X^2 < \infty$.

- We call X and Y **uncorrelated** if $\mathbf{E}X^2, \mathbf{E}Y^2 < \infty$ and

$$\rho_{X,Y} := \frac{\mathbf{E}XY - \mathbf{E}X\mathbf{E}Y}{\sqrt{\text{var}X\text{var}Y}} = 0.$$

Otherwise, that is if $\rho_{X,Y} \neq 0$, X and Y are correlated. $\rho_{X,Y}$ is called the correlation coefficient between X and Y . If X and Y are independent, then they are uncorrelated.

- We say that X and Y are **partially uncorrelated given Z** if

$$\rho_{X,Y \mid Z} := \frac{\rho_{X,Y} - \rho_{X,Z}\rho_{Z,Y}}{\sqrt{(1 - \rho_{X,Z}^2)(1 - \rho_{Z,Y}^2)}} = 0.$$

The following interpretation of partial correlation is important: $\rho_{X,Y \mid Z}$ equals the correlation between residuals after linearly regressing X on Z and Y on Z .

- In general, we have

$$\begin{aligned} \rho_{X,Y \mid Z} = 0 & \not\Rightarrow X \perp\!\!\!\perp Y \mid Z & \text{and} \\ \rho_{X,Y \mid Z} \neq 0 & \not\Rightarrow X \not\perp\!\!\!\perp Y \mid Z. \end{aligned}$$

The latter holds because a linear regression does not necessarily remove all the dependence from Z in X : after linearly regressing X on Z , there might still be dependence between the residuals and Z .

- Given finitely many data we do not expect the empirical correlation (or any independence measure) to be exactly zero. We therefore make use of statistical hypothesis tests. To test for vanishing correlation, we can use the empirical correlation coefficient and a t -test (for Gaussian variables) or Fisher's z -transform [e.g. `cor.test` in RProject, 2015].

As an independence test, we may use a χ^2 -test for discrete or discretized data or the Hilbert-Schmidt Independence Criterion (HSIC), see [Gretton et al., 2008]. As

usual, the null hypothesis is chosen to be vanishing correlation or independence of the variables. Note, however, that in causal inference we do not necessarily want to treat type I error and type II error equally. We will see in Section 4 that some methods for causal structure learning make use of both independences and dependences.

- In a slight abuse of notation we consider sets of variables $\mathbf{B} \subseteq \mathbf{X}$ as a single multivariate variable.

For an introduction to measure theory, see for example [Dudley, 2002].

1.3 Graphs

We start with some basic notation for graphs. Consider finitely many random variables $\mathbf{X} = (X_1, \dots, X_p)$ with index set $\mathbf{V} := \{1, \dots, p\}$, joint distribution $\mathbb{P}^{\mathbf{X}}$ and density $p(\mathbf{x})$.

Definition 1.3.1 A **graph** $\mathcal{G} = (\mathbf{V}, \mathcal{E})$ consists of (finitely many) **nodes** or **vertices** \mathbf{V} and **edges** $\mathcal{E} \subseteq \mathbf{V}^2$ with $(v, v) \notin \mathcal{E}$ for any $v \in \mathbf{V}$.

We now introduce graph terminology that we require later. Most of the definitions can be found in Spirtes et al. [2000], Koller and Friedman [2009] and Lauritzen [1996], for example. The terminology is meant to be self-explanatory, it is widely used. When reading papers it usually suffices to check some details in the definitions; e.g, is a node descendant of itself?

- Let $\mathcal{G} = (\mathbf{V}, \mathcal{E})$ be a graph with $\mathbf{V} := \{1, \dots, p\}$ and corresponding random variables $\mathbf{X} = (X_1, \dots, X_p)$. A graph $\mathcal{G}_1 = (\mathbf{V}_1, \mathcal{E}_1)$ is called a **subgraph** of \mathcal{G} if $\mathbf{V}_1 = \mathbf{V}$ and $\mathcal{E}_1 \subseteq \mathcal{E}$; we then write $\mathcal{G}_1 \leq \mathcal{G}$. If additionally, $\mathcal{E}_1 \neq \mathcal{E}$, \mathcal{G}_1 is a **proper subgraph** of \mathcal{G} .
- A node i is called a **parent** of j if $(i, j) \in \mathcal{E}$ and $(j, i) \notin \mathcal{E}$ and a **child** if $(j, i) \in \mathcal{E}$ and $(i, j) \notin \mathcal{E}$. The set of parents of j is denoted by $\mathbf{PA}_j^{\mathcal{G}}$, the set of its children by $\mathbf{CH}_j^{\mathcal{G}}$. Two nodes i and j are **adjacent** if either $(i, j) \in \mathcal{E}$ or $(j, i) \in \mathcal{E}$. We call \mathcal{G} **fully connected** if all pairs of nodes are adjacent. We say that there is an **undirected edge** between two adjacent nodes i and j if $(i, j) \in \mathcal{E}$ and $(j, i) \in \mathcal{E}$. An edge between two adjacent nodes is **directed** if it is not undirected. We then write $i \rightarrow j$ for $(i, j) \in \mathcal{E}$. Three nodes are called an **immorality** or a **v-structure** if one node is a child of the two others that themselves are not adjacent. The **skeleton** of \mathcal{G} does not take the directions of the edges into account: it is the graph $(\mathbf{V}, \tilde{\mathcal{E}})$ with $(i, j) \in \tilde{\mathcal{E}}$, if $(i, j) \in \mathcal{E}$ or $(j, i) \in \mathcal{E}$.
- A **path** in \mathcal{G} is a sequence of (at least two) distinct vertices i_1, \dots, i_n , such that there is an edge between i_k and i_{k+1} for all $k = 1, \dots, n - 1$. If $i_k \rightarrow i_{k+1}$ for all k we speak of a **directed path** from i_1 to i_n and call i_n a **descendant** of i_1 . In this work, i is neither a descendant nor a non-descendant of itself. We denote all descendants of i by $\mathbf{DE}_i^{\mathcal{G}}$ and all non-descendants of i , excluding i , by $\mathbf{ND}_i^{\mathcal{G}}$. If $i_{k-1} \rightarrow i_k$ and $i_{k+1} \rightarrow i_k$, i_k is called a **collider relative to this path**.
- \mathcal{G} is called a **partially directed acyclic graph (PDAG)** if there is no directed cycle, i.e., if there is no pair (j, k) with directed paths from j to k and from k to j . \mathcal{G} is called a **directed acyclic graph (DAG)** if it is a PDAG and all edges are directed.

- In a DAG, a path between i_1 and i_n is **blocked by a set \mathbf{S}** (with neither i_1 nor i_n in \mathbf{S}) whenever there is a node i_k , such that one of the following two possibilities holds:
 1. $i_k \in \mathbf{S}$ and $i_{k-1} \rightarrow i_k \rightarrow i_{k+1}$ or $i_{k-1} \leftarrow i_k \leftarrow i_{k+1}$ or $i_{k-1} \leftarrow i_k \rightarrow i_{k+1}$
 2. $i_{k-1} \rightarrow i_k \leftarrow i_{k+1}$ and neither i_k nor any of its descendants is in \mathbf{S} .

We say that two disjoint subsets of vertices \mathbf{A} and \mathbf{B} are **d -separated** by a third (also disjoint) subset \mathbf{S} if every path between nodes in \mathbf{A} and \mathbf{B} is blocked by \mathbf{S} .

- Given a DAG \mathcal{G} , we obtain the undirected **moralized graph** \mathcal{G}^{mor} of \mathcal{G} by connecting the parents of each node and removing the directions of the edges.
- In a slight abuse of notation we identify the nodes $j \in \mathbf{V}$ with variables X_j from a random vector $\mathbf{X} = (X_1, \dots, X_p)$, see Section 1.2, the context should clarify the meaning.

Definition 1.3.2 Given a DAG \mathcal{G} , we say that a $\pi \in S_p$, that is a bijective mapping

$$\pi : \{1, \dots, p\} \rightarrow \{1, \dots, p\},$$

is a *topological (or causal) ordering* of the variables if it satisfies

$$\pi(i) < \pi(j) \quad \text{if} \quad j \in \mathbf{DE}_i^{\mathcal{G}}.$$

Because of the acyclic structure of the DAG, there is always a topological ordering (see below). But this order does not have to be unique. The node $\pi^{-1}(1)$ is a source node, $\pi^{-1}(p)$ a sink node.

Proposition 1.3.3 *For each DAG there is a topological ordering.*

Proof. We need to show that each DAG has a node without any ancestors: start with any node and move to one of its parents (if there are any). You will never visit a parent that you have seen before (if you did there had been a directed cycle). At latest after $p - 1$ steps you reach a node without any parent. \square

Definition 1.3.4 We can represent a DAG $\mathcal{G} = (V, \mathcal{E})$ over p nodes with a binary $p \times p$ matrix A (taking values 0 or 1):

$$A_{i,j} = 1 \quad \Leftrightarrow \quad (i, j) \in \mathcal{E}.$$

A is called the **adjacency matrix** of \mathcal{G} .

Remark 1.3.5 (i) Let A be the adjacency matrix for DAG \mathcal{G} . The entry (i, j) of A^2 equals the number of paths of length 2 from i to j because of

$$A_{i,j}^2 = \sum_k A_{ik} A_{kj}.$$

| p | number of DAGs with p nodes |
|-----|---|
| 1 | 1 |
| 2 | 3 |
| 3 | 25 |
| 4 | 543 |
| 5 | 29281 |
| 6 | 3781503 |
| 7 | 1138779265 |
| 8 | 783702329343 |
| 9 | 1213442454842881 |
| 10 | 4175098976430598143 |
| 11 | 31603459396418917607425 |
| 12 | 521939651343829405020504063 |
| 13 | 18676600744432035186664816926721 |
| 14 | 1439428141044398334941790719839535103 |
| 15 | 237725265553410354992180218286376719253505 |
| 16 | 83756670773733320287699303047996412235223138303 |
| 17 | 62707921196923889899446452602494921906963551482675201 |
| 18 | 99421195322159515895228914592354524516555026878588305014783 |
| 19 | 332771901227107591736177573311261125883583076258421902583546773505 |
| 20 | 2344880451051088988152559855229099188899081192234291298795803236068491263 |

Table 1.2: The number of DAGs depending on the number p of nodes, taken from <http://oeis.org/A003024> (Feb 2015).

(ii) In general, we have

$$A_{ij}^k = \# \text{ paths of length } k \text{ from } i \text{ to } j$$

(iii) When the identity is a causal order, the adjacency matrix is upper triangular, i.e., only the upper-right half of the matrix contains non-zeros.

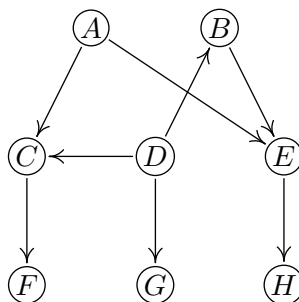
(iv) We may want to use sparse matrices when the graph is sparse in order to save space and/or computation time.

The number of DAGs with p nodes have been studied by Robinson [1970, 1973], and independently by Stanley [1973]. The number of such matrices (or DAGs) is growing very quickly in p , see Table 1.3. McKay [2004] proves the following equivalent description of DAGs which had been conjectured by Eric W. Weisstein.

Theorem 1.3.6 *The matrix A is an adjacency matrix of a DAG \mathcal{G} if and only if $A + Id$ is a 0 – 1 matrix and has eigenvalues strictly greater than zero.*

1.4 Exercises

Exercise 1.4.1 For the following graph \mathcal{G}



write down

- the non-descendants of D ,
- all variables that are d -separated from A given F, D .
- all sets of variables that you can condition on in order to d -separate A and D .

Exercise 1.4.2 Which graphs satisfy the following d -separation statements? (Assume, that these are all d -separations that can be found in the graphs.)

- Consider graphs with three nodes A, B and C such that

| \cdot | AND | \cdot | d -separated by |
|---------|-------|---------|-------------------|
| A | | C | $\{B\}$ |

- Consider graphs with four nodes A, B, C and D such that

| \cdot | AND | \cdot | d -separated by |
|---------|-------|---------|-------------------|
| A | | C | \emptyset |
| A | | D | $\{B\}$ |
| A | | D | $\{B, C\}$ |
| D | | C | $\{B\}$ |
| D | | C | $\{B, A\}$ |

Chapter 2

Structural equation models

Structural equation models have been used for a long time in fields like agriculture or social sciences [e.g., Wright, 1921a, Bollen, 1989]. Model selection, for example, was done by fitting different structures that were considered as reasonable given the prior knowledge about the system. These candidate structures were then compared using goodness of fit tests. In Section 4, we consider the question of identifiability.

2.1 Definitions and first properties

Definition 2.1.1 A *structural equation model (SEM)* (also called a functional model) is defined as a tuple $\mathcal{S} := (\mathcal{S}, \mathbb{P}^{\mathbf{N}})$, where $\mathcal{S} = (S_1, \dots, S_p)$ is a collection of p equations

$$S_j : \quad X_j = f_j(\mathbf{PA}_j, N_j), \quad j = 1, \dots, p, \quad (2.1)$$

where $\mathbf{PA}_j \subseteq \{X_1, \dots, X_p\} \setminus \{X_j\}$ are called *parents of X_j* and $\mathbb{P}^{\mathbf{N}} = \mathbb{P}^{N_1, \dots, N_p}$ is the joint distribution of the noise variables, which we require to be jointly independent, i.e., $\mathbb{P}^{\mathbf{N}}$ is a product distribution. The graph of a structural equation model is obtained simply by drawing direct edges from each parent to its direct effects, i.e., from each variable X_k occurring on the right-hand side of equation (2.1) to X_j , see Figure 2.1. We henceforth assume this graph to be acyclic. According to the notation defined in Section 1.3, \mathbf{PA}_j are the parents of X_j .

Proposition 2.1.2 *Because of the acyclic structure an SEM defines a unique distribution over the variables (X_1, \dots, X_p) such that $X_j \stackrel{d}{=} f_j(\mathbf{PA}_j, N_j)$ for $j = 1, \dots, p$.*

Proof. Using a topological ordering π we can write each node j as a function of the noise terms N_k with $\pi(k) \leq \pi(j)$ (use the structural equations iteratively). That is,

$$X_j = g_j((N_k)_{k: \pi(k) \leq \pi(j)}).$$

□

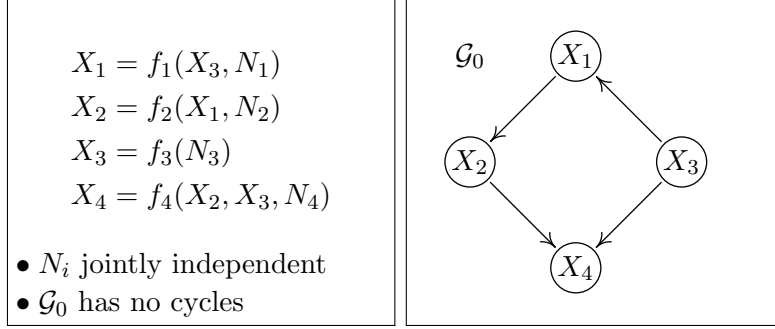


Figure 2.1: Example of a structural equation model (SEM) (left) with corresponding graph (right). There is only one topological ordering π (that satisfies $3 \mapsto 1$, $1 \mapsto 2$, $2 \mapsto 3$, $4 \mapsto 4$).

We use the SEM to define not only the distribution of observed data but also so-called interventional distributions (see Remark 2.2.5, for example). These are formally defined in Definition 2.2.1.

- Remark 2.1.3** (i) It may be helpful to think about generating n samples from this distribution: one first samples $(\mathbf{N}_1, \dots, \mathbf{N}_n) \stackrel{\text{iid}}{\sim} \mathbb{P}^{\mathbf{N}}$ and then subsequently uses the structural equations (starting from a source node $\pi^{-1}(1)$, then $\pi^{-1}(2)$, and so on) to generate samples from the X_j .
- (ii) Definition 2.1.1 is purely mathematical, we relate SEMs to reality in Remark 2.2.5. The parents \mathbf{PA}_j may then be thought of as the direct causes of X_j . An SEM specifies how the \mathbf{PA}_j affect X_j . Note that for many authors, SEMs already have a causal meaning. In this script, we try to separate mathematical from the causal language.
- (iii) In physics (chemistry, biology, ...), we would usually expect that such causal relationships occur in time, and are governed by sets of coupled differential equations. Under certain assumptions such as stable equilibria, one can derive an SEM that describes how the equilibrium states of such a dynamical system will react to physical interventions on the observables involved [Mooij et al., 2013]. In this lecture, we do not deal with these issues but take the SEM as our starting point instead.
- (iv) The model class of SEMs, i.e. the set of distributions that can be generated by an SEM, is the set of *all* distributions. We will see later (Proposition 2.5.2) that each distribution can be generated by many SEM's with a fully connected graph, for example.
- (v) It seems surprising that the two SEMs $\mathbf{S}_1 : X = N_X, Y = N_Y$ and $\mathbf{S}_2 : X = N_X, Y = 0 \cdot X + N_Y$ correspond to different graphs; see also causal minimality (Definition 2.4.10).

- (vi) This is one of the reasons why we should not use the structural equations (2.1) as usual equations. They should be thought of as a tool that tells us how to generate a distribution (see Proposition 2.1.2) and the intervention distributions (see Section 2.2).
- (vii) The goal in Chapter 4 will be to estimate the causal structure from the joint distribution. Remark (iv) shows that we will need additional assumptions. It turns out that finding a causal order π is difficult. Assume that π is given, i.e. we have:

$$\begin{aligned} X &= N_X \\ Y &= f(X, N_Y) \\ Z &= g(Y, Z, N_Z) \end{aligned}$$

with unknown f, g, N_X, N_Y, N_Z . Deciding whether α, β and/or γ equals zero is a well-studied significance problem in “traditional” statistics (herefore, one often assumes an easier model class, e.g. additive noise).

2.2 Interventions

We are now ready to use the structure of SEMs to construct the “other distributions” $\tilde{\mathbb{P}}^{\mathbf{X}}$ from $\mathbb{P}^{\mathbf{X}}$.

Definition 2.2.1 [Intervention Distribution] Consider a distribution $\mathbb{P}^{\mathbf{X}}$ that has been generated from an SEM $\mathcal{S} := (\mathcal{S}, \mathbb{P}^{\mathbf{N}})$. We can then replace one (or more) structural equations (without generating cycles in the graph) and obtain a new SEM $\tilde{\mathcal{S}}$. We call the distributions in the new SEM *intervention distributions* and say that the variables whose structural equation we have replaced have been “intervened on”. We denote the new distribution by¹

$$\mathbb{P}_{\tilde{\mathcal{S}}}^{\mathbf{X}} = \mathbb{P}_{\mathcal{S}}^{\mathbf{X} | do(X_j = \tilde{f}(\tilde{\mathbf{P}}\mathbf{A}_j, \tilde{N}_j))}.$$

The set of noise variables in \mathcal{S} now contains both some “new” \tilde{N} ’s and some “old” N ’s and is required to be mutually independent.

When $\tilde{f}(\tilde{\mathbf{P}}\mathbf{A}_j, \tilde{N}_j)$ puts a point mass on a real value a , we simply write $\mathbb{P}_{\tilde{\mathcal{S}}}^{\mathbf{X} | do(X_j = a)}$ and call this a **perfect** intervention². An intervention with $\tilde{\mathbf{P}}\mathbf{A}_j = \mathbf{P}\mathbf{A}_j$ is called **imperfect**³. It’s a special case of a **stochastic** intervention [Korb et al., 2004], in

¹Although the set of parents can change arbitrarily (as long as they are not introducing cycles), we mainly consider interventions, for which the new set of parents $\tilde{\mathbf{P}}\mathbf{A}_j$ is either empty or equals $\mathbf{P}\mathbf{A}_j$.

²This is also referred to as an **ideal, structural** [Eberhardt and Scheines, 2007], **surgical** [Pearl, 2009], **independent** or **deterministic** [Korb et al., 2004] intervention.

³This has also been referred to as a **parametric** [Eberhardt and Scheines, 2007] or **dependent** intervention [Korb et al., 2004] or simply as a **mechanism change** [Tian and Pearl, 2001]. Unfortunately, the term **soft** intervention can either mean the same thing [Eberhardt and Scheines, 2007] and is also used for an intervention that increases the chances that a node takes a particular value [Eaton and Murphy, 2007, Markowetz et al., 2005]

which the marginal distribution of the intervened variable has positive variance.

(Because of acyclicity the set of allowed interventions depends on the graph induced by \mathcal{S} .) It turns out that this simple concept is a powerful tool to model differences in distributions and to understand causal relationships. We try to illustrate this with a couple of examples.

Example 2.2.2 [“Cause-Effect”] Suppose that $\mathbb{P}^{(X,Y)}$ is induced by a structural equation model \mathcal{S}

$$X = N_X \tag{2.2}$$

$$Y = 4 \cdot X + N_Y \tag{2.3}$$

with $N_X, N_Y \stackrel{\text{iid}}{\sim} \mathcal{N}(0, 1)$ and graph $X \rightarrow Y$. Then,

$$\begin{aligned} \mathbb{P}_{\mathcal{S}}^Y &= \mathcal{N}(0, 17) \neq \mathcal{N}(8, 1) = \mathbb{P}_{\mathcal{S}}^{Y|do(X=2)} = \mathbb{P}_{\mathcal{S}}^{Y|X=2} \\ &\neq \mathcal{N}(12, 1) = \mathbb{P}_{\mathcal{S}}^{Y|do(X=3)} = \mathbb{P}_{\mathcal{S}}^{Y|X=3} . \end{aligned}$$

Intervening on X changes the distribution of Y .

But on the other hand,

$$\mathbb{P}_{\mathcal{S}}^{X|do(Y=2)} = \mathcal{N}(0, 1) = \mathbb{P}_{\mathcal{S}}^X = \mathbb{P}_{\mathcal{S}}^{X|do(Y=314159265)} \neq \mathbb{P}_{\mathcal{S}}^{X|Y=2} .$$

No matter how strongly we intervene on Y , the distribution of X remains what it was before. This model behavior corresponds well to our intuition of X is “causing” Y : no matter how much we whiten someone’s teeth, this will not have any effect on his smoking habits.

The asymmetry between cause and effect can also be formulated as an independence statement: When we replace the structural equation for Y with $Y = \tilde{N}_Y$, we break the dependence between X and Y : in $\mathbb{P}_{\mathcal{S}}^{X,Y|do(Y=\tilde{N}_Y)}$ we find $X \perp\!\!\!\perp Y$. This does not hold for $\mathbb{P}_{\mathcal{S}}^{X,Y|do(X=\tilde{N}_X)}$ as long as $\text{var}(\tilde{N}_X) \neq 0$: the correlation between X and Y is non-zero.

We use the latter statement in the preceding Example 2.2.2 for defining the existence of a (total) causal effect.

Definition 2.2.3 [total causal effect] Given an SEM \mathcal{S} , there is a **(total) causal effect** from X to Y if and only if

$$X \not\perp\!\!\!\perp Y \quad \text{in } \mathbb{P}_{\mathcal{S}}^{\mathbf{X}|do(X=\tilde{N}_X)}$$

for some variable \tilde{N}_X .

There are several equivalent statements.

Proposition 2.2.4 *Given an SEM S , the following statements are equivalent*

- (i) *There is a causal effect from X to Y .*
- (ii) *There are x^Δ and x^\square , such that $\mathbb{P}_S^{Y|do(X=x^\Delta)} \neq \mathbb{P}_S^{Y|do(X=x^\square)}$.*
- (iii) *There is x^Δ , such that $\mathbb{P}_S^{Y|do(X=x^\Delta)} \neq \mathbb{P}_S^Y$.*
- (iv) *$X \not\perp\!\!\!\perp Y$ in $\mathbb{P}_S^{X,Y|do(X=\tilde{N}_X)}$ for any \tilde{N}_X that has full support.*

The proof can be found in Appendix A.2.1.

Remark 2.2.5 [the “correct” SEM] So far SEMs are mathematical objects. We regard them as models for a data generating process both with and without interventions in real life. It is a complicated model though. Instead of modeling “just” a joint distribution (as we can model a physical process with a Poisson process, for example) we now model the system in an observational state and under perturbations at the same time.

Formally, we say that an SEM S over $\mathbf{X} = (X_1, \dots, X_p)$ is a correct model (the “correct SEM”) for the underlying data generating process if the observational distribution is correct and all interventional distributions $\mathbb{P}_S^{\mathbf{X}|do(X_j=\tilde{N}_j)}$ correspond to distributions that we obtain from randomized experiments⁴. Importantly, an SEM is therefore falsifiable (if we can do the randomized experiments).

For the rest of this section we usually provide the correct SEM. Under what kind of assumptions we can obtain the SEM from real data is the question of Chapter 4.

Example 2.2.6 [Randomized trials] In randomized trials we randomly assign the treatment T according to \tilde{N}_T to a patient (this may include a placebo). In the SEM, this is modeled with observing data from the distribution $\mathbb{P}_S^{\mathbf{X}|do(T=\tilde{N}_T)}$. If we then still find a dependence between the treatment and recovery, for example, we conclude that T has a total causal effect on the recovery.

The idea of using randomized trials for causal inference was described (using different mathematical language) by C.S. Peirce [Peirce, 1883, Peirce and Jastrow, 1885] and later by J. Neyman [Splawa-Neyman et al., 1990, a translated and edited version of the original article] and R.A. Fisher [Fisher, 1925], for applications in agriculture.

One of the first examples of a randomized experiment was performed by James Lind. During the 18th century Great Britain lost more soldiers due to scurvy than to enemy action. James Lind thought that scurvy is a putrefaction of the body and expected acids to be helpful. In 1747, he treated 12 sailors who caught the disease in 6 different ways: with apple cider, drops of sulfuric acid, vinegar, sea water, two oranges and one lemon and barley water respectively. After a couple of days the two subjects treated

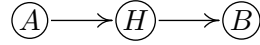
⁴This includes the assumption that there is an agreement about what a randomized experiment should look like.

with citrus fruits had recovered and the two people drinking cider showed first signs of recovery [Wikipedia, 2015].

Example 2.2.7 [Nicolai’s running-and-health example] The underlying (“correct”) SEM that generated the data has the following form:

$$\mathbf{S} : \begin{aligned} A &= N_A \\ H &= A \oplus N_H \\ B &= H \oplus N_B \end{aligned}$$

with graph



where $N_A \sim \text{Ber}(1/2)$, $N_H \sim \text{Ber}(1/3)$ and $N_B \sim \text{Ber}(1/20)$ are independent. The symbol \oplus denotes addition modulo 2 (i.e. $1 \oplus 1 = 0$). Although B is in some sense a better predictor for H than A (e.g. the mutual information between B and H is larger than the mutual information between A and H), an intervention on A has a larger influence on H than intervening on B . More precisely, we have that

$$\mathbb{P}_S^{H|do(B=1)} = \mathbb{P}_S^H \quad (\text{forcing } B \text{ to be one})$$

and

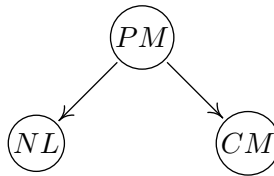
$$\mathbb{P}_S^{H|do(A=1)} = \text{Ber}(2/3) \neq \text{Ber}(1/2) = \mathbb{P}_S^H \quad (\text{forcing } A \text{ to be one})$$

We now revisit the example about myopia (the example about chocolate and Nobel prizes works analogously).

Example 2.2.8 [Myopia, cont.] Assume that the underlying (“correct”) SEM is of the form

$$\mathbf{S} : \begin{aligned} PM &= N_{PM} \\ NL &= f(PM, N_{NL}) \\ CM &= g(PM, N_{CM}) \end{aligned}$$

where PM stands for parent myopia, NL for night light and CM for child myopia. The corresponding graph is



Quinn et al. [1999] found that $NL \not\perp\!\!\!\perp CM$ but if we replace the structural equation of NL with $NL = \tilde{N}_{NL}$, we have $NL \perp\!\!\!\perp CM$ in the intervention distribution (since $CM = g(N_{PM}, N_{CM})$). This holds for any variable \tilde{N}_{NL} , in particular for variables with full support. Thus, there is no causal effect from NL to CM .

In general, we have that

Proposition 2.2.9 (i) *If there is no directed path from X to Y , then there is no causal effect.*

(ii) *Sometimes there is a directed path but no causal effect.*

The proof can be found in Appendix A.2.2.

2.3 Counterfactuals

The definition and interpretation of counterfactuals has received a lot of attention in literature. They concern the following situation: assume you are playing poker and as a starting hand you have $\clubsuit J$ and $\clubsuit 3$ (sometimes called a “lumberjack” - tree and a jack); you fold because you estimate the probability of winning not to be high enough. The flop, however, turns out to be $\clubsuit 4$, $\clubsuit Q$ and $\clubsuit 2$. The reaction is a typical counterfactual statement: “If I had stayed in the game, my chances would have been good.”

Definition 2.3.1 Consider an SEM $\mathcal{S} := (\mathbf{S}, \mathbb{P}^{\mathbf{N}})$ over nodes \mathbf{X} . Given some observations \mathbf{x} , we define a *counterfactual SEM* by replacing the distribution of noise variables:

$$\mathcal{S}_{\mathbf{X}=\mathbf{x}} := (\mathbf{S}, \mathbb{P}_{\mathcal{S}, \mathbf{X}=\mathbf{x}}^{\mathbf{N}}),$$

where $\mathbb{P}_{\mathcal{S}, \mathbf{X}=\mathbf{x}}^{\mathbf{N}} := \mathbb{P}^{\mathbf{N}} | \mathbf{X}=\mathbf{x}$. The new set of noise variables need not be mutually independent anymore. *Counterfactual statements* can now be seen as *do*-statements in the new counterfactual SEM⁵.

This definition can be generalized such that we observe not the full vector $\mathbf{X} = \mathbf{x}$ but only some of the variables.

Example 2.3.2 Consider the following SEM

$$\begin{aligned} X &= N_X \\ Y &= X^2 + N_Y \\ Z &= 2 \cdot Y + X + N_Z \end{aligned}$$

with $N_X, N_Y, N_Z \stackrel{\text{iid}}{\sim} \mathcal{N}(0, 1)$. Now, assume that we observe $(X, Y, Z) = (1, 2, 4)$. Then $\mathbb{P}_{\mathcal{S}, \mathbf{X}=\mathbf{x}}^{\mathbf{N}}$ puts a point mass on $(N_X, N_Y, N_Z) = (1, 1, -1)$. We therefore have the counterfactual statement (in the context of $(X, Y, Z) = (1, 2, 4)$): “ Z would have been 11, had X been 2.” Mathematically, this means that $\mathbb{P}_{\mathcal{S}, \mathbf{X}=\mathbf{x}}^{Z | \text{do}(X=2)}$ has a point mass on 11.

In the same way, we obtain “ Y would have been 5, had X been 2.” and “ Z would have been 10, had Y been 5.”

⁵for simplicity, we consider only *do*-statements, for which the replaced structural equation contains a new noise variable that is independent of all other noise variables

Example 2.3.3 Consider the following made up scenario: a patient with poor eyesight comes to the hospital and goes blind ($B = 1$) after the doctor suggests the treatment $T = 1$. Let us assume that the correct SEM has the form

$$S: \begin{array}{lcl} T & = & N_T \\ B & = & T \cdot N_B + (1 - T) \cdot (1 - N_B) \end{array}$$

with $N_B \sim Ber(0.01)$ and corresponding graph $T \rightarrow B$. The question: “What would have happened had the doctor decided to give treatment $T = 0$?” can be answered with

$$\mathbb{P}_{S, B=1, T=1}^{B | do(T=0)} = Ber(0),$$

i.e.,

$$\mathbb{P}_{S, B=1, T=1}(B = 0 | do(T = 0)) = 1,$$

the patient would have been cured ($B = 0$) if the doctor had given him treatment $T = 0$. Because of

$$\begin{aligned} \mathbb{P}_S(B = 0 | do(T = 1)) &= 0.99 \quad \text{and} \\ \mathbb{P}_S(B = 0 | do(T = 0)) &= 0.01, \end{aligned}$$

however, we can still argue that the doctor acted optimally (according to his knowledge).

Counterfactual statements depend strongly on the structure of the SEM. The following example shows two SEMs that agree on all observational and interventional statements but predict different counterfactual statements.

Example 2.3.4 Let $N_1, N_2 \sim Ber(0.5)$ and $N_3 \sim U(\{0, 1, 2\})$, such that the three variables are jointly independent. That is, N_1, N_2 have a Bernoulli distribution with parameter 0.5 and N_3 is uniformly distributed on $\{0, 1, 2\}$. We define two different SEMs, first consider \mathcal{S}_A :

$$\begin{aligned} X_1 &= N_1 \\ X_2 &= N_2 \\ X_3 &= (1_{N_3 > 0} \cdot X_1 + 1_{N_3 = 0} \cdot X_2) \cdot 1_{X_1 \neq X_2} + N_3 \cdot 1_{X_1 = X_2}. \end{aligned}$$

If X_1 and X_2 have different values, depending on N_3 we either choose $X_3 = X_1$ or $X_3 = X_2$. Otherwise $X_3 = N_3$. Now, \mathcal{S}_B differs from \mathcal{S}_A only in the latter case:

$$\begin{aligned} X_1 &= N_1 \\ X_2 &= N_2 \\ X_3 &= (1_{N_3 > 0} \cdot X_1 + 1_{N_3 = 0} \cdot X_2) \cdot 1_{X_1 \neq X_2} + (2 - N_3) \cdot 1_{X_1 = X_2}. \end{aligned}$$

It can be checked that both SEMs generate the same observational distribution, which satisfies causal minimality with respect to the graph $X_1 \rightarrow X_3 \leftarrow X_2$. They also generate the same intervention distributions, for any possible intervention. But the

two models differ in a counterfactual statement. Suppose, we have seen a sample $(X_1, X_2, X_3) = (1, 0, 0)$ and we are interested in the counterfactual question, what X_3 would have been if X_1 had been 0. From both SEMs it follows that $N_3 = 0$, and thus the two SEMs \mathcal{S}_A and \mathcal{S}_B “predict” different values for X_3 under a counterfactual change of X_1 (namely 0 and 2 respectively).

If we want to use an estimated SEM to predict counterfactual questions, this example shows that we require assumptions that let us distinguish between \mathcal{S}_A or \mathcal{S}_B .

We now summarize some properties of counterfactuals.

- Remark 2.3.5** (i) Counterfactual statements are not transitive. In Example 2.3.2 we found that given the observation $(X, Y, Z) = (1, 2, 4)$, Y would have been 5, had X been 2 and Z would have been 10, had Y been 5 but Z would have not been 10 had X been 2.
- (ii) Humans often think in counterfactuals: “I should have taken the train.”, “Do you remember our flight to New York on Sep 11th 2000? Imagine we would have taken the flight one year later!” and “Imagine we would have invested in CHF last year.” are only few examples. Interestingly, this sometimes even concerns situations in which we made optimal decisions (based on the available information). Assume, someone offers you \$10,000 if you predict the result of a coin flip, you guess ‘heads’ and lose. How many people would think: “Why didn’t I say ‘tails’?” Discussing whether counterfactual statements contain any information that can help us making better decisions in future is interesting but lies beyond this work.
- (iii) Similarly, we cannot provide details about the role of counterfactuals in our law system. The question whether counterfactuals should be taken as a basis of verdicts, for example, seems interesting to us though (see Example 2.3.3).
- (iv) Thinking about counterfactuals has been done since a long time; it is a popular tool of historians. Titus Livius, for example, discusses in 25BC what would have happened if Alexander the Great had not died in Asia and had attacked Rome [Geradin and Girgenson, 2011].
- (v) We can think of interventional statements as a mathematical construct for (randomized) experiments. For counterfactual statements, there is no apparent correspondence in the real world. But if there is none, these statements may be considered as being not falsifiable and therefore as non-scientific according to Popper [e.g. Popper, 2002].

2.4 Markov property, faithfulness and causal minimality

We now develop some language that helps us to formalize some ideas that we have had in the preceding sections.

2.4.1 Markov property

The Markov property is a commonly used assumption that is on the basis of graphical modeling. When a distribution is Markov with respect to a graph, this graph encodes certain independencies in the distribution that we can exploit for efficient computation or data storage. The Markov property exists for both directed and undirected graphs and it is well known that these two classes encode different sets of independencies. In causal inference, however, we are mainly interested in directed graphs. While many introductions to causal inference start with the Markov property as the underlying assumption, we will derive it as a property of SEMs.

Definition 2.4.1 [Markov property] Given a DAG \mathcal{G} and a joint distribution $\mathbb{P}^{\mathbf{X}}$, this distribution is said to satisfy

- (i) the **global Markov property** with respect to the DAG \mathcal{G} if

$$\mathbf{A}, \mathbf{B} \text{ } d\text{-sep. by } \mathbf{C} \Rightarrow \mathbf{A} \perp\!\!\!\perp \mathbf{B} \mid \mathbf{C}$$

for all disjoint sets $\mathbf{A}, \mathbf{B}, \mathbf{C}$,

- (ii) the **local Markov property** with respect to the DAG \mathcal{G} if each variable is independent of its non-descendants given its parents, and
- (iii) the **Markov factorization property** with respect to the DAG \mathcal{G} if

$$p(\mathbf{x}) = p(x_1, \dots, x_p) = \prod_{j=1}^p p(x_j \mid x_{\mathbf{PA}_j^{\mathcal{G}}})$$

(here, we have to assume that $\mathbb{P}^{\mathbf{X}}$ has a density p).

It turns out that as long as the joint distribution has a density⁶ these three definitions are equivalent.

Theorem 2.4.2 *If $\mathbb{P}^{\mathbf{X}}$ has a density p (with respect to a product measure), then all Markov properties in Definition 2.4.1 are equivalent.*

The proof can be found as Theorem 3.27 in [Lauritzen, 1996], for example.

Example 2.4.3 A distribution $\mathbb{P}^{X_1, X_2, X_3, X_4}$ is Markov with respect to the graph \mathcal{G}_0 shown in Figure 2.1 if, according to (i) or (ii), $X_2 \perp\!\!\!\perp X_3 \mid X_1$ and $X_1 \perp\!\!\!\perp X_4 \mid X_2, X_3$, or, according to (iii),

$$p(x_1, x_2, x_3, x_4) = p(x_3)p(x_1 \mid x_3)p(x_2 \mid x_1)p(x_4 \mid x_2, x_3).$$

We will see later in Proposition 2.5.1 that the distribution generated from the SEM shown on the left hand side in Figure 2.1 on page 20 is Markov w.r.t. \mathcal{G}_0 .

⁶In this script, we always consider densities with respect to Lebesgue or counting measure. For this theorem it suffices if the distribution is absolutely continuous w.r.t. a product measure.

Definition 2.4.4 [Markov equivalence class of graphs] We denote by $\mathcal{M}(\mathcal{G})$ the set of distributions that are Markov with respect to \mathcal{G} :

$$\mathcal{M}(\mathcal{G}) := \{\mathbb{P} : \mathbb{P} \text{ satisfies the global (or local) Markov property w.r.t. } \mathcal{G}\}.$$

Two DAGs \mathcal{G}_1 and \mathcal{G}_2 are **Markov equivalent** if $\mathcal{M}(\mathcal{G}_1) = \mathcal{M}(\mathcal{G}_2)$. This is the case if and only if \mathcal{G}_1 and \mathcal{G}_2 satisfy the same set of d -separations, that means the Markov condition entails the same set of (conditional) independence conditions. The set of all DAGs that are Markov equivalent to some DAG (a so-called Markov equivalence class) can be represented by a **completed PDAG** $\text{CPDAG}(\mathcal{G}) = (V, \mathcal{E})$. This graph satisfies $(i, j) \in \mathcal{E}$ if and only if one member of the Markov equivalence class does.

Verma and Pearl [1991] showed that:

Lemma 2.4.5 *Two DAGs are Markov equivalent if and only if they have the same skeleton and the same immoralities.*

The following figure Figure 2.2 shows an example of two Markov equivalent graphs. The graphs share the same skeleton and both of them have the immorality $Z \rightarrow V \leftarrow U$.

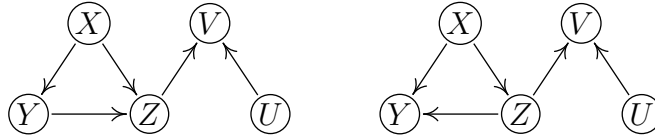


Figure 2.2: Two Markov-equivalent DAGs.

Remark 2.4.6 Consider a graph $\mathcal{G} = (\mathbf{V}, \mathcal{E})$ and a target node Y . The *Markov blanket* of Y is the smallest set M such that

$$Y \text{ } d\text{-sep } \mathbf{V} \setminus (\{Y\} \cup M) \text{ given } M.$$

If $\mathbb{P}^{\mathbf{X}}$ is Markov w.r.t. \mathcal{G} , then

$$Y \perp\!\!\!\perp \mathbf{V} \setminus (\{Y\} \cup M) \text{ given } M.$$

If we have a powerful regression technique, we only need to include the variables in M for predicting Y . Given the Markov blanket, the other variables do not provide any further information about Y .

Remark 2.4.7 [Reichenbach’s common cause principle] Reichenbach’s common cause principle [Reichenbach, 1956] states that when the random variables X and Y are dependent, there must be a “causal explanation” for this dependence:

- X is (possibly indirectly) causing Y or

- Y is (possibly indirectly) causing X or
- there is a (possibly unobserved) confounder T that (possibly indirectly) causes both X and Y .

Here, we do not further specify the meaning of the word “causing”.

Proposition 2.4.8 *Assume that any pair of variables X and Y can be embedded into a larger system in the following sense: there exists a correct SEM over the collection \mathbf{X} of random variables that contains X and Y with graph \mathcal{G} . Then the Reichenbach’s common cause principle follows from the Markov property in the following sense: If X and Y are dependent, then there is*

- *either a directed path from X to Y*
- *or from Y to X*
- *or there is a node T with a directed path from T to X and from T to Y .*

Proof. The proof is immediate: Given dependent variables X and Y we embed them into a larger system of random variables with graph \mathcal{G} . Because of the Markov property, \mathcal{G} contains an unblocked path between X and Y . \square

In Reichenbach’s principle, we start with two dependent random variables and obtain a valid statement. In real applications, however, it might be that we have implicitly conditioned on a third variable (“selection bias”). As the following example shows⁷, this may lead to a dependence between X and Y , although there none of the three conditions hold.

Example 2.4.9 Let us assume that whether you study engineering in Zurich ($Z = 1$) is determined only by the fact whether you like nature ($N = 1$) and whether you think ETH is a great university ($U = 1$). More precisely, assume that the correct SEM has the form:

$$\begin{aligned} N &= N_N, \\ U &= N_U, \\ Z &= \text{OR}(N, U) \oplus N_Z, \end{aligned}$$

where $N_N, N_U \stackrel{\text{iid}}{\sim} \text{Ber}(0.5)$, $N_Z \sim \text{Ber}(0.1)$ and $\text{OR}(N, U)$ equals one if either $N = 1$ or $U = 1$ and zero otherwise. Again, \oplus is addition modulo 2, see Example 2.2.7. As we can see from the SEM, N and U are assumed to be independent. If you ask engineering students *in Zurich*, however, i.e. you condition on $Z = 1$, the answers to whether they like nature or ETH become anti-correlated: if someone is not a fan of nature, he probably likes ETH and vice versa (otherwise he would have not studied at ETH). We have that

$$N \not\perp\!\!\!\perp U \mid Z = 1.$$

⁷The author thanks Marloes Maathuis for pointing out this comment and Dominik Janzing for the example.

The Markov assumption gives us the ability to read off independencies from the graph structure. Faithfulness (defined in the following section) allows us to infer dependencies from the graph structure, see Example 2.4.9.

2.4.2 Faithfulness and causal minimality

Definition 2.4.10 (i) $\mathbb{P}^{\mathbf{X}}$ is said to be **faithful to the DAG \mathcal{G}** if

$$\mathbf{A}, \mathbf{B} \text{ } d\text{-sep. by } \mathbf{C} \Leftarrow \mathbf{A} \perp\!\!\!\perp \mathbf{B} \mid \mathbf{C}$$

for all disjoint sets $\mathbf{A}, \mathbf{B}, \mathbf{C}$ (compare this to the global Markov condition).

(ii) A distribution satisfies **causal minimality** with respect to \mathcal{G} if it is Markov with respect to \mathcal{G} , but not to any proper subgraph of \mathcal{G} .

Faithfulness is not very intuitive at first glance. We now give an example of a distribution that is Markov but not faithful with respect to some DAG \mathcal{G}_1 . This is achieved by making two paths cancel each other and creating an independence that is not implied by the graph structure.

Example 2.4.11 Consider the two graphs in the following figure.



We first look at a linear Gaussian SEM that corresponds to the left graph \mathcal{G}_1 .

$$\begin{aligned} X &= N_X, \\ Y &= aX + N_Y, \\ Z &= bY + cX + N_Z, \end{aligned}$$

with normally distributed noise variables $N_X \sim \mathcal{N}(0, \sigma_X^2)$, $N_Y \sim \mathcal{N}(0, \sigma_Y^2)$ and $N_Z \sim \mathcal{N}(0, \sigma_Z^2)$ that are jointly independent. This is an example of a linear Gaussian structural equation model with graph \mathcal{G}_1 , see Definition 2.1.1. Now, if $a \cdot b + c = 0$, the distribution is not faithful with respect to \mathcal{G}_1 since we obtain $X \perp\!\!\!\perp Z$; more precisely, it is not triangle-faithful [Zhang and Spirtes, 2008].

Correspondingly, we consider a SEM that corresponds to graph \mathcal{G}_2 :

$$\begin{aligned} X &= \tilde{N}_X, \\ Y &= \tilde{a}X + \tilde{b}Z + \tilde{N}_Y, \\ Z &= \tilde{N}_Z, \end{aligned}$$

with all $\tilde{N}_i \sim \mathcal{N}(0, \tau_i^2)$ jointly independent. If we choose $\tau_X^2 = \sigma_X^2$, $\tilde{a} = a$, $\tau_Z^2 = b^2\sigma_Y^2 + \sigma_Z^2$, $\tilde{b} = (b\sigma_Y^2)/(b^2\sigma_Y^2 + \sigma_Z^2)$ and $\tau_Y^2 = \sigma_Y^2 - (b^2\sigma_Y^4)/(b^2\sigma_Y^2 + \sigma_Z^2)$, both models lead to the covariance matrix

$$\Sigma = \begin{pmatrix} \sigma_X^2 & a\sigma_X^2 & 0 \\ a\sigma_X^2 & a^2\sigma_X^2 + \sigma_Y^2 & b\sigma_Y^2 \\ 0 & b\sigma_Y^2 & b^2\sigma_Y^2 + \sigma_Z^2 \end{pmatrix}$$

and thus to the same observational distribution. It can be checked that the distribution is faithful with respect to \mathcal{G}_2 if $\tilde{a}, \tilde{b} \neq 0$ and all $\tilde{\tau}_i > 0$.

The distribution from Example 2.4.11 is faithful with respect to \mathcal{G}_2 , but not with respect to \mathcal{G}_1 . Nevertheless, for both models, causal minimality is satisfied if none of the parameters vanishes: the distribution is not Markov to any proper subgraph of \mathcal{G}_1 or \mathcal{G}_2 since removing an arrow would correspond to a new (conditional) independence that does not hold in the distribution. Note that \mathcal{G}_2 is not a proper subgraph of \mathcal{G}_1 . In general, causal minimality is weaker than faithfulness:

Remark 2.4.12 If $\mathbb{P}^{\mathbf{X}}$ is faithful and Markov with respect to \mathcal{G} , then causal minimality is satisfied.

This is due to the fact that any two nodes that are not directly connected by an edge can be d -separated.

It turns out that in most model classes, identifiability is impossible to obtain without causal minimality: we cannot distinguish between $Y = f(X) + N_Y$ and $Y = c + N_Y$, for example, if f is allowed to be constant. At first, we therefore look at an equivalent formulation of causal minimality in the case of SEMs.

Proposition 2.4.13 *Consider the random vector $\mathbf{X} = (X_1, \dots, X_p)$ and assume that the joint distribution has a density with respect to a product measure. Suppose that $\mathbb{P}^{\mathbf{X}}$ is Markov with respect to \mathcal{G} . Then $\mathbb{P}^{\mathbf{X}}$ satisfies causal minimality with respect to \mathcal{G} if and only if $\forall X_j \forall Y \in \mathbf{PA}_j^{\mathcal{G}}$ we have that $X_j \not\perp\!\!\!\perp Y \mid \mathbf{PA}_j^{\mathcal{G}} \setminus \{Y\}$.*

Proof. See Appendix A.2.5. □

2.5 Some more properties of SEMs

Pearl [2009] shows in Theorem 1.4.1 that the law $\mathbb{P}^{\mathbf{X}}$ generated by an SEM is Markov with respect to its graph.

Proposition 2.5.1 *Assume that $\mathbb{P}^{\mathbf{X}}$ is generated by an SEM with graph \mathcal{G} . Then, $\mathbb{P}^{\mathbf{X}}$ is Markov with respect to \mathcal{G} .*

We can now come back to the question how large the class of SEMs is. More precisely, we are interested in the question: “Give a distribution $\mathbb{P}^{\mathbf{X}}$, how many different SEMs can generate this distribution? This can be answered with the following proposition⁸.

⁸Similar but weaker statements than Proposition 2.5.2 can be found in Druzdzel and Simon [1993], Druzdzel and van Leijen [2001], Janzing and Schölkopf [2010].

Proposition 2.5.2 *Consider X_1, \dots, X_p and let $\mathbb{P}^{\mathbf{X}}$ have a strictly positive density with respect to Lebesgue measure and assume it is Markov with respect to \mathcal{G} . Then there exists an SEM $(\mathcal{S}, \mathbb{P}^{\mathbf{N}})$ with graph \mathcal{G} that generates the distribution $\mathbb{P}^{\mathbf{X}}$.*

Proof. See Appendix A.2.3. □

Remark 2.5.3 Why do we primarily work with SEMs and not just with graphs and the Markov condition (i.e. graphical models)? Formally, structural equation models contain strictly more information than their corresponding graph and law (e.g. counterfactual statements) and hence also more information than the family of all intervention distributions together with the observational distribution. It is debatable though, whether this additional information is useful. Maybe more importantly, we will see later that restricting the function class in SEMs can lead to identifiability of the causal structure. Those assumptions are easier to phrase in the language of SEMs compared to graphical models.

2.6 Exercises

Exercise 2.6.1 *Why can we d -separate any two nodes in a DAG \mathcal{G} that are not directly connected by an edge. Use this statement to prove Remark 2.4.12.*

Chapter 3

Using the known underlying causal structure

In the following chapters we will make use of an invariance statement. We first state it as a tautology in the hope that this helps the reader to remember it:

“If we replace only the structural equation for X_j ,
we replace only the structural equation for X_j .”

More precisely, we mean that given an SEM \mathcal{S} , we have

$$p_{\tilde{\mathcal{S}}}(x_k \mid x_{pa(k)}) = p_{\mathcal{S}}(x_k \mid x_{pa(k)}) \quad (3.1)$$

for any SEM $\tilde{\mathcal{S}}$ that is constructed from \mathcal{S} by replacing the structural equation(s) for (some) X_j but not the one for X_k . Equation (3.1) shows that causal relationships are autonomous under interventions, it is therefore sometimes called “autonomy”, but also “structural invariance” or “separability”. Aldrich [1989] provides a brief overview of the historical development in economy. Interestingly, Aldrich [1989] argues that the “‘most basic’ question one can ask about a relation should be: How autonomous is it?” [?, preface]. Other relevant references include work from Frisch’s assistant Trygve Haavelmo [Haavelmo, 1944, Girshick and Haavelmo, 1947]. For a discussion and more references see also [Pearl, 2009, chapter 1.4]. Schölkopf et al. [2012] discusses the potential relevance of autonomy for machine learning.

3.1 Adjustment formulas

3.1.1 Truncated factorization, G -computation formula or manipulation theorem

We deduce a formula from (3.1) that became known under three different names: “truncated factorization” [Pearl, 1993a], “ G -computation formula” [Robins, 1986] and “manipulation theorem” [Spirtes et al., 1993]. Its importance stems from the fact that it allows us to compute statements about distributions that we have never seen data from.

Consider an SEM \mathcal{S} with structural equations

$$X_j = f_j(X_{pa(j)}, N_j)$$

and density $p_{\mathcal{S}}$. Because of the Markov property we have

$$p_{\mathcal{S}}(x_1, \dots, x_p) = \prod_{j=1}^p p_{\mathcal{S}}(x_j | x_{pa(j)}).$$

Now consider the SEM $\tilde{\mathcal{S}}$ which evolves from \mathcal{S} after $do(X_k = \tilde{N}_k)$, where \tilde{N}_k allows for the density \tilde{p} . Again, it follows from the Markov assumption that

$$p_{\mathcal{S}, do(X_k = \tilde{N}_k)}(x_1, \dots, x_p) = \prod_{j=1}^p p_{\mathcal{S}, do(X_j = \tilde{N}_j)}(x_j | x_{pa(j)}) = \prod_{j \neq k} p_{\mathcal{S}}(x_j | x_{pa(j)}) \tilde{p}(x_k). \quad (3.2)$$

As a special case we obtain

$$p_{\mathcal{S}, do(X_k = a)}(x_1, \dots, x_p) = \begin{cases} \prod_{j \neq k} p_{\mathcal{S}}(x_j | x_{pa(j)}) & \text{if } x_k = a \\ 0 & \text{otherwise.} \end{cases} \quad (3.3)$$

It immediately follows that conditioning and intervening with $do()$ becomes equivalent for any variable that does not have any parents (w.l.o.g. let X_1 be such a source node):

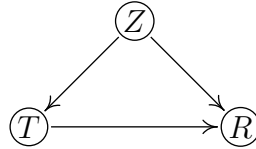
$$p_{\mathcal{S}}(x_2, \dots, x_p | x_1 = a) = \frac{p(x_1 = a) \prod_{j=2}^p p_{\mathcal{S}}(x_j | x_{pa(j)})}{p(x_1 = a)} = p_{\mathcal{S}, do(X_1 = a)}(x_2, \dots, x_p). \quad (3.4)$$

In general, however, intervening and conditioning are usually two different things.

3.1.2 Invariances and adjusting

Equations (3.2) and (3.3) are widely applicable but sometimes a bit cumbersome to use. We will now learn about some practical alternatives. Therefore, we recall the kidney stone Example 1.1.3 that we will be able to generalize.

Example 3.1.1 [kidney stones, cont.] Assume that the true underlying SEM allows for the graph



Here, Z is the size of the stone, T the treatment and R the recovery (all binary). Consider further the two SEMs \mathcal{S}_A and \mathcal{S}_B that we obtain after replacing the structural equation for T with $T = A$ and $T = B$ respectively. Let us call the corresponding

resulting probability distributions $\mathbb{P}_{\mathcal{S}_A}$ and $\mathbb{P}_{\mathcal{S}_B}$. Given that we are diagnosed with a kidney stone *without knowing its size*, we should base our choice of treatment on a comparison between

$$\mathbf{E}_{\mathcal{S}_A} R = \mathbb{P}_{\mathcal{S}_A}(R = 1) = \mathbb{P}_{\mathcal{S}}(R = 1 \mid do(T = A))$$

and

$$\mathbf{E}_{\mathcal{S}_B} R = \mathbb{P}_{\mathcal{S}_B}(R = 1) = \mathbb{P}_{\mathcal{S}}(R = 1 \mid do(T = B)).$$

Given that we have observed data from \mathcal{S} , how can we estimate these quantities? Consider the following computation

$$\mathbb{P}_{\mathcal{S}_A}(R = 1) = \sum_{z=0}^1 \mathbb{P}_{\mathcal{S}_A}(R = 1, T = A, Z = z) \quad (3.5)$$

$$= \sum_{z=0}^1 \mathbb{P}_{\mathcal{S}_A}(R = 1 \mid T = A, Z = z) \mathbb{P}_{\mathcal{S}_A}(T = A, Z = z) \quad (3.6)$$

$$= \sum_{z=0}^1 \mathbb{P}_{\mathcal{S}_A}(R = 1 \mid T = A, Z = z) \mathbb{P}_{\mathcal{S}_A}(Z = z) \quad (3.7)$$

$$\stackrel{(3.1)}{=} \sum_{z=0}^1 \mathbb{P}_{\mathcal{S}}(R = 1 \mid T = A, Z = z) \mathbb{P}_{\mathcal{S}}(Z = z). \quad (3.8)$$

The last step contains the key idea: again, we have made use of (3.1). We can estimate $\mathbb{P}_{\mathcal{S}_A}(R = 1)$ from the empirical data shown in Table 1.1 and obtain

$$\mathbb{P}_{\mathcal{S}_A}(R = 1) \approx 0.93 \times \frac{357}{700} + 0.73 \times \frac{343}{700} = 0.832.$$

It is important to realize that this is different from $\mathbb{P}_{\mathcal{S}}(R = 1 \mid T = 1) = 0.78$. Analogously, we obtain

$$\mathbb{P}_{\mathcal{S}_B}(R = 1) \approx 0.87 \times \frac{357}{700} + 0.69 \times \frac{343}{700} \approx 0.782,$$

and we conclude that we rather go for treatment A . (We have not checked whether there is a statistically significance difference between the treatments but from a decision theoretic point of view we do not need to do so.)

The derivation above could also be seen as an implication from (3.3) but we will see in Proposition 3.1.4 that the idea of this alternative computation carries over to more complicated settings.

Definition 3.1.2 [valid adjustment set] Consider an SEM \mathcal{S} over nodes \mathbf{V} and let $Y \notin \mathbf{PA}_X$ (otherwise we have $p_{\mathcal{S}, do(X=x)}(y) = p_{\mathcal{S}}(y)$). We call a set $\mathbf{Z} \subseteq \mathbf{V} \setminus \{X, Y\}$ a valid adjustment set for X and Y if

$$p_{\mathcal{S}, do(X=x)}(y) = \sum_{\mathbf{z}} p_{\mathcal{S}}(y \mid x, \mathbf{z}) p_{\mathcal{S}}(\mathbf{z}). \quad (3.9)$$

Here, the sum (could also be an integral) is over the range of \mathbf{Z} , i.e., over all values \mathbf{z} that \mathbf{Z} can take.

In Example 3.1.1 above, $\mathbf{Z} = \{Z\}$ is a valid adjustment set. We will now investigate which sets we can use for adjusting. We use the same idea as in Example 3.1.1 and write (for any set \mathbf{Z})

$$\begin{aligned} p_{\mathcal{S}, do(X=x)}(y) &= \sum_{\mathbf{z}} p_{\mathcal{S}, do(X=x)}(y, \mathbf{z}) \\ &= \sum_{\mathbf{z}} p_{\mathcal{S}, do(X=x)}(y \mid x, \mathbf{z}) p_{\mathcal{S}, do(X=x)}(\mathbf{z}). \end{aligned}$$

If these conditionals are invariant, i.e.,

$$p_{\mathcal{S}, do(X=x)}(y \mid x, \mathbf{z}) = p_{\mathcal{S}}(y \mid x, \mathbf{z}) \quad \text{and} \quad p_{\mathcal{S}, do(X=x)}(\mathbf{z}) = p_{\mathcal{S}}(\mathbf{z}), \quad (3.10)$$

we can deduce (as above) that \mathbf{Z} is a valid adjustment set. We therefore address the question, which conditionals remain invariant under the intervention $do(X = x)$.

Remark 3.1.3 [Characterization of invariant conditionals] Consider an SEM \mathcal{S} with structural equations

$$X_j = f_j(\mathbf{PA}_j, N_j)$$

and an intervention $do(X_k = x_k)$. Analogously to what is done in [Pearl, 2009, Chapter 3.2.2], for example, we can now construct a new SEM \mathcal{S}^* that equals \mathcal{S} but has one more variable I that indicates whether the intervention took place or not. More precisely, I is a parent of X_k and does not have any other neighbors. The corresponding structural equations are

$$\begin{aligned} I &= N_I \\ X_j &= f_j(\mathbf{PA}_j, N_j) \quad \text{for } j \neq k \\ X_k &= \begin{cases} f_k(\mathbf{PA}_k, N_k) & \text{if } I = 0 \\ x_k & \text{otherwise} \end{cases}, \end{aligned}$$

where $N_I \sim Ber(0.5)$. Thus, $I = 0$ corresponds to the observational setting and $I = 1$ to the interventional setting. More precisely, using (3.4), we obtain

$$\begin{aligned} p_{\mathcal{S}^*}(x_1, \dots, x_p \mid I = 0) &= p_{\mathcal{S}^*, do(I=0)}(x_1, \dots, x_p) \\ &= p_{\mathcal{S}}(x_1, \dots, x_p) \end{aligned}$$

and similarly

$$p_{\mathcal{S}^*}(x_1, \dots, x_p \mid I = 1) = p_{\mathcal{S}, do(X_k=x_k)}(x_1, \dots, x_p). \quad (3.11)$$

Using the Markov condition for \mathcal{S}^* it thus follows for variables A and a set of variables \mathbf{B} that

$$p_{\mathcal{S}}(a \mid \mathbf{b}) = p_{\mathcal{S}, do(X_j=x_j)}(a \mid \mathbf{b}) \iff A \text{ } d\text{-sep } I \mid \mathbf{B} \quad \text{in } \mathcal{G}^*. \quad (3.12)$$

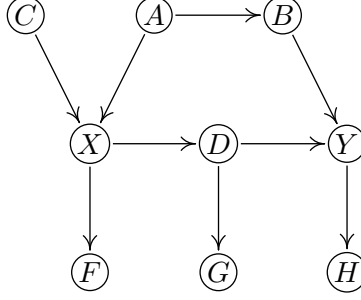


Figure 3.1: Only the path $X \leftarrow A \rightarrow B \rightarrow Y$ is a “backdoor path” from X to Y .

We are now able to continue the argument from before. Equation (3.10) is satisfied for sets \mathbf{Z} , for which we have

$$Y \text{ } d\text{-sep}_{\mathcal{G}^*} I \mid X, \mathbf{Z} \quad \text{and} \quad \mathbf{Z} \text{ } d\text{-sep}_{\mathcal{G}^*} I .$$

The subscript \mathcal{G}^* means that the d -separation statement is required to hold in \mathcal{G}^* . This immediately implies the first two statements of the following proposition.

Proposition 3.1.4 (i) “parent adjustment”:

$$\mathbf{Z} := \mathbf{PA}_j$$

is a valid adjustment set.

(ii) “backdoor-criterion”: Any \mathbf{Z} with

- \mathbf{Z} contains no descendant of X AND
- \mathbf{Z} blocks all paths from X to Y entering X through the backdoor ($X \leftarrow \dots$, see Figure 3.1.2)

is a valid adjustment set.

(iii) “towards necessity”: Any \mathbf{Z} with

- \mathbf{Z} contains no descendant of any node on a directed path from X to Y (except for descendants of X that are not on a directed path from X to Y) AND
- \mathbf{Z} blocks all non-directed paths from X to Y

is a valid adjustment set.

Only the third statement [Shpitser et al., 2010] requires some explanation: we can add any node Z_0 to a valid adjustment set that satisfies $Z_0 \perp\!\!\!\perp Y \mid X$ because then

$$\begin{aligned} \sum_{\mathbf{z}, z_0} p(y \mid x, \mathbf{z}, z_0) p(\mathbf{z}, z_0) &= \sum_{\mathbf{z}} p(y \mid x, \mathbf{z}) \sum_{z_0} p(\mathbf{z}, z_0) \\ &= \sum_{\mathbf{z}} p(y \mid x, \mathbf{z}) p(\mathbf{z}) . \end{aligned}$$

In fact, *all* valid adjustment sets can be characterized by Proposition 3.1.4 (iii) [Shpitser et al., 2010].

Example 3.1.5 [Adjustment in linear Gaussian systems] Consider a linear Gaussian SEM \mathcal{S} over variables \mathbf{V} with $\{X, Y\}, \mathbf{Z} \subseteq \mathbf{V}$. Sometimes, we want to summarize a causal effect from X to Y by a single real number instead of looking at $p_{\mathcal{S}, do(X=x)}(y)$ for all x . As a first approximation we may look at the expectation of this distribution and then take the derivative with respect to x (given that X is continuous):

$$\frac{\partial}{\partial x} \mathbf{E}_{\mathcal{S}, do(X=x)} Y .$$

In general, this is still a function of x . In Gaussian systems, however, this function turns out to be constant. Assume that \mathbf{Z} is a valid adjustment set for (X, Y) . The Gaussian distribution of \mathbf{V} implies that $Y | X, \mathbf{Z}$ follows a Gaussian distribution, too; its mean is

$$aX + \mathbf{b}^t \mathbf{Z}$$

for some a and \mathbf{b} . If there is exactly one directed path from X to Y , then a equals the product of the path coefficients. If there is no directed path, then $a = 0$ and if there are different paths, a can be computed using the Wright's formula [Wright, 1921b]. It follows from (3.9) that

$$\frac{\partial}{\partial x} \mathbf{E}_{\mathcal{S}, do(X=x)} Y = a . \quad (3.13)$$

Remark 3.1.6 It is not the case that all sets are valid adjustment sets. Therefore, it is not always a good idea to adjust for as many variables as possible, for example, cf. Berkson's paradox [Berkson, 1946].

Example 3.1.7 [Simpson's Paradox] Example 1.1.3 on page 9 is well-known for the following reason: we have

$$\begin{aligned} \mathbb{P}_{\mathcal{S}}(R = 1 | T = A) &< \mathbb{P}_{\mathcal{S}}(R = 1 | T = B) && \text{but} \\ \mathbb{P}_{\mathcal{S}}(R = 1 | do(T = A)) &> \mathbb{P}_{\mathcal{S}}(R = 1 | do(T = B)) , \end{aligned} \quad (3.14)$$

see Example 3.1.1. Suppose that we have not measured the confounder Z (size of the stone) and furthermore that we do not even know about its existence. We might then hypothesize that $T \rightarrow R$ is the correct graph. If we denote this (wrong) SEM by $\tilde{\mathcal{S}}$, we can rewrite (3.14) as

$$\begin{aligned} \mathbb{P}_{\tilde{\mathcal{S}}}(R = 1 | do(T = A)) &< \mathbb{P}_{\tilde{\mathcal{S}}}(R = 1 | do(T = B)) && \text{but} \\ \mathbb{P}_{\mathcal{S}}(R = 1 | do(T = A)) &> \mathbb{P}_{\mathcal{S}}(R = 1 | do(T = B)) . \end{aligned} \quad (3.15)$$

Due to the model misspecification, the causal inference statement gets reversed! Although A is the more effective drug, we propose to use B . What happens if there is yet

another confounder that we did not correct for? If we are unlucky, it could be that we have to reverse the conclusion once more if we include this variable. In principle, this could lead to an arbitrarily long sequence of reversed causal conclusions (see Exercises).

This means that we have to be really careful when writing down the underlying graph. In some situations, we know the DAG from the protocol how the data have been recorded. If the medical doctors assigning the treatments, for example, did not have any knowledge about the patient other than the size of the kidney stone, there cannot be any other confounder than the size of the stone. Recent work investigates, whether we can check for confounders if we are willing to make further assumptions on the data generating process [g. Janzing et al., 2009, Sgouritsa et al., 2013].

Summarizing, the Simpson’s paradox is not so much of a paradox but rather an example of how sensitive causal analysis could be with respect to model misspecifications.

3.2 Alternative identification of interventional distributions

Again, consider an SEM over variables \mathbf{V} . Sometimes, we can compute interventional distributions $p_{\mathcal{S}, do(X=x)}$ in other ways than the adjustment formula (3.9). Let us therefore call an interventional distribution $p_{\mathcal{S}, do(X=x)}(y)$ *identifiable* if it can be computed from the observational distribution and the graph structure. If there is a valid adjustment set for (X, Y) , for example, $p_{\mathcal{S}, do(X=x)}(y)$ is certainly identifiable. Judea Pearl has developed the so-called *do*-calculus that contains of three rules [Pearl, 2009, Theorem 3.4.1]. Given a graph \mathcal{G} and disjoint subsets $\mathbf{X}, \mathbf{Y}, \mathbf{Z}$ and \mathbf{W} , we have

1. “Insertion/deletion of observations”:

$$p_{\mathcal{S}, do(\mathbf{X}=\mathbf{x})}(\mathbf{y} \mid \mathbf{z}, \mathbf{w}) = p_{\mathcal{S}, do(\mathbf{X}=\mathbf{x})}(\mathbf{y} \mid \mathbf{w})$$

if \mathbf{Y} *d*-separates \mathbf{Z} given \mathbf{X}, \mathbf{W} in a graph where incoming edges in \mathbf{X} have been removed.

2. “Action/observation exchange”:

$$p_{\mathcal{S}, do(\mathbf{X}=\mathbf{x}, \mathbf{Z}=\mathbf{z})}(\mathbf{y} \mid \mathbf{w}) = p_{\mathcal{S}, do(\mathbf{X}=\mathbf{x})}(\mathbf{y} \mid \mathbf{z}, \mathbf{w})$$

if \mathbf{Y} *d*-separates \mathbf{Z} given \mathbf{X}, \mathbf{W} in a graph where incoming edges in \mathbf{X} and outgoing edges from \mathbf{Z} have been removed.

3. “Insertion/deletion of actions”:

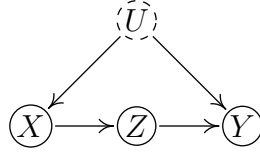
$$p_{\mathcal{S}, do(\mathbf{X}=\mathbf{x}, \mathbf{Z}=\mathbf{z})}(\mathbf{y} \mid \mathbf{w}) = p_{\mathcal{S}, do(\mathbf{X}=\mathbf{x})}(\mathbf{y} \mid \mathbf{w})$$

if \mathbf{Y} *d*-separates \mathbf{Z} given \mathbf{X}, \mathbf{W} in a graph where incoming edges in \mathbf{X} and $\mathbf{Z}(\mathbf{W})$ have been removed. Here, $\mathbf{Z}(\mathbf{W})$ is the subset of nodes in \mathbf{Z} that are not ancestors of any node in \mathbf{W} in a graph that is obtained from \mathcal{G} from removing all edges into \mathbf{X} .

Theorem 3.2.1 *The following statements can be proved*

- *The rules are complete [Shpitser and Pearl, 2006], that is all identifiable intervention distributions can be computed by an iterative application of these three rules.*
- *In fact, there is an algorithm, proposed by Tian [2002] that is guaranteed [Huang and Valtorta, 2006, Shpitser and Pearl, 2006] to find all identifiable interventional distributions.*

Example 3.2.2 [Front-door adjustment] Let \mathcal{S} be an SEM with corresponding graph

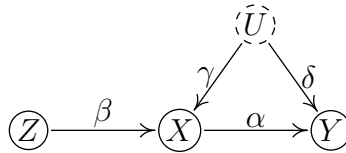


If we do not observe U , we cannot apply the backdoor criterion. In fact, there is no valid adjustment set. But still, provided that $p_{\mathcal{S}}(x, z) > 0$, the *do*-calculus provides us with

$$p_{\mathcal{S}, do(X=x)}(y) = \sum_z p_{\mathcal{S}}(z | x) \sum_{\tilde{x}} p_{\mathcal{S}}(y | \tilde{x}, z) p_{\mathcal{S}}(\tilde{x}). \quad (3.16)$$

3.3 Instrumental variables

Instrumental variables date back to the 1920s [Wright, 1928] and are widely used in practice [e.g. Imbens and Angrist, 1994, Bowden and Turkington, 1990]. Although there exist numerous extensions and alternative methods, here, we focus on the essential idea. Consider a linear Gaussian SEM with the following corresponding graph



Here, the coefficient α is the quantity of interest (see Example 3.1.5) but not directly accessible because of the hidden common cause U . Because U is independent of X , we can regard $\gamma U + N_X$ in

$$X = \beta Z + \gamma U + N_X$$

as noise. It becomes apparent that we can therefore consistently estimate the coefficient β and therefore have access to βZ . From

$$Y = \alpha X + \delta U + N_Y = \alpha \beta Z + (\alpha \gamma + \delta) U + N_Y$$

it is clear that we can then consistently estimate α . Thus, we first regress X on Z and then regress Y on the predicted values of X (predicted from the first regression). This method is commonly referred to as “two-stage-least-squares”. It makes heavy use of the following assumptions

- linear SEMs,
- non-zero β (in the case of small or vanishing β , Z is often called a “weak instrument”),
- the independence between U and Z , and
- the absence of a direct influence from Z to Y .

3.4 Potential Outcomes

t.b.w.

3.5 Exercises

Exercise 3.5.1 *Prove the backdoor criterion Proposition 3.1.4 (ii).*

Exercise 3.5.2 *Prove the frontdoor criterion (3.16) starting with*

$$p_{\mathcal{S}, do(X=x)}(y) = \sum_z p_{\mathcal{S}, do(X=x)}(y \mid z, x) p_{\mathcal{S}, do(X=x)}(z)$$

and then using rules 2 and 3 from the do-calculus.

Chapter 4

Causal structure learning

In this chapter, we first state some known identifiability results and then briefly introduce causal discovery methods (e.g. independence-based and score-based methods).

4.1 Structure identifiability

We have seen in Proposition 2.5.2 that any distribution could have been generated from many SEMs with different graphs. We therefore require further assumptions in order to obtain identifiability results. We discuss some of those assumptions in the following subsections.

4.1.1 Faithfulness

If the distribution $\mathbb{P}^{\mathbf{X}}$ is Markov and faithful with respect to the underlying DAG \mathcal{G}^0 , we have a one-to-one correspondence between d -separation statements in the graph \mathcal{G}^0 and the corresponding conditional independence statements in the distribution. All graphs outside the correct Markov equivalence class of \mathcal{G}^0 can therefore be rejected because they impose conditional independences that do not hold in $\mathbb{P}^{\mathbf{X}}$. Since both the Markov condition and faithfulness put restrictions *only* on the conditional independences in the joint distribution, it is also clear that we are not able to distinguish between two Markov equivalent graphs, i.e. between two graphs that entail exactly the same set of (conditional) independences (see for example Figure 2.2 on page 29). More precisely, the Markov equivalence class of \mathcal{G}^0 , represented by $\text{CPDAG}(\mathcal{G}^0)$ is identifiable from $\mathbb{P}^{\mathbf{X}}$.

Lemma 4.1.1 *Assume that $\mathbb{P}^{\mathbf{X}}$ is Markov and faithful with respect to \mathcal{G}^0 . Then, for each graph $\mathcal{G} \in \text{CPDAG}(\mathcal{G})$, we find an SEM that generates the distribution $\mathbb{P}^{\mathbf{X}}$. Furthermore, the distribution $\mathbb{P}^{\mathbf{X}}$ is not Markov and faithful to any graph $\mathcal{G} \notin \text{CPDAG}(\mathcal{G})$.*

Proof. The first statement follows directly from Proposition 2.5.2 and the second statement is a reformulation of Definition 2.4.4. \square

The key idea of independence- (or constraint-)based methods (Section 4.2) is to assume faithfulness and then to estimate the correct Markov equivalence class of graphs.

4.1.2 Additive noise models

Proposition 2.5.2 shows that any distribution could have been generated from many SEMs with different graphs. For many distributions, however, the functions f_j appearing in the proof are rather complicated. It turns out that we can obtain identifiability results if we do not allow for arbitrary complex functions, i.e. if we restrict the function class. In the following subsections 4.1.3 and 4.1.4 we will assume that the noise acts in an additive way.

Definition 4.1.2 [Additive Noise Model] We call an SEM \mathcal{S} an Additive Noise Model if the structural equations are of the form

$$X_j = f_j(\mathbf{PA}_j) + N_j, \quad (4.1)$$

that is, if the noise acts additively. For simplicity, let us further assume that the functions f_j are continuous and the noise variables N_j have a strictly positive density.

For these models causal minimality (Section 2.4.2) reduces to the condition that each function f_j is not constant in any of its arguments:

Proposition 4.1.3 *Consider a distribution generated by a model (4.1) and assume that the functions f_j are not constant in any of its arguments, i.e., for all j and $i \in \mathbf{PA}_j$ there are some $x_{\mathbf{PA}_j \setminus \{i\}}$ and some $x_i \neq x'_i$ such that*

$$f_j(x_{\mathbf{PA}_j \setminus \{i\}}, x_i) \neq f_j(x_{\mathbf{PA}_j \setminus \{i\}}, x'_i).$$

Then the joint distribution satisfies causal minimality with respect to the corresponding graph. Conversely, if there is a j and i such that $f_j(x_{\mathbf{PA}_j \setminus \{i\}}, \cdot)$ is constant, causal minimality is violated.

Proof. See Appendix A.4.1 □

Some of the following results assume causal minimality. This seems a plausible assumption since we will in general not be able to detect whether a variable depends on another variable in a constant way. Intuitively, we require that a function really “depends” on its arguments.

Given the restricted class of SEMs described in (4.1), what can we say about identifiability? Again, the answer is negative because the linear Gaussian SEMs, for example, is not identifiable, see Example 4.1.5 and Exercise 4.5.2. It turns out, however, that this case is exceptional in the following sense. For almost all other combinations of functions and distributions, we obtain identifiability. All the nonidentifiable cases have been characterized [Zhang and Hyvärinen, 2009, Peters et al., 2014]. Another non-identifiable example different from the linear Gaussian case is shown in the right plot in Figure 4.1. Its details can be found in Example 25 in [Peters et al., 2014]. Table 4.1.2 shows some of the known identifiability results.

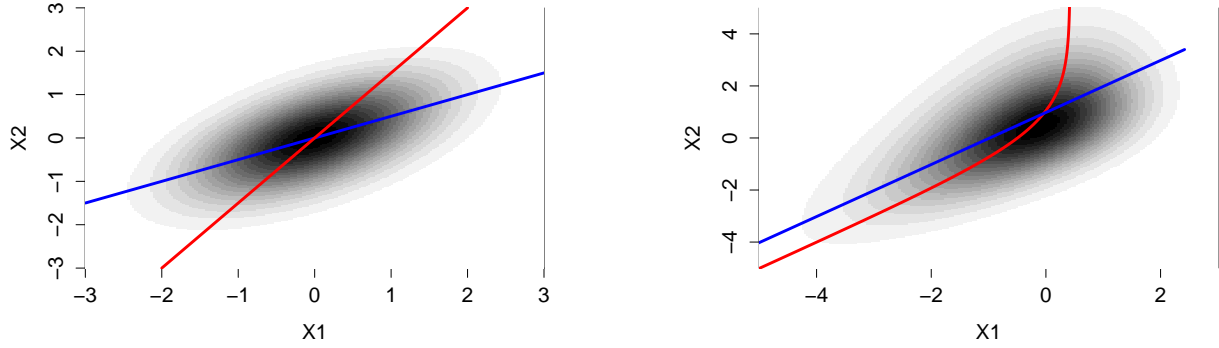


Figure 4.1: Joint density over X_1 and X_2 for two non-identifiable examples. The left panel shows Example 4.1.5 (linear Gaussian case) and the right panel shows a slightly more complicated example, with “fine-tuned” parameters for function, input and noise distribution (the latter plot is based on kernel density estimation). The blue function corresponds to the forward model $X_2 = f_2(X_1) + N_2$, the red function to the backward model $X_1 = \tilde{f}_1(X_2) + \tilde{N}_1$.

| type of structural equation | | conditions | DAG identif. | see |
|-----------------------------|---|--------------|--------------|---------------|
| general SEM: | $X_i = f_i(X_{\mathbf{PA}_i}, N_i)$ | - | X | Prop. 2.5.2 |
| additive noise model: | $X_i = f_i(X_{\mathbf{PA}_i}) + N_i$ | nonlin. fct. | ✓ | Thm 4.1.9(i) |
| causal additive model: | $X_i = \sum_{k \in \mathbf{PA}_i} f_{ik}(X_k) + N_i$ | nonlin. fct. | ✓ | Thm 4.1.9(ii) |
| linear Gaussian: | $X_i = \sum_{k \in \mathbf{PA}_i} \beta_{ik} X_k + N_i$ | linear fct. | X | Exerc. 4.5.2 |

Table 4.1: Summary of some known identifiability results for Gaussian noise

Remark 4.1.4 There have been several extensions to the framework of additive noise models (4.1). For example, Zhang and Hyvärinen [2009] allow for a post-nonlinear transformation of the variables. Peters et al. [2011] consider additive noise models for discrete variables. Janzing et al. [2009] investigate what happens if there exists a hidden common cause.

In the following two subsections, we will look at two specific identifiable examples in more detail: the linear non-Gaussian case (Section 4.1.3) and the nonlinear Gaussian case (Section 4.1.4). Although more general results are available [Peters et al., 2014], we concentrate on those two examples because for them, precise conditions can be stated easily.

4.1.3 Linear non-Gaussian acyclic models

The work introduced by Shimizu et al. [2006], Kano and Shimizu [2003] covers the general case, the idea is maybe best understood in the case of two variables:

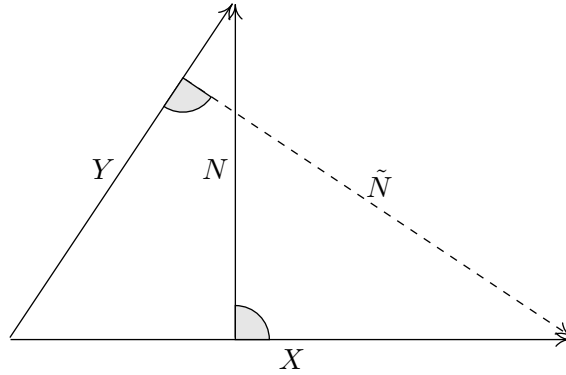
Example 4.1.5

$$Y = \phi X + N, \quad N \perp\!\!\!\perp X,$$

where X and N are normally distributed with mean zero. It can be checked that

$$X = \tilde{\phi} Y + \tilde{N}, \quad \tilde{N} \perp\!\!\!\perp Y,$$

with $\tilde{\phi} = \frac{\phi \text{var}(X)}{\phi^2 \text{var}(X) + \sigma^2} \neq \frac{1}{\phi}$ and $\tilde{N} = X - \tilde{\phi} Y$. The following figure depicts this example in \mathcal{L}_2 , [e.g. Peters, 2008] with the dot product representing the covariance.



If we consider non-Gaussian noise, however, the structural equation model becomes identifiable.

Proposition 4.1.6 *Let X and Y be two random variables, for which*

$$Y = \phi X + N, \quad N \perp\!\!\!\perp X, \quad \phi \neq 0$$

holds. Then we can reverse the process, i.e. there exists $\psi \in \mathbb{R}$ and a noise \tilde{N} , such that

$$X = \psi Y + \tilde{N}, \quad \tilde{N} \perp\!\!\!\perp Y,$$

if and only if X and N are Gaussian distributed.

The proof (Appendix A.4.2) is based on a characterization of the Gaussian distribution that was proved independently by Skitovič and Darmois [Skitovič, 1954, 1962, Darmois, 1953].

Theorem 4.1.7 *[Darmois-Skitovich] Let X_1, \dots, X_n be independent, non-degenerate random variables. If the two linear combinations*

$$\begin{aligned} l_1 &= a_1 X_1 + \dots + a_n X_n, & a_i &\neq 0 \\ l_2 &= b_1 X_1 + \dots + b_n X_n, & b_i &\neq 0 \end{aligned}$$

are independent, each X_i is normally distributed.

This result holds in the multivariate case, too. Shimizu et al. [2006] prove it using Independent Component Analysis (ICA) [Comon, 1994, Theorem 11], which itself is proved using the Darmois-Skitovic theorem.

Theorem 4.1.8 *[Shimizu et al. [2006]] Assume an SEM with graph \mathcal{G}_0*

$$X_j = \sum_{k \in \mathbf{PA}_j^{\mathcal{G}_0}} \beta_{jk} X_k + N_j, \quad j = 1, \dots, p \quad (4.2)$$

where all N_j are jointly independent and non-Gaussian distributed with strictly positive density¹. Additionally, for each $j \in \{1, \dots, p\}$ we require $\beta_{jk} \neq 0$ for all $k \in \mathbf{PA}_j^{\mathcal{G}_0}$. Then, the graph \mathcal{G}_0 is identifiable from the joint distribution.

The authors call this model a linear non-Gaussian acyclic model (LiNGAM) and provide a practical method based on ICA that can be applied to a finite amount of data. Later, an improved version of this method has been proposed in [Shimizu et al., 2011].

Interestingly, there is an alternative proof for Theorem 4.1.8: Theorem 28 in [Peters et al., 2014] extends bivariate identifiability results as Proposition 4.1.6 to the multivariate case. This trick will also be used for nonlinear additive models.

4.1.4 Nonlinear Gaussian additive noise models

We have seen that the graph structure of an additive noise models becomes identifiable if we assume the function to be linear and the noise to be non-Gaussian. Alternatively, we can exploit the nonlinearity of functions. The result is easiest to state with Gaussian noise:

Theorem 4.1.9 *(i) Let $\mathbb{P}^{\mathbf{X}} = \mathbb{P}^{X_1, \dots, X_p}$ be generated by an SEM with*

$$X_j = f_j(\mathbf{PA}_j) + N_j,$$

¹The condition of a strictly positive density was missing in the original version of this thesis. This condition is necessary although this might not be apparent on first sight of the original paper [Shimizu et al., 2006].

with normally distributed noise variables $N_j \sim \mathcal{N}(0, \sigma_j^2)$ and three times differentiable functions f_j that are not linear in any component: denote the parents \mathbf{PA}_j of X_j by $X_{k_1}, \dots, X_{k_\ell}$, then the function $f_j(x_{k_1}, \dots, x_{k_{a-1}}, \cdot, x_{k_{a+1}}, \dots, x_{k_\ell})$ is assumed to be nonlinear for all a and some $x_{k_1}, \dots, x_{k_{a-1}}, x_{k_{a+1}}, \dots, x_{k_\ell} \in \mathbb{R}^{\ell-1}$.

(ii) As a special case, let $\mathbb{P}^{\mathbf{X}} = \mathbb{P}^{X_1, \dots, X_p}$ be generated by an SEM with

$$X_j = \sum_{k \in \mathbf{PA}_j} f_{j,k}(X_k) + N_j, \quad (4.3)$$

with normally distributed noise variables $N_j \sim \mathcal{N}(0, \sigma_j^2)$ and three times differentiable, nonlinear functions $f_{j,k}$. This model is known as a causal additive model (CAM).

In both cases (i) and (ii), we can identify the corresponding graph \mathcal{G}_0 from the distribution $\mathbb{P}^{\mathbf{X}}$. The statements remain true if the noise distributions for source nodes, i.e., nodes with no parents, are allowed to have a non-Gaussian density with full support on the real line \mathbb{R} (the proof remains identical).

The proof is omitted. The statement can be found as Corollary 31 in [Peters et al., 2014].

4.1.5 Data from different environments (not only observational data)

We now assume that we observe data from different environments $e \in \mathcal{E}$. We model this with

$$\mathbf{X}^e \sim \mathbb{P}^e,$$

where each variable X_j^e for different e denotes the same (physical) quantity, measured in different environments. We will talk about a variable X in different environments, which is a light abuse of notation. From each of the environments, we assume to observe n^e i.i.d. samples.

Known intervention targets A first type of methods assumes that the different environments are generated from different interventional settings. In the case that the intervention targets $\mathcal{I}^e \subseteq \{1, \dots, p\}$ are known, several methods have been proposed. Assuming faithfulness and a specific type of intervention, Tian and Pearl [2001], Hauser and Bühlmann [2012] define and characterize the interventional equivalence classes of graphs; that is the class of graphs that can explain the observed distributions. Eberhardt et al. [2005] investigate how many intervention experiments are necessary (in the worst case) in order to identify the graph.

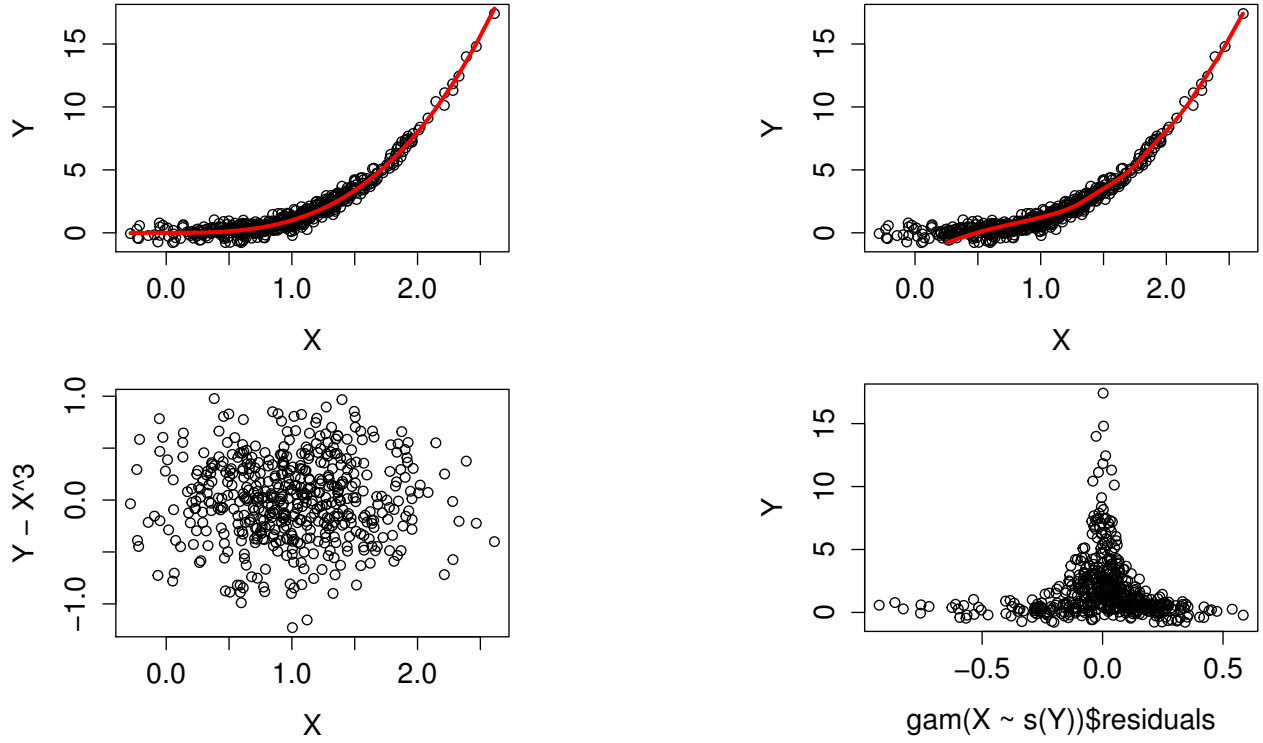


Figure 4.2: The data set contains i.i.d. data points from a distribution $\mathbb{P}^{(X,Y)}$ that has been generated from an additive noise model $Y = X^3 + N_Y$ with normally distributed noise N_Y . The left plots show the correct model and the independent residuals. Fitting a model in the backward direction $X = g(Y) + M_X$ leads to residuals that are dependent on the input (right hand side). (Here, regression is performed with `gam` from the R-package `mgcv` [Wood, 2011].) This corresponds to the identifiability proved in Theorem 4.1.9.

Unknown intervention targets Let us now consider a slightly different setting. Instead of learning the whole causal structure, we may consider a target variable Y and try to learn its causal parents. That is, we have

$$(\mathbf{X}^e, Y^e) \sim \mathbb{P}^e.$$

for $e \in \mathcal{E}$. We may then assume that there is a set \mathbf{PA}_Y such that the conditional

$$\mathbb{P}^{Y^e | \mathbf{PA}_Y^e} = \mathbb{P}^{Y^f | \mathbf{PA}_Y^f},$$

for all $e, f \in \mathcal{E}$. This assumption is satisfied if the distributions are generated by an underlying SEM and the different environments correspond to different intervention distributions, for which Y has not been intervened on [Peters et al., 2015]. Having said that, the assumption is more general and does not require an underlying SEM. One can consider the collection \mathcal{A} of *all* sets \mathbf{A} of variables that lead to “invariant prediction”, i.e., we have

$$\mathbb{P}^{Y^e | \mathbf{A}^e} = \mathbb{P}^{Y^f | \mathbf{A}^f},$$

for all $e, f \in \mathcal{E}$ and for all $\mathbf{A} \in \mathcal{A}$. It is not difficult to see (Exercise 4.5.3) that the variables appearing in all those sets must be direct causes of Y :

$$\bigcap_{\mathbf{A} \in \mathcal{A}} \mathbf{A} \subseteq \mathbf{PA}_Y. \quad (4.4)$$

In the case of SEMs and interventions, it is further possible to write down sufficient conditions for the identifiability of the set of [Peters et al., 2015].

Tian and Pearl [2001] also address the question of identifiability with unknown intervention targets. They do not specify a target variable and focus on changes in marginal distributions rather than conditionals.

4.1.6 Modularity and Independence of cause and mechanism (bivariate case)

For two variables the difficulty of causal discovery can be seen from the following symmetric equation

$$p(x_2 | x_1)p(x_1) = p(x_1 | x_2)p(x_2), \quad (4.5)$$

where the left (or right) hand side corresponds to the Markov factorization of $p(x_1, x_2)$ if the distribution is Markov w.r.t $X_1 \rightarrow X_2$ (or $X_2 \rightarrow X_1$).

Modularity [Pearl, 2009, and references therein] or autonomy [Haavelmo, 1944, Aldrich, 1989] describe the assumption that changing one of the structural equations leaves the other structural equations invariant, see the invariance principle described in Section 3.1.2. This leads to an asymmetry in Equation (4.5): intervening on the cause C changes its distribution $p(c)$ but not the conditional distribution $p(e | c)$ of the effect E given cause C . Intervening

on E , however, is expected to change both $p(e)$ and $p(c|e)$. Hoover [1990] uses this for identification of cause and effects in economics.

Another related way to break the symmetry in (4.5) is by assuming that $p(\text{effect}|\text{cause})$ is in some sense “independent” of $p(\text{cause})$. The hope is that this “independence” will not hold between $p(\text{cause}|\text{effect})$ and $p(\text{effect})$.

Different formalizations of this idea, in particular formalizations of “independence”, are given by Janzing et al. [2012], Sgouritsa et al. [2015], Zscheischler et al. [2011].

4.2 Independence-based methods

Independence-based methods assume that the distribution is faithful to the underlying DAG and therefore estimate the underlying CPDAG from conditional independences in $\mathbb{P}^{\mathbf{X}}$.

Estimation of skeleton Most methods first concentrate on estimating the skeleton and only later try to orient as many edges as possible. For the skeleton search it is useful to know that

Lemma 4.2.1 (i) *Two nodes X, Y in a graph $(\mathbf{X}, \mathcal{E})$ are adjacent if and only if they are d -connected given all subsets $S \subseteq \mathbf{V} \setminus \{X, Y\}$.*

(ii) *If two nodes X, Y in a graph $(\mathbf{X}, \mathcal{E})$ are not adjacent, then they are d -separated by either \mathbf{PA}_X or \mathbf{PA}_Y .*

Using Lemma 4.2.1(i), we have that if two variables are always dependent, no matter what other variables one conditions on, these two variables must be adjacent. This reasoning is used in the IC algorithm [Pearl, 2009] or in the SGS algorithm [Spirtes et al., 2000]; it is an example of how properties of the joint distribution can help to infer parts of the graph structure. The PC algorithm [Spirtes et al., 2000] uses Lemma 4.2.1(ii) instead of Lemma 4.2.1(i) in order to avoid conditioning on all possible subsets and therefore improve the computation time. Especially for sparse graphs, this furthermore has the advantage of not necessarily conditioning on large sets of variables.

Orientation of edges According to Lemma 2.4.5, we might be able to orient the immoralities (or v -structures) in the graph. If two nodes are not directly connected in the obtained skeleton, there must be a set that d -separates these nodes. Suppose that the skeleton contains the structure $X - Y - Z$ with no direct edge between X and Z ; let further S denote the corresponding d -separation set S . The structure $X - Y - Z$ is an immorality and can therefore be oriented as $X \rightarrow Y \leftarrow Z$ if and only if $Y \notin S$. After the orientation of immoralities, we may be able to orient some further edges in order to avoid cycles, for example. One set of such orientation rules has been shown to be complete and is known as Meek’s orientation rules [Meek, 1995].

Conditional independence tests In the two preceding paragraphs we have assumed the existence of an independence oracle that tells us whether a specific (conditional) independence is or is not present in the distribution. In practice, however, we have to infer this statement from a finite amount of data. There is some recent work on kernel-based tests [Fukumizu et al., 2008, Tillman et al., 2010, Zhang et al., 2011] but in general, conditional independence tests are difficult to perform in practice [e.g. Bergsma, 2004] if one does not restrict the variables to follow a Gaussian distribution, for example. In the latter case, we can test for vanishing partial correlation, see Section 1.2.

4.3 Score-based methods

Although the roots for score-based methods for causal inference may date back even further, we mainly refer to [Geiger and Heckerman, 1994, Heckerman, 1997, Chickering, 2002] and references therein.

Best scoring graph Given the data \mathcal{D} from a vector \mathbf{X} of variables, i.e. n i.i.d. samples, the idea is to assign a score $S(\mathcal{D}, \mathcal{G})$ to each graph \mathcal{G} and search over the space of DAGs for the best scoring graph.

$$\hat{\mathcal{G}} := \underset{\mathcal{G} \text{ DAG over } \mathbf{X}}{\operatorname{argmax}} S(\mathcal{D}, \mathcal{G}) \quad (4.6)$$

There are several possibilities to define such a scoring function. Often a parametric model is assumed (e.g. linear Gaussian equations or multinomial distributions), which introduces a set of parameters $\theta \in \Theta$.

(Penalized) likelihood For each graph we may consider the maximum likelihood estimator $\hat{\theta}$. We may then define a different score function by the Bayesian Information Criterion (BIC)

$$S(\mathcal{D}, \mathcal{G}) = \log p(\mathcal{D} | \hat{\theta}, \mathcal{G}) - \frac{d}{2} \log n,$$

where n is the sample size. Chickering [2002] discusses, how these two approaches can be related using work by Haughton [1988].

Since the search space of all DAGs is growing super-exponentially in the number of variables [e.g. Chickering, 2002], greedy search algorithms is applied to solve Equation (4.6): at each step there is a candidate graph and a set of neighboring graphs. For all these neighbors one computes the score and considers the best-scoring graph as the new candidate. If none of the neighbors obtains a better score, the search procedure terminates (not knowing whether one obtained only a local optimum). Clearly, one therefore has to define a neighborhood relation. Starting from a graph \mathcal{G} , we may define all graphs as neighbors from \mathcal{G} that can be obtained by removing, adding or reversing one edge. In the linear Gaussian case, for example, one cannot distinguish between Markov equivalent graphs. It turns out that in

those cases it is beneficial to change the search space to Markov equivalence classes instead of DAGs. The greedy equivalence search (GES) [Chickering, 2002] starts with the empty graph and consists of two-phases. In the first phase, edges are added until a local maximum is reached; in the second phase, edges are removed until a local maximum is reached, which is then given as an output of the algorithm.

Bayesian formalization We may define priors $p_{pr}(\mathcal{G})$ and $p_{pr}(\theta)$ over DAGs and parameters and consider the log posterior as a score function (note that $p(\mathcal{D})$ is constant over all DAGs):

$$S(\mathcal{D}, \mathcal{G}) := \log p(\mathcal{G} | \mathcal{D}) \propto \log p_{pr}(\mathcal{G}) + \log p(\mathcal{D} | \mathcal{G}),$$

where $p(\mathcal{D} | \mathcal{G})$ is the marginal likelihood

$$p(\mathcal{D} | \mathcal{G}) = \int_{\theta \in \Theta} p(\mathcal{D} | \mathcal{G}, \theta) p_{pr}(\theta) d\theta.$$

Here, $\hat{\mathcal{G}}$ is the mode of the posterior distribution, which is usually called maximum a posteriori (or MAP) estimator. Instead of a MAP estimator, one may be interested in the full posterior distribution over DAGs. In principle, even finer information as output is possible. One can average over all graphs to get a posterior of the hypothesis about the existence of a specific edge, for example.

In the case of parametric models, we call two graphs \mathcal{G}_1 and \mathcal{G}_2 *distribution equivalent* if for each parameter θ_1 there is a corresponding parameter θ_2 , such that the distribution obtained from \mathcal{G}_1 in combination with θ_1 is the same as the distribution obtained from graph \mathcal{G}_2 with θ_2 , and vice versa. It can be shown (see Exercise 4.5.1) that in the linear Gaussian case, for example, two graphs are distribution-equivalent if and only if they are Markov equivalent. One may therefore argue that $p(\mathcal{D} | \mathcal{G}_1)$ and $p(\mathcal{D} | \mathcal{G}_2)$ should be the same for Markov equivalent graphs \mathcal{G}_1 and \mathcal{G}_2 . Heckerman and Geiger [1995] discusses how to choose the prior over parameters accordingly.

Exact Methods There is a lot of interesting research that tries to scale up exact methods. Here, “exact” means that they aim at finding (one of) the best scoring graphs for a given finite data sets. Greedy search techniques are often heuristic and have guarantees only in the limit of infinite data.

In the Bayesian setting, Koivisto and Sood [2004], Koivisto [2006] compute marginal probabilities over edges.

The integer linear programming framework (probably added later) is studied by [De Campos and Ji, 2011, Cussens, 2011, Studený and Haws, 2014, Jaakkola et al., 2010, Sheehan et al., 2014, and others].

For a dynamic programming approach consider the work by [Silander and Myllymak, 2006, and references therein].

4.4 Methods for different environments

Here, we obtain one sample $\mathbf{X}_1^e, \dots, \mathbf{X}_{n_e}^e$ for each environment $e \in \mathcal{E}$.

Known intervention targets Each setting corresponds to an interventional experiment and we have additional knowledge of the intervention targets $\mathcal{I}^e \subseteq \{1, \dots, p\}$. Cooper and Yoo [1999] incorporate the intervention effects as mechanism changes into a Bayesian framework. For perfect interventions, Hauser and Bühlmann [2015] considers the linear Gaussian SEMs and proposes the Greedy Interventional Equivalence Search (GIES), a modified version of the GES algorithm that we briefly described in Section 4.3.

Unknown intervention targets Eaton and Murphy [2007] do not assume that the targets of the different interventions are known. Instead, they introduce for each $e \in \mathcal{E}$ intervention nodes I_e [see also Pearl, 1993b], and assume that they have no incoming edges; for each data point only one of those intervention nodes is active. Then, standard techniques can be applied to the enlarged model with $p + \#\mathcal{E}$ variables.

Tian and Pearl [2001] propose to test whether the marginal distributions change in the different settings and use this information to infer parts of the graph structure. They even combine this method with an independence-based method.

Peters et al. [2015] compute tests (at level α) in order to obtain an estimate $\hat{\mathcal{A}}$ for the set \mathcal{A} in (4.4). Because the true set of parents \mathbf{PA}_Y is obtained in $\hat{\mathcal{A}}$ with high probability $(1 - \alpha)$, we have the coverage statement

$$\bigcap_{\mathbf{A} \in \hat{\mathcal{A}}} \mathbf{A} \subseteq \mathbf{PA}_Y$$

with high probability $(1 - \alpha)$. Note that this approach does not even require that the different data sets correspond to different interventions.

4.5 Exercises

Exercise 4.5.1 *Prove that for linear Gaussian SEMs, two graphs \mathcal{G}_1 and \mathcal{G}_2 are distribution equivalent if and only if they are Markov equivalent.*

Exercise 4.5.2 *Consider a distribution $\mathbb{P}^{\mathbf{X}}$ that has been generated from a linear Gaussian SEM S . Prove that for any DAG \mathcal{G} such that $\mathbb{P}^{\mathbf{X}}$ is Markov w.r.t. \mathcal{G} there is a corresponding SEM $S_{\mathcal{G}}$ generating $\mathbb{P}^{\mathbf{X}}$.*

Exercise 4.5.3 *Prove Equation (4.4).*

Appendix A

Proofs

A.1 Proofs from Chapter 1

A.2 Proofs from Chapter 2

A.2.1 Proof of Proposition 2.2.4

Proof. In order to simplify notation we write X_1 instead of X and X_2 instead of Y . First, the truncated factorization formula (3.3) implies

$$\begin{aligned} p_S^{X_2 | do(X_1=x_1)}(x_2) &= \int \prod_{j \neq 1} p_j(x_j | x_{pa(j)}) dx_3 \cdots dx_p \\ &= \int \prod_{j \neq 1} p_j(x_j | x_{pa(j)}) \frac{\tilde{p}(x_1)}{\tilde{p}(x_1)} dx_3 \cdots dx_p \\ &= p_S^{X_2 | X_1=x_1, do(X_1=\tilde{N}_1)}(x_2) \end{aligned} \quad (\text{A.1})$$

if \tilde{N}_1 puts positive mass on x_1 , i.e., $\tilde{p}(x_1) > 0$. The other statement that we need is

$$X_2 \not\perp\!\!\!\perp X_1 \text{ in } \mathbb{Q} \iff \exists x_1^\Delta, x_1^\square \text{ with } q(x_1^\Delta), q(x_1^\square) > 0 \text{ and } \mathbb{Q}^{X_2 | X_1=x_1^\Delta} \neq \mathbb{Q}^{X_2 | X_1=x_1^\square} \quad (\text{A.2})$$

and

$$X_2 \not\perp\!\!\!\perp X_1 \text{ in } \mathbb{Q} \iff \exists x_1^\Delta \text{ with } q(x_1^\Delta) > 0 \text{ and } \mathbb{Q}^{X_2 | X_1=x_1^\Delta} \neq \mathbb{Q}^{X_2}. \quad (\text{A.3})$$

We then have for any \hat{N}_1 with full support

$$\begin{aligned} (i) &\xrightarrow{(\text{A.2})} \exists x_1^\Delta, x_1^\square \text{ with pos. density under } \tilde{N}_1 \text{ s.t. } \mathbb{P}_S^{X_2 | X_1=x_1^\Delta, do(X_1=\tilde{N}_1)} \neq \mathbb{P}_S^{X_2 | X_1=x_1^\square, do(X_1=\tilde{N}_1)} \\ &\xrightarrow{(\text{A.1})} (ii) \\ &\xrightarrow{(\text{A.1})} \exists x_1^\Delta, x_1^\square \text{ with pos. density under } \hat{N}_1 \text{ s.t. } \mathbb{P}_S^{X_2 | X_1=x_1^\Delta, do(X_1=\hat{N}_1)} \neq \mathbb{P}_S^{X_2 | X_1=x_1^\square, do(X_1=\hat{N}_1)} \\ &\xrightarrow{(\text{A.2})} (iv) \\ &\xrightarrow{(\text{trivial})} (i) \end{aligned}$$

We further have that $(ii) \xRightarrow{\text{(trivial)}} (iii)$ and that $\mathbb{P}_{\mathcal{S}}^{X_2} = \mathbb{P}_{\mathcal{S}}^{X_2 | do(X_1 = N_1^*)}$ with N_1^* having the same distribution as $\mathbb{P}_{\mathcal{S}}^{X_2}$. The latter implies

$$\begin{aligned}
\neg(i) &\implies X_2 \perp\!\!\!\perp X_1 \text{ in } \mathbb{P}_{\mathcal{S}}^{\mathbf{X} | do(X_1 = N_1^*)} \\
&\xRightarrow{(A.3)} \mathbb{P}_{\mathcal{S}}^{X_2 | X_1 = x^\Delta | do(X_1 = N_1^*)} = \mathbb{P}_{\mathcal{S}}^{X_2 | do(X_1 = N_1^*)} \text{ for all } x^\Delta \text{ with } p_1(x^\Delta) > 0 \\
&\xRightarrow{(A.1)} \mathbb{P}_{\mathcal{S}}^{X_2 | do(X_1 = x^\Delta)} = \mathbb{P}_{\mathcal{S}}^{X_2} \text{ for all } x^\Delta \text{ with } p_1(x^\Delta) > 0 \\
&\xRightarrow{\neg(ii)} \neg(iii)
\end{aligned}$$

□

A.2.2 Proof of Proposition 2.2.9

Proof. (i) follows directly from the Markov property of the interventional SEM: after removing the incoming edges into X , X and Y are d -separated if there is no direct path from X to Y .

(ii) can be proved by counter example: e.g.

$$\begin{aligned}
X &= N_X \\
Z &= 2X + N_Z \\
Y &= 4X - 2Z + N_Y
\end{aligned}$$

Because $Y = -2N_Z + N_Y$, we have $X \perp\!\!\!\perp Y$ for all N_X .

□

A.2.3 Proof of Proposition 2.5.2

Proof. Let N_1, \dots, N_p be independent and uniformly distributed between 0 and 1. We then define $X_j = f_j(X_{\mathbf{PA}_j}, N_j)$ with

$$f_j(x_{\mathbf{PA}_j}, n) = F_{X_j | X_{\mathbf{PA}_j} = x_{\mathbf{PA}_j}}^{-1}(n)$$

where $F_{X_j | X_{\mathbf{PA}_j} = x_{\mathbf{PA}_j}}$ is the inverse cdf from X_j given $X_{\mathbf{PA}_j} = x_{\mathbf{PA}_j}$.

□

A.2.4 Proof of Theorem 2.4.2

Proof. proof sketch for equiv. of markov properties

□

A.2.5 Proof of Proposition 2.4.13

Proof. “if”: Assume that causal minimality is not satisfied. Then, there is an X_j and a $Y \in \mathbf{PA}_j^{\mathcal{G}}$, such that $\mathbb{P}^{\mathbf{X}}$ is also Markov with respect to the graph obtained when removing the edge $Y \rightarrow X_j$ from \mathcal{G} .

“only if”: If $\mathbb{P}^{\mathbf{X}}$ has a density, the Markov condition is equivalent to the Markov factorization [Lauritzen, 1996, Theorem 3.27]. Assume that $Y \in \mathbf{PA}_j^{\mathcal{G}}$ and $X_j \perp\!\!\!\perp Y \mid \mathbf{PA}_j^{\mathcal{G}} \setminus \{Y\}$. Then $P(\mathbf{X}) = P(X_j \mid \mathbf{PA}_j^{\mathcal{G}} \setminus \{Y\}) \prod_{k \neq j} P(X_k \mid \mathbf{PA}_k^{\mathcal{G}})$, which implies that $\mathbb{P}^{\mathbf{X}}$ is Markov w.r.t. \mathcal{G} without $Y \rightarrow X_j$. \square

A.3 Proofs from Chapter 3

A.4 Proofs from Chapter 4

A.4.1 Proof of Proposition 4.1.3

Proof. Assume causal minimality is not satisfied. We can then find a j and $i \in \mathbf{PA}_j$ with $X_j = f_j(X_{\mathbf{PA}_j \setminus \{i\}}, X_i) + N_j$ that does not depend on X_i if we condition on all other parents $\mathbf{PA}_j \setminus \{i\}$ (Proposition 2.4.13). Let us denote $\mathbf{PA}_j \setminus \{X_i\}$ by X_A . For the function f_j it follows that $f_j(x_A, x_i) = c_{x_A}$ for \mathbb{P}^{X_A, X_i} -almost all (x_A, x_i) . Indeed, assume without loss of generality that $\mathbf{E}N_j = 0$, take the mean of $X_j \mid \mathbf{PA}_j^{\mathcal{G}_0} = (x_A, x_i)$ and use e.g. (2b) from Dawid [1979]. The continuity of f_j implies that f_j is constant in its last argument. \square

The converse statement follows from Proposition 2.4.13, too. \square

A.4.2 Proof of Proposition 4.1.6

We first prove the following lemma, which should be clear intuitively.

Lemma A.1 *Let X and ϵ be two independent variables and assume ϵ to be non-deterministic. Then*

$$\epsilon \not\perp\!\!\!\perp (X + \epsilon).$$

Proof. Of course the proof becomes trivial if the variables have finite variance. Then $\mathbf{cov}(X, X + \epsilon) = \mathbf{var}(X) > 0$. For the general case, however, the argumentation is a bit more complex. Assume $N \perp\!\!\!\perp (X + \epsilon)$. Then for every $u, v \in \mathbb{R}$:

$$\begin{aligned} \varphi_{(\epsilon, X+\epsilon)}(u, v) &= \mathcal{E} [\exp(iu\epsilon + iv\epsilon + ivX)] \\ &= \mathcal{E} [\exp(iu\epsilon + iv\epsilon) \cdot \exp(ivX)] \\ &= \mathcal{E} [\exp(iu\epsilon + iv\epsilon)] \cdot \mathcal{E} [\exp(ivX)] \\ &= \varphi_{\epsilon}(u + v) \cdot \varphi_X(v). \end{aligned}$$

We also have

$$\begin{aligned} \varphi_{(\epsilon, X+\epsilon)}(u, v) &= \mathcal{E} [\exp(iu\epsilon + iv\epsilon + ivX)] \\ &= \mathcal{E} [\exp(iu\epsilon) \cdot \exp(iv\epsilon + ivX)] \\ &= \mathcal{E} [\exp(iu\epsilon)] \cdot \mathcal{E} [\exp(iv\epsilon + ivX)] \\ &= \varphi_{\epsilon}(u) \cdot \varphi_{(\epsilon+X)}(v) \\ &= \varphi_{\epsilon}(u) \cdot \varphi_{\epsilon}(v) \cdot \varphi_X(v). \end{aligned}$$

We know that $\varphi_X(0) = 1$ and that characteristic functions are continuous. Thus there exists a non-empty open interval $V = (-r, r) \subset \mathbb{R}$, such that $|\varphi_X(v)| > 0 \forall v \in V$. Thus we have for all $u \in \mathbb{R}$ and $v \in V$:

$$\varphi_\epsilon(u + v) = \varphi_\epsilon(u) \cdot \varphi_\epsilon(v).$$

Note that this is still true for an arbitrary $v \in \mathbb{R}$: Choose $n \in \mathbb{N}$, such that $\|v/n\| \leq r$. It follows

$$\begin{aligned} \varphi_\epsilon(u + v) &= \varphi_\epsilon\left(u + (n-1)\frac{v}{n} + \frac{v}{n}\right) \\ &= \varphi_\epsilon\left(u + (n-1)\frac{v}{n}\right) \cdot \varphi_\epsilon\left(\frac{v}{n}\right) \\ &\vdots \\ &= \varphi_\epsilon(u) \cdot \varphi_\epsilon\left(\frac{v}{n}\right)^n = \varphi_\epsilon(u) \cdot \varphi_\epsilon(v) \end{aligned}$$

Then we know

$$\varphi_\epsilon(u) = z^u \quad \text{for some } z \in \setminus\{c \in \mathbb{C} : \operatorname{Im} c = 0, \operatorname{Re} c < 0\}.$$

We can write $z = \exp(a + ib)$ and since $\|\varphi_\epsilon\|_\infty \leq 1$ we deduce that $a = 0$. It follows

$$\varphi_\epsilon(u) = \exp(ib \cdot u).$$

Because of the uniqueness of characteristic functions this implies $\mathbb{P}(\epsilon = b) = 1$ and ϵ is degenerate. \square

Proof of Proposition 4.1.6 If X and N are Gaussian distributed, the statement follows from Example 4.1.5. Conversely, we assume that

$$\begin{aligned} Y &= \phi X + N \\ \text{and } \tilde{N} &= (1 - \phi\psi)X - \psi N \end{aligned}$$

are independent. Distinguish between the following cases:

1. $(1 - \phi\psi) \neq 0$ and $\psi \neq 0$

Here, Theorem 4.1.7 implies that X, N and thus also Y, \tilde{N} are normally distributed.

2. $\psi = 0$

We have $(1 - \phi\psi)X \perp\!\!\!\perp \phi X + N$. $\psi = 0$ implies

$$X \perp\!\!\!\perp \phi X + N,$$

which is a contradiction to Lemma A.1.

3. $(1 - \phi\psi) = 0$

It follows $-\psi N \perp\!\!\!\perp \phi X + N$. Thus

$$N \perp\!\!\!\perp \phi X + N$$

and we can apply Lemma A.1 again. \square

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