Graphical Models

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These notes will be updated as the course goes on. If you find any mistakes or omissions, I'd be very grateful to be informed.

Administration

The course webpage is at

`http://www.stats.ox.ac.uk/~evans/gms/`

Here you will find problem sheets, slides and links to any other materials (including videos of the lectures).

Problem Sheets and Classes

There will be four problem sheets, and four associated classes.

Part C and OMMS students should sign-up for classes via the online system.

Resources

Books are useful, though not required. Here are the main ones this course is based on.

1. S.L. Lauritzen, *Graphical Models*, Oxford University Press, 1996.

The 'bible' of graphical models, and much of the first half of this course is based on this. One complication is that the book makes a distinction between two different types of vertex, which can make some ideas look more complicated.

2. M.J. Wainwright and M.I. Jordan, *Graphical Models, Exponential Families, and Variational Inference*, Foundations and Trends in Machine Learning, 2008.

Relevant for the later part of the course, and for understanding much of the computational advantages of graphical models. Available for free at `https://people.eecs.berkeley.edu/~wainwrig/Papers/WaiJor08_FTML.pdf`.

3. J. Pearl, *Causality*, third edition, Cambridge, 2013.

Book dealing with the causal interpretation of directed models, which we will touch upon.

4. D. Koller and N. Friedman, *Probabilistic Graphical Models: Principles and Techniques*, MIT Press, 2009.

A complementary book, written from a machine learning perspective.

5. A. Agresti *Categorical Data Analysis*, 3rd Edition, John Wiley & Sons, 2013.

As the name suggests, covers most of the material we will use for discussing contingency tables and log-linear models, as well as some data examples. Available for free at `https://mybiostats.files.wordpress.com/2015/03/3rd-ed-alan_agresti_categorical_data_analysis.pdf`.

Recommended Prerequisites

Knowledge of Part A Probability and Statistics is assumed. Part B Applied Statistics (especially GLMs) and Foundations of Statistical Inference would be useful, but are not essential.

Aims and Objectives

This course will give an overview of the use of graphical models as a tool for statistical inference. Graphical models relate the structure of a graph to the structure of a multivariate probability distribution, usually via conditional independence constraints. This has two broad uses: first, conditional independence can provide vast savings in computational effort, both in terms of the representation of large multivariate models and in performing inference with them; this makes graphical models very popular for dealing with big data problems. Second, conditional independence can be used as a tool to discover hidden structure in data, such as that relating to the direction of causality or to unobserved processes. As such, graphical models are widely used in genetics, medicine, epidemiology, statistical physics, economics, the social sciences and elsewhere.

Students will develop an understanding of the use of conditional independence and graphical structures for dealing with multivariate statistical models. They will appreciate how this is applied to causal modelling, and to computation in large-scale statistical problems.

Contents

1 Introduction

The modern world is replete with sources of massively multivariate data, sometimes called 'big data'. In many cases, the number of variables being measured (p) exceeds the number of samples available (n), and in almost all cases the number of possible ways of classifying individuals is greater than n.

Examples:

- There are around 25,000 human genes, which gives more possible human genomes than humans who have ever existed. Even if a gene is present, whether or not it is expressed depends upon other genes and also environmental factors. Good genetic data sets might have a few hundred thousand individuals in, the best ones perhaps a million. How do we study what effect these genes have on diseases, or on each other's expression?
- A doctor has to diagnose one (or more) of hundreds of different possible diseases in a patient with a handful out of thousands of possible symptoms, and with a few pieces of information about his medical history. She can perhaps order some tests to provide evidence in favour of one condition or another. How should she decide whether the evidence is behind a particular condition?
- Photographs are typically made up of millions of pixels, each of which can take one of $256^3 \approx 17$ million colours. How do we train a computer to recognize the object in an image?

The nature of these data sets leads to two related challenges: the first is statistical, and the second computational. Both are features of the so-called *curse of dimensionality*. The statistical problems are easy to see: suppose I ask 1,000 people 10 questions each with two answers. This gives $2^{10} = 1024$ possible response patterns, so that it is impossible to observe all the response patterns, and in practice we won't observe most of them even once. How can we sensibly estimate the probability of those missing response patterns in future?

The computational problem is related. Suppose now that I *know* the distribution of outcomes, so I have $P(X_V = x_V)$ for every $x_V \in \mathcal{X}_V$. How can I compute the marginal probability of a particular variable? Well:

$$P(X_i = x_i) = \sum_{x_{V\setminus\{i\}}} P(X_V = x_V).$$

But notice that, if $p = |V|$ is large, say 1,000 variables, then this sum could easily involve $2^{1000} \approx 10^{301}$ terms! Even for a very fast computer this is completely infeasible, and of course we would not be able to store all the probabilities in the first place.

Each of these examples—although theoretically massive—has a lot of underlying structure that makes the problem potentially tractable. Particular medical symptoms are closely tied to particular diseases, with probabilities that we understand. Adjacent pixels in photographs are often almost the same; if every pixel were completely different we would never discern an image.

Graphical models provide a convenient way of modelling this structure, and make it computationally feasible to perform calculations with the networks.

2 Conditional Independence

The primary tool we will use to provide statistical and computationally feasible models is conditional independence. This ensures that distributions factorize into smaller pieces that can be evaluated separately and quickly.

2.1 Independence

Recall that two discrete variables X and Y are *independent* if

$$P(X = x, Y = y) = P(X = x) \cdot P(Y = y) \qquad \forall x \in \mathcal{X}, y \in \mathcal{Y}.$$

Note that this is equivalent to

$$P(X = x \,|\, Y = y) = P(X = x) \qquad \text{whenever } P(Y = y) > 0, \forall x \in \mathcal{X}.$$

In other words, knowing the value of Y gives us no information about the distribution of X; we say that Y is **irrelevant** for X. Similarly, two variables with joint density f_{XY} are independent if

$$f_{XY}(x, y) = f_X(x) \cdot f_Y(y) \qquad \forall x \in \mathcal{X}, y \in \mathcal{Y}.$$

The qualification that these expressions hold for all $(x, y) \in \mathcal{X} \times \mathcal{Y}$, a product space, is very important[1], and sometimes forgotten.

Example 2.1. Suppose that X, W are independent Exponential(λ) random variables. Define $Y = X + W$. Then the joint density of X and Y is

$$f_{XY}(x, y) = \begin{cases} \lambda^2 e^{-\lambda y} & \text{if } y > x > 0, \\ 0 & \text{otherwise} \end{cases}.$$

Note that the expression within the valid range for x, y factorizes, so when performing the usual change of variables one may mistakenly conclude that X and Y are independent.

2.2 Conditional Independence

Given random variables X, Y we denote the joint density $p(x, y)$, and call

$$p(y) = \int_{\mathcal{X}} p(x, y)\, dx.$$

the **marginal density** (of Y). The **conditional density** of X given Y is defined as any function $p(x \,|\, y)$ such that

$$p(x, y) = p(y) \cdot p(x \,|\, y).$$

Note that if $p(y) > 0$ then the solution is unique and given by the familiar expression

$$p(x \,|\, y) = \frac{p(x, y)}{p(y)}.$$

[1] Of course, for continuous random variables densities are only defined up to a set of measure zero, so the condition should really read 'almost everywhere'. We will ignore such measure theoretic niceties in this course.

Definition 2.2. Let X, Y be random variables defined on a product space $\mathcal{X} \times \mathcal{Y}$; let Z be a third random variable, and let the joint density be $p(x, y, z)$. We say that X and Y are *conditionally independent* given Z if

$$p(x \,|\, y, z) = p(x \,|\, z), \qquad \forall x \in \mathcal{X}, y \in \mathcal{Y}, z \in \mathcal{Z} \text{ such that } p(y, z) > 0.$$

When this holds we write $X \perp\!\!\!\perp Y \mid Z\,[p]$, possibly omitting the p for brevity.

In other words, once $Z = z$ is known, the value of Y provides no *additional* information that would allow us to predict or model X. If Z is degenerate—that is, there is some z such that $P(Z = z) = 1$, then the definition above is the same as saying that X and Y are independent. This is called *marginal independence*, and denoted $X \perp\!\!\!\perp Y$.

Example 2.3. Let $X_1, \ldots, X_k$ be a Markov chain. Then X_k is independent of $X_1, \ldots, X_{k-2}$ conditional upon X_{k-1}:

$$P(X_k = x \mid X_{k-1} = x_{k-1}, \cdots, X_1 = x_1) = P(X_k = x \mid X_{k-1} = x_{k-1})$$

for all $x, x_{k-1}, \ldots, x_1$. That is, $X_k \perp\!\!\!\perp X_1, \ldots, X_{k-2} \mid X_{k-1}$. This is known as the *Markov property*, or memoryless property.

Although the definition of conditional independence appears to be asymmetric in X and Y, in fact it is not: if X gives no additional information about Y then the reverse is also true, as the following theorem shows.

Theorem 2.4. *Let X, Y, Z be random variables on a Cartesian product space. The following are equivalent.*

(i) $p(x \,|\, y, z) = p(x \,|\, z)$ *for all x, y, z such that $p(y, z) > 0$;*

(ii) $p(x, y \,|\, z) = p(x \,|\, z) \cdot p(y \,|\, z)$ *for all x, y, z such that $p(z) > 0$;*

(iii) $p(x, y, z) = p(y, z) \cdot p(x \,|\, z)$ *for all x, y, z;*

(iv) $p(z) \cdot p(x, y, z) = p(x, z) \cdot p(y, z)$ *for all x, y, z;*

(v) $p(x, y, z) = f(x, z) \cdot g(y, z)$ *for some functions f, g and all x, y, z.*

Proof. Note that $p(y, z) > 0$ implies $p(z) > 0$, so (i) $\implies$ (ii) follows from multiplying by $p(y \,|\, z)$, and (ii) $\implies$ (iii) by multiplying by $p(z)$. (iii) $\implies$ (i) directly.

The equivalence of (iii) and (iv) is also clear (note that if $p(z) = 0$ then both sides of (iii) are 0), and (iii) implies (v). It remains to prove that (v) implies the others. Suppose that (v) holds. Then

$$p(y, z) = \int p(x, y, z)\, dx = g(y, z) \int f(x, z)\, dx = g(y, z) \cdot \tilde{f}(z).$$

If $\tilde{f}(z) > 0$ (which happens whenever $p(z) > 0$) we have

$$p(x, y, z) = \frac{f(x, z)}{\tilde{f}(z)} p(y, z).$$

But by definition $f(x, z)/\tilde{f}(z)$ is $p(x \,|\, y, z)$, and it does not depend upon y, so we obtain (iii). $\square$

Conditional independence is a complicated and often unintuitive notion, as the next example illustrates.

Example 2.5 (Simpson's Paradox)**.** Below is a famous data set that records the races of the victim and defendants in various murder cases in Florida between 1976 and 1987, and whether or not the death penalty was imposed upon the killer. The data are presented as counts, though we can turn this into an empirical probability distribution by dividing by the total, 674.

Victim	White	
Defendant	White	Black
Yes	53	11
No	414	37

Victim	Black	
Defendant	White	Black
Yes	0	4
No	16	139

The marginal table has

Defendant	White	Black
Yes	53	15
No	430	176

Here we see that the chance of receiving a death sentence is approximately independent of the defendant's race. $P(\text{Death} \mid \text{White}) = 53/(53 + 430) = 0.11$, $P(\text{Death} \mid \text{Black}) = 15/(15 + 176) = 0.08$. (One could fiddle the numbers to obtain exact independence.)

However, restricting only to cases where the victim is white we see that black defendants have nearly a 1/3 chance of receiving the death penalty, compared to about 1/8 for whites. And for black victims the story is the same, a handful of blacks were were sentenced to death while no white defendants were. (In fact we will see in Chapter 3.4 that this conditional dependence is not statistically significant either, but for the purposes of this discussion this doesn't matter: we could multiply all the numbers by 10 and get a data set in which the correlations *are* significant. For more on this data set, take a look at Example 2.3.2 in the book *Categorical Data Analysis* by Agresti).

The previous example teaches us the valuable lesson that marginal independence does not imply conditional independence (nor vice versa). More generally, conditioning on additional things may result in dependence being induced. However, there are properties that relate conditional independences, the most important of which are given in the next theorem.

Theorem 2.6 (Graphoid Axioms)**.** *Conditional independence satisfies the following properties, sometimes called the* graphoid axioms*.*

1. $X \perp\!\!\!\perp Y \mid Z \implies Y \perp\!\!\!\perp X \mid Z$;
2. $X \perp\!\!\!\perp Y, W \mid Z \implies X \perp\!\!\!\perp Y \mid Z$;
3. $X \perp\!\!\!\perp Y, W \mid Z \implies X \perp\!\!\!\perp W \mid Y, Z$;
4. $X \perp\!\!\!\perp W \mid Y, Z$ *and* $X \perp\!\!\!\perp Y \mid Z \implies X \perp\!\!\!\perp Y, W \mid Z$;
5. *if* $p(x, y, z, w) > 0$, *then* $X \perp\!\!\!\perp W \mid Y, Z$ *and* $X \perp\!\!\!\perp Y \mid W, Z \implies X \perp\!\!\!\perp Y, W \mid Z$.

These properties are sometimes referred to respectively as symmetry, decomposition, weak union, contraction and intersection.

Proof. 1. Symmetry follows from Theorem 2.4

2. Starting from $p(x, y, w \mid z) = p(x \mid z)p(y, w \mid z)$ and integrating out w gives $p(x, y \mid z) = p(x \mid z)p(y \mid z)$.

3. and 4: see Examples sheet.

5. By Theorem 2.4 we have $p(x, y, w, z) = f(x, y, z)g(y, w, z)$ and $p(x, y, w, z) = \tilde{f}(x, w, z)\tilde{g}(y, w, z)$. By positivity, taking ratios shows that

$$\begin{aligned} f(x, y, z) &= \frac{\tilde{f}(x, w, z)\tilde{g}(y, w, z)}{g(y, w, z)} \\ &= \frac{\tilde{f}(x, w_0, z)\tilde{g}(y, w_0, z)}{g(y, w_0, z)} \end{aligned}$$

for any w_0, since the LHS does not depend upon w; now we see that the right hand side is a function of x, z times a function of y, z, so

$$f(x, y, z) = a(x, z) \cdot b(y, z).$$

Plugging into the first expression gives the result. □

Remark 2.7. Properties 2–4 can be combined into a single 'chain rule':

$$X \perp\!\!\!\perp W \mid Y, Z \qquad \text{and} \qquad X \perp\!\!\!\perp Y \mid Z \qquad \iff \qquad X \perp\!\!\!\perp Y, W \mid Z.$$

The fifth property is often extremely useful (as we shall see), but doesn't generally hold if the distribution is not positive: see the Examples Sheet.

Remark 2.8. Since the events $\{Y = y\}$ and $\{Y = y, h(Y) = h(y)\}$ are equal for any (measurable) function h, it follows that

$$p(x \mid y, z) = p(x \mid y, h(y), z).$$

This can be used to prove that

$$X \perp\!\!\!\perp Y \mid Z \quad \implies \quad X \perp\!\!\!\perp h(Y) \mid Z \quad \text{and} \quad X \perp\!\!\!\perp Y \mid h(Y), Z,$$

both of which are very useful facts.

2.3 Statistical Inference

Conditional independence crops up in various areas of statistics; here is an example that should be familiar.

Example 2.9. Suppose that $X \sim f_\theta$ for some parameter $\theta \in \Theta$. We say that $T \equiv t(X)$ is a *sufficient statistic* for θ if the likelihood can be written as

$$L(\theta \mid X = x) = f_\theta(x) = g(t(x), \theta) \cdot h(x).$$

Note that under a Bayesian interpretation of θ, this is equivalent to saying that $X \perp\!\!\!\perp \theta \mid T$.

Conditional independence can also give huge computational advantages for dealing with complex distributions and large datasets. Take random variables X, Y, Z on a product space with joint density

$$p_\theta(x, y, z) = g_\eta(x, y) \cdot h_\zeta(y, z), \qquad \forall x, y, z, \theta,$$

for some functions g, h, where $\theta = (\eta, \zeta)$ is a Cartesian product.

Then suppose we wish to find the maximum likelihood estimate of θ; well this is just $\hat{\theta} = (\hat{\eta}, \hat{\zeta})$ where

$$\hat{\eta} = \arg\max_\eta \prod_{i=1}^n g_\eta(x_i, y_i), \qquad \hat{\zeta} = \arg\max_\zeta \prod_{i=1}^n h_\zeta(y_i, z_i).$$

So we can maximize these two pieces separately. Notice in particular that we don't need all the data in either case!

If in a Bayesian mood, we might impose a prior $\pi(\eta, \zeta) = \pi(\eta)\pi(\zeta)$. Then

$$\begin{aligned}
\pi(\eta, \zeta \mid \boldsymbol{x}, \boldsymbol{y}, \boldsymbol{z}) &\propto \pi(\eta) \cdot \pi(\zeta) \cdot \prod_i g_\eta(x_i, y_i) \cdot h_\zeta(y_i, z_i) \\
&= \left\{ \pi(\eta) \prod_i g_\eta(x_i, y_i) \right\} \cdot \left\{ \pi(\zeta) \prod_i h_\zeta(y_i, z_i) \right\} \\
&\propto \pi(\eta \mid \boldsymbol{x}, \boldsymbol{y}) \cdot \pi(\zeta \mid \boldsymbol{y}, \boldsymbol{z}).
\end{aligned}$$

Applying Theorem 2.4(ii) we see that $\eta \perp\!\!\!\perp \zeta \mid \boldsymbol{X}, \boldsymbol{Y}, \boldsymbol{Z}$, and so we can perform inference about this distribution for the two pieces separately (e.g. by running an MCMC procedure or finding the posterior mode).

Indeed, each piece only requires part of the data, and for large problems this can be a tremendous computational saving.

3 Exponential Families and Contingency Tables

For much of the rest of the course we will be dealing with collections of random variables $X_V \equiv (X_v : v \in V)$, indexed by a set $V = \{1, \ldots, p\}$. Each X_v takes values in the set $\mathcal{X}_v$. For a subset of the variables $A \subseteq V$, we write X_A to denote $(X_v : v \in A)$.

3.1 Exponential Families

Let $p(\cdot; \theta)$ be a collection of probability densities over $\mathcal{X}$ indexed by $\theta \in \Theta$. We say that p is an *exponential family* if it can be written as

$$p(x; \theta) = \exp\left\{ \sum_i \theta_i \phi_i(x) - A(\theta) - C(x) \right\}.$$

If Θ is a non-empty open set then the family is said to be *regular*. The functions ϕ_i are the *sufficient statistics*, and the components θ_i are called the *canonical parameters* (or natural parameters). We can replace the sum with an inner product of vectors $\theta = (\theta_i)$ and $\phi = (\phi_i(x))$:

$$p(x; \theta) = \exp\left\{ \langle \theta, \phi(x) \rangle - A(\theta) - C(x) \right\}.$$

The function $A(\theta)$ is the *cumulant function*, and must be chosen so that the distribution normalizes, i.e.

$$A(\theta) = \log \int \exp\left\{ \langle \theta, \phi(x) \rangle - C(x) \right\} \, dx.$$

$Z(\theta) \equiv e^{A(\theta)}$ is also called the *partition function*.

Lemma 3.1. *We have*

$$\nabla A(\theta) = \mathbb{E}_\theta \phi(X), \qquad \nabla \nabla^T A(\theta) = \mathrm{Cov}_\theta \, \phi(X).$$

Consequently $A(\theta)$ (and $-\log p(x; \theta)$) are convex in θ. In addition, the map $\mu(\theta) : \theta \mapsto \nabla A(\theta)$ is bijective, and called the mean function.

Proof. For the first part,

$$\begin{aligned}
e^{A(\theta)} \frac{\partial}{\partial \theta_i} A(\theta) &= \frac{\partial}{\partial \theta_i} e^{A(\theta)} \\
&= \frac{\partial}{\partial \theta_i} \int \exp\left\{ \langle \theta, \phi(x) \rangle - C(x) \right\} \, dx \\
&= \int \frac{\partial}{\partial \theta_i} \exp\left\{ \langle \theta, \phi(x) \rangle - C(x) \right\} \, dx \\
&= \int \phi_i(x) \exp\left\{ \langle \theta, \phi(x) \rangle - C(x) \right\} \, dx \\
&= e^{A(\theta)} \int \phi_i(x) \exp\left\{ \langle \theta, \phi(x) \rangle - A(\theta) - C(x) \right\} \, dx \\
&= e^{A(\theta)} \mathbb{E}_\theta \phi_i(X).
\end{aligned}$$

The result for the Hessian follows similarly. The convexity of $-\log p(x; \theta) = A(\theta) - \langle \theta, \phi(x) \rangle$ is now immediate from the fact that its Hessian is a non-negative definite matrix. That $\mu(\theta)$ is bijective requires *strict* convexity; i.e. that the Hessian is positive definite. This follows from a slight extension to the above (see the book by Wainwright and Jordan, Proposition 3.1). □

The property of convexity plays an important role in the computational advantages of exponential families. Convex functions are easy to work with for the purposes of optimization: in particular, they do not contain multiple local minima.

Example 3.2. Let $X \sim \text{Poisson}(\lambda)$. We have

$$p_\lambda(x) = e^{-\lambda}\frac{\lambda^x}{x!} = \frac{1}{x!}\exp\{x\log\lambda - \lambda\}.$$

Clearly the canonical parameter is $\theta = \log\lambda$, so we can rewrite as

$$p_\theta(x) = \frac{1}{x!}\exp\left\{\theta x - e^\theta\right\},$$

giving $A(\theta) = e^\theta$ (which is convex, as expected). Note that $A'(\theta) = A''(\theta) = e^\theta = \lambda$, which is indeed the mean and variance of a Poisson distribution.

3.2 Empirical Moment Matching

To find the maximum likelihood estimate in an exponential family, we maximize the log-likelihood (ignoring C, since it is constant in θ)

$$\begin{aligned} l(\theta; X^{(1)}, \ldots, X^{(n)}) &= \left\langle \sum_{i=1}^n \phi(X^{(i)}), \theta \right\rangle - nA(\theta) \\ n^{-1} l(\theta; X^{(1)}, \ldots, X^{(n)}) &= \langle \overline{\phi(X)}, \theta\rangle - A(\theta) \end{aligned}$$

where $\overline{\phi(X)} = n^{-1}\sum_i \phi(X^{(i)})$ is the sample mean of the sufficient statistics. To maximize this, we can differentiate and set to zero, obtaining

$$\overline{\phi(X)} - \nabla A(\theta) = 0,$$

so in other words when we choose θ so that $\mathbb{E}_\theta\phi(X) = \overline{\phi(X)}$: the mean of the sufficient statistics matches the empirical mean from the data.

Note also that if we differentiate just with respect to θ_i, we obtain the same result for each sufficient statistic separately; hence if we update the parameters to match the moment $\overline{\phi_i(X)} = \mathbb{E}_\theta\phi_i(X)$, then we increase the log-likelihood. If we iterate this over i, we will converge to the global maximum likelihood estimate, because the log-likelihood is a (strictly) concave and differentiable function.

3.3 Multivariate Gaussian Distribution

Let $X_V = (X_1, \ldots, X_p)^T \in \mathbb{R}^p$ be a random vector. Let $\mu \in \mathbb{R}^p$ and $\Sigma \in \mathbb{R}^{p\times p}$ be a positive definite symmetric matrix. We say that X_V has a **multivariate Gaussian distribution** with parameters μ and Σ if the joint density is

$$f(x_V) = \frac{1}{(2\pi)^{p/2}|\Sigma|^{1/2}}\exp\left\{-\frac{1}{2}(x_V-\mu)^T\Sigma^{-1}(x_V-\mu)\right\}, \qquad x_V \in \mathbb{R}^p.$$

This is also called the multivariate normal distribution. The **concentration matrix** is $K \equiv \Sigma^{-1}$.

We can rewrite this as

$$f(x_V) = \frac{1}{(2\pi)^{p/2}} \exp\left\{-\frac{1}{2}x_V^T K x_V + \mu^T K x_V - \frac{1}{2}\mu^T K \mu + \frac{1}{2}\log|K|\right\}, \qquad x_V \in \mathbb{R}^p.$$

Noting that $x_V^T K x_V = \sum_{i,j} k_{ij} x_i x_j$ we see that this is an exponential family with canonical parameters K and $\eta \equiv -K\mu$, and sufficient statistics $\phi(x_V) = (x_V, -\frac{1}{2}x_V x_V^T)$.

We then obtain that $2A(\theta) = 2A(K, \eta) = \eta^T K^{-1}\eta - \log|K|$, which by differentiating[2], gives

$$\begin{aligned}\nabla_\eta A(\theta) &= K^{-1}\eta = \mu \\ 2\nabla_K A(\theta) &= -K^{-1} - K^{-1}\eta\eta^T K^{-1} = -\Sigma - \mu\mu^T,\end{aligned}$$

and these are indeed the expectations of the sufficient statistics. By the previous observation that maximum likelihood estimation corresponds to moment matching for exponential families, this means that the MLEs are $\hat{\mu} = \overline{X}_V$ and $\hat{\Sigma} = \overline{X_V X_V'} - \overline{X}_V \overline{X}_V^T$.

Proposition 3.3. *Let X_V have a multivariate Gaussian distribution with concentration matrix $K = \Sigma^{-1}$. Then $X_i \perp\!\!\!\perp X_j \mid X_{V\setminus\{i,j\}}$ if and only if $k_{ij} = 0$, where k_{ij} is the corresponding entry in the concentration matrix.*

Proof. The log-density is

$$\log f(x_V) = -\frac{1}{2}(x_V - \mu)^T K (x_V - \mu) + \text{const}$$

where the constant term does not depend upon x_V. It is clear that the only term involving both x_i and x_j is $-k_{ij}(x_i - \mu_i)(x_j - \mu_j)$. Hence, $k_{ij} = 0$ if and only if the log-density has separate terms for each of x_i and x_j. □

We will return to the multivariate Gaussian distribution in Chapter 5.

3.4 Contingency Tables

In this section we will assume that our variables X_v are discrete with a finite set of levels $\mathcal{X}_v \equiv \{1, \ldots, d_v\}$. Though we use integers as labels, they can represent something completely arbitrary and unordered such as religion, social preference, or a car model.

Given a vector of these categories $X_V^{(i)} = (X_1^{(i)}, \ldots, X_p^{(i)})$ sampled over individuals $i = 1, \ldots, n$, it is helpful to cross-tabulate their responses. Define:

$$n(x_V) \equiv \sum_{i=1}^{n} \mathbb{1}\{X_1^{(i)} = x_1, \ldots, X_p^{(i)} = x_p\},$$

i.e. the number of individuals who have the response pattern x_V. These counts are the sufficient statistics for a multinomial model, whose log-likelihood is

$$l(p; \boldsymbol{n}) = \sum_{x_V} n(x_V) \log p(x_V), \qquad p(x_V) \geq 0, \quad \sum_{x_V} p(x_V) = 1$$

[2]Here I use matrix calculus, see for example, "The Matrix Cookbook", available here (though note this is not examinable!): `https://www.math.uwaterloo.ca/~hwolkowi/matrixcookbook.pdf`

Letting 0_V mean the vector of zeros, we can rewrite this as

$$l(p; \boldsymbol{n}) = \sum_{x_V \neq 0_V} n(x_V) \log p(x_V)/p(0_V) + n \log p(0_V),$$

We immediately obtain that the multinomial distribution is an exponential family with sufficient statistics given by the counts $n(x_V)$, and canonical parameters given by the ratios of log-probabilities. The cumulant function is $-\log p(0_V)$, but it should be written as a function of the canonical parameters; you can check that this gives

$$-\log p(0_V) = \log \left(1 + \sum_{x_V \neq 0_V} e^{\theta(x_V)} \right)$$

for $\theta(x_V) = \log p(x_V)/p(0_V)$, which is convex. Note that canonical parameters are only unique up to linear transformations; in particular, we could have used a different reference value. We will use an alternative parameterization below.

Each possibility x_V is called a *cell* of the table. Given a subset of the responses $A \subseteq V$ we may be interested in the *marginal table*:

$$n(x_A) \equiv \sum_{x_B} n(x_A, x_B),$$

where $B = V \setminus A$.

Example 3.4. Consider the death penalty data again:

Victim	White	
Defendant	White	Black
Yes	53	11
No	414	37

Victim	Black	
Defendant	White	Black
Yes	0	4
No	16	139

The marginal table has

Defendant	White	Black
Yes	53	15
No	430	176

3.5 Computation

As noted in the introduction, even a moderately sized contingency table will cause statistical problems in practice due to the *curse of dimensionality*. If we have k binary variables, then the contingency table will have 2^k cells. Even for $k = 10$ we will have over a thousand possibilities, and for $k = 50$ there are too many to cells to store in a computer's memory.

Conditional independence can help, however; suppose that $X_A \perp\!\!\!\perp X_B \mid X_S$ for some $A \cup B \cup S = V$, so that we have

$$p(x_V) = p(x_S) \cdot p(x_A \mid x_S) \cdot p(x_B \mid x_S).$$

Now we can store each of these factors in computer memory separately, which means $2^s + 2^{a+s} + 2^{b+s} = 2^s(1 + 2^a + 2^b)$ cells instead of 2^{s+a+b}. This is a considerable saving

if s is small and the minimum of a and b is not too small. With respect to calculations, if we want to find $P(X_v = 1)$ and $v \in A$, then we need only sum over the 2^{s+a} entries in $p(x_S) \cdot p(x_A \mid x_S)$ rather than the 2^{a+b+s} entries in $p(x_V)$.

Of course, if there are other conditional independences present then one might imagine that further computational savings become possible: indeed this is correct, and is one of the main ideas behind graphical models.

3.6 Log-linear models

The *log-linear* parameters for $p(x_V) > 0$ are defined by the relation

$$\begin{aligned}\log p(x_V) &= \sum_{A \subseteq V} \lambda_A(x_A) \\ &= \lambda_\emptyset + \lambda_1(x_1) + \cdots + \lambda_V(x_V),\end{aligned}$$

and the identifiability constraint $\lambda_A(x_A) = 0$ whenever $x_a = 1$ for some $a \in A$. (Other identifiability constraints can also be used.)

In the case of binary variables (that is, each variable takes only two states, $d_v = 2$, $\mathcal{X}_v = \{1, 2\}$), there is only one possibly non-zero level for each log-linear parameter $\lambda_A(x_A)$, which is when $x_A = (2, \ldots, 2)$. In this case we will simply write $\lambda_A = \lambda_A(2, \ldots, 2)$. We will proceed under this assumption from now on.

Example 3.5. Consider a 2×2 table with probabilities $\pi_{ij} = P(X = i, Y = j)$. The log-linear parametrization has

$$\begin{aligned}\log \pi_{11} &= \lambda_\emptyset & \log \pi_{21} &= \lambda_\emptyset + \lambda_X \\ \log \pi_{12} &= \lambda_\emptyset + \lambda_Y & \log \pi_{22} &= \lambda_\emptyset + \lambda_X + \lambda_Y + \lambda_{XY}.\end{aligned}$$

From this we can deduce that

$$\lambda_{XY} = \log \frac{\pi_{11}\pi_{22}}{\pi_{21}\pi_{12}}.$$

The quantity $\exp \lambda_{XY}$ is called the *odds ratio* between X and Y, and is a fundamental quantity in statistical inference.

Multinomial models can be fitted as Poisson GLMs using the following fact:

Proposition 3.6. *Let $X_i \sim \text{Poisson}(\mu_i)$ independently, and let $N = \sum_{i=1}^k X_i$. Then,*

$$\begin{aligned}N &\sim \text{Poisson}\left(\textstyle\sum_i \mu_i\right) \\ (X_1, \ldots, X_k)^T \mid N = n &\sim \text{Multinom}(n, (\pi_1, \ldots, \pi_k)^T),\end{aligned}$$

where $\pi_i = \mu_i / \sum_j \mu_j$.

3.7 Conditional Independence

Log-linear parameters provide a convenient way of expressing conditional independence constraints, since factorization of a density is equivalent to an additive separation of the log-density.

Theorem 3.7. *Let $p > 0$ be a discrete distribution on X_V with associated log-linear parameters λ_C, $C \subseteq V$. The conditional independence $X_a \perp\!\!\!\perp X_b \mid X_{V\setminus\{a,b\}}$ holds if and only if $\lambda_C = 0$ for all $\{a, b\} \subseteq C \subseteq V$.*

Proof. See examples sheet. □

If there is a conditional independence, then the log-linear parameters can be calculated by just looking at the distribution of each 'piece' of the conditional independence separately. For example, suppose that $X_A \perp\!\!\!\perp X_B \mid X_C$, where $A \cup B \cup C = V$. Then by Theorem 2.4, we have

$$p(x_C) \cdot p(x_A, x_B, x_C) = p(x_A, x_C) \cdot p(x_B, x_C),$$

and hence

$$\log p(x_A, x_B, x_C) = \log p(x_A, x_C) + \log p(x_B, x_C) - \log p(x_C).$$

Then applying the log-linear expansions to each term, we get

$$\sum_{W \subseteq V} \lambda_W(x_W) = \sum_{W \subseteq A \cup C} \lambda_W^{AC}(x_W) + \sum_{W \subseteq B \cup C} \lambda_W^{BC}(x_W) - \sum_{W \subseteq C} \lambda_W^{C}(x_W),$$

where λ_{BC} By equating terms we can see that

$$\begin{aligned}
\lambda_W(x_W) &= \lambda_W^{AC}(x_W) && \text{for any } W \subseteq A \cup C \text{ with } W \cap A \neq \emptyset \\
\lambda_W(x_W) &= \lambda_W^{BC}(x_W) && \text{for any } W \subseteq B \cup C \text{ with } W \cap B \neq \emptyset \\
\lambda_W(x_W) &= \lambda_W^{AC}(x_W) + \lambda_W^{BC}(x_W) - \lambda_W^{C}(x_W) && \text{for any } W \subseteq C.
\end{aligned}$$

So under this conditional independence, the log-linear parameters for $p(x_V)$ are easily obtainable from those for $p(x_A, x_C)$ and $p(x_B, x_C)$.

Example 3.8. Let us now try applying this to our death penalty dataset using R. The file `deathpen.txt` is available on the class website.

```
> df <- read.table("deathpen.txt", header=TRUE)
> df


  DeathPen Defendant Victim freq
1      Yes     White  White   53
2       No     White  White  414
3      Yes     Black  White   11
4       No     Black  White   37
5      Yes     White  Black    0
6       No     White  Black   16
7      Yes     Black  Black    4
8       No     Black  Black  139
```

We can fit log-linear models using the `glm()` command with a Poisson response. This gives the model DeathPen $\perp\!\!\!\perp$ Defendant | Victim.

```
> mod1 <- glm(freq ~ DeathPen*Victim + Defendant*Victim,
+                 family=poisson, data=df)
> summary(mod1)$coefficients
```

The output (edited for brevity) is:

```
Coefficients:
                            Estimate Std. Error z value Pr(>|z|)
(Intercept)                   4.0610     0.1258  32.283  < 2e-16 ***
DeathPenNo                    1.9526     0.1336  14.618  < 2e-16 ***
VictimBlack                  -4.9711     0.5675  -8.760  < 2e-16 ***
DefendantBlack               -2.2751     0.1516 -15.010  < 2e-16 ***
DeathPenNo:VictimBlack        1.7045     0.5237   3.255  0.00114 **
VictimBlack:DefendantBlack    4.4654     0.3041  14.685  < 2e-16 ***
```

We can verify that the coefficient of Victim-Defendant is the same as the marginal log odds-ratio between those two variables by fitting a model that ignores whether or not the death penalty was administered:

```
> mod2 <- glm(freq ~ Defendant*Victim,
+                 family=poisson, data=df)
> summary(mod2)$coefficients
```

```
                            Estimate Std. Error z value Pr(>|z|)
(Intercept)                  5.45318    0.04627  117.84   <2e-16 ***
DefendantBlack              -2.27513    0.15157  -15.01   <2e-16 ***
VictimBlack                 -3.37374    0.25423  -13.27   <2e-16 ***
DefendantBlack:VictimBlack   4.46538    0.30407   14.69   <2e-16 ***
```

Note that the parameter estimates relating to the Defendant's race (and their standard errors) are the same as in the larger model.

It is perhaps easier just to recover the predicted counts under the model:

```
> count1 <- predict(mod1, type="response")
> count1

      1       2       3       4       5       6       7       8
 58.035 408.965   5.965  42.035   0.403  15.597   3.597 139.403
```

Compare these to the actual counts: a goodness of fit test can be performed by using Pearson's χ^2 test or (almost equivalently) by looking at the residual deviance of the model.

4 Undirected Graphical Models

Conditional independence is, in general, a rather complicated object. In fact, one can derive a countably infinite number of properties like those in Theorem 2.6 to try to describe it. Graphical models are a class of conditional independence models with particularly nice properties. In this section we introduce *undirected graphical models*.

4.1 Undirected Graphs

Definition 4.1. Let V be a finite set. An *undirected graph* $\mathcal{G}$ is a pair (V, E) where:

- V are the *vertices*;
- $E \subseteq \{\{i, j\} : i, j \in V, i \neq j\}$ is a set of unordered distinct pairs of V, called *edges*.

We represent graphs by drawing the vertices (also called *nodes*) and then joining pairs of vertices by a line if there is an edge between them.

Example 4.2. The graph in Figure 4.1(a) has five vertices and six edges:

$$V = \{1, 2, 3, 4, 5\};$$
$$E = \{\{1, 2\}, \{1, 3\}, \{2, 3\}, \{3, 4\}, \{3, 5\}, \{4, 5\}\}.$$

We write $i \sim j$ if $\{i, j\} \in E$, and say that i and j are *adjacent* in the graph. The vertices adjacent to i are called the *neighbours* of i, and the set of neighbours is often called the *boundary* of i and denoted $\mathrm{bd}_{\mathcal{G}}(i)$.

A *path* in a graph is a sequence of adjacent vertices, without repetition. For example, $1 - 2 - 3 - 5$ is a path in the graph in Figure 4.1(a). However $3 - 1 - 2 - 3 - 4$ is not a path, since the vertex 3 appears twice. The *length* of a path is the number of edges in it. There is trivially a path of length zero from each vertex to itself.

Definition 4.3 (Separation)**.** Let $A, B, S \subseteq V$. We say that A and B are *separated by* S in $\mathcal{G}$ (and write $A \perp_s B \mid S\,[\mathcal{G}]$) if every path from any $a \in A$ to any $b \in B$ contains at least one vertex in S.

For example, $\{1, 2\}$ is separated from $\{5\}$ by $\{3\}$ in Figure 4.1(a).

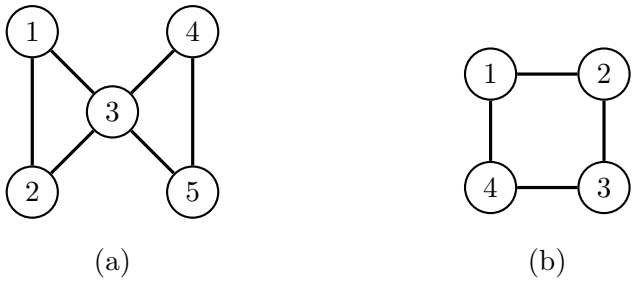
Note that there is no need for A, B, S to be disjoint for the definition to make sense, though in practice this is usually assumed.

Given a subset of vertices $W \subseteq V$, we define the *induced subgraph* $\mathcal{G}_W$ of $\mathcal{G}$ to be the graph with vertices W, and all edges from $\mathcal{G}$ whose endpoints are contained in W. For example, the induced subgraph of Figure 4.1(a) over $\{2, 3, 5\}$ is the graph $2 - 3 - 5$.

We remark that A and B are separated by S (where $S \cap A = S \cap B = \emptyset$) if and only if A and B are separated by $\emptyset$ in $\mathcal{G}_{V \setminus S}$.

4.2 Markov Properties

A graphical model is a statistical model based on the structure of a graph. We associate each vertex v with a random variable X_v, and infer structure (a model) on the joint



(a) (b)

Figure 4.1: Two undirected graphs.

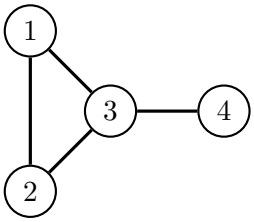


Figure 4.2: An undirected graph.

distribution of the random variables from the structure of the graph. In all the examples we consider, the model will be defined by conditional independences arising from missing edges in the graph.

Definition 4.4. Let $\mathcal{G}$ be a graph with vertices V, and let p be a probability distribution over the random variables X_V. We say that p satisfies the *pairwise Markov property* for $\mathcal{G}$ if

$$i \not\sim j \text{ in } \mathcal{G} \implies X_i \perp\!\!\!\perp X_j \mid X_{V\setminus\{i,j\}} \, [p].$$

In other words, whenever an edge is missing in $\mathcal{G}$ there is a corresponding conditional independence in p.

Example 4.5. Looking at the graph in Figure 4.2, we see that there are two missing edges, $\{1, 4\}$ and $\{2, 4\}$. Therefore a distribution obeys the pairwise Markov property for this graph if and only if $X_1 \perp\!\!\!\perp X_4 \mid X_2, X_3$ and $X_2 \perp\!\!\!\perp X_4 \mid X_1, X_3$.

Note that, if the distribution is positive then we can apply Property 5 of Theorem 2.6 to obtain that $X_1, X_2 \perp\!\!\!\perp X_4 \mid X_3$.

The word 'Markov' is used by analogy with Markov chains, in which a similar independence structure is observed. In fact, undirected graph models are often called *Markov random fields* or *Markov networks* in the machine learning literature.

Definition 4.6. We say that p satisfies the *global Markov property* for $\mathcal{G}$ if for any disjoint sets A, B, S

$$A \perp_s B \mid S \text{ in } \mathcal{G} \implies X_A \perp\!\!\!\perp X_B \mid X_S \, [p].$$

In other words, whenever a separation is present in $\mathcal{G}$ there is a corresponding conditional independence in p.

Proposition 4.7. *The global Markov property implies the pairwise Markov property.*

Proof. If $i \not\sim j$ then clearly any path from i to j first visits a vertex in $V \setminus \{i, j\}$. Hence $V \setminus \{i, j\}$ separates i and j. □

We will shortly see that the pairwise property 'almost' implies the global property.

It is common, though a pet peeve of your lecturer, to confuse a 'graph' with a 'graphical model'. A graph is—as should now be clear from the definitions above—a purely mathematical (as opposed to statistical) object; a graphical model is a statistical model that is based on the structure of a graph.

4.3 Cliques and Factorization

The pairwise Markov property implies a conditional independence involving all the variables represented in a graph for each edge that is missing from the graph; from Theorem 2.4 it is therefore a factorization on the joint distribution. A natural question is whether these separate factorizations can be combined into a single constraint on the joint distribution; in this section we show that they can, at least for positive distributions.

Definition 4.8. Let $\mathcal{G}$ be a graph with vertices V. We say C is *complete* if $i \sim j$ for every $i, j \in C$. A maximal complete set is called a *clique*. We will denote the set of cliques in a graph by $\mathcal{C}(\mathcal{G})$.

The cliques of Figure 4.1(a) are $\{1, 2, 3\}$ and $\{3, 4, 5\}$, and the complete sets are any subsets of these vertices. Note that $\{v\}$ is trivially complete in any graph.

The graph in Figure 4.1(b) has cliques $\{1, 2\}$, $\{2, 3\}$, $\{3, 4\}$ and $\{1, 4\}$.

Definition 4.9. Let $\mathcal{G}$ be a graph with vertices V. We say a distribution with density p *factorizes according to* $\mathcal{G}$ if

$$p(x_V) = \prod_{C \in \mathcal{C}(\mathcal{G})} \psi_C(x_C) \tag{1}$$

for some functions ψ_C. The functions ψ_C are called *potentials*.

Recalling Theorem 2.4, it is clear that this factorization implies conditional independence constraints. In fact, it implies those conditional independence statements given by the global Markov property.

Theorem 4.10. *If $p(x_V)$ factorizes according to $\mathcal{G}$, then p obeys the global Markov property with respect to $\mathcal{G}$.*

Proof. Suppose that S separates A and B in $\mathcal{G}$. Let $\tilde{A}$ be the set of vertices that are connected to A by paths in $\mathcal{G}_{V \setminus S}$; in particular, $B \cap \tilde{A} = \emptyset$. Let $\tilde{B} = V \setminus (\tilde{A} \cup S)$, so that $\tilde{A}$ and $\tilde{B}$ are separated by S, $V = \tilde{A} \cup \tilde{B} \cup S$, and $A \subseteq \tilde{A}$, $B \subseteq \tilde{B}$.

Every clique in $\mathcal{G}$ must be a subset of either $\tilde{A} \cup S$ or $\tilde{B} \cup S$, since there are no edges between $\tilde{A}$ and $\tilde{B}$. Hence we can write

$$\begin{aligned} \prod_{C \in \mathcal{C}} \psi_C(x_C) &= \prod_{C \in \mathcal{C}_A} \psi_C(x_C) \cdot \prod_{C \in \mathcal{C}_B} \psi_C(x_C) \\ &= f(x_{\tilde{A}}, x_S) \cdot f(x_{\tilde{B}}, x_S). \end{aligned}$$

and hence $X_{\tilde{A}} \perp\!\!\!\perp X_{\tilde{B}} \mid X_S$. Then applying property 2 of Theorem 2.6 gives $X_A \perp\!\!\!\perp X_B \mid X_S$. □

Theorem 4.11 (Hammersley-Clifford Theorem)**.** *If $p(x_V) > 0$ obeys the pairwise Markov property with respect to $\mathcal{G}$, then p factorizes according to $\mathcal{G}$.*

The proof of this is omitted, but if of interest it can be found in Lauritzen's book.

We can now summarize our Markov properties as follows:

$$\text{factorization} \implies \text{global Markov property} \implies \text{pairwise Markov property},$$

and if p is positive, then we also have

$$\text{pairwise Markov property} \implies \text{factorization},$$

so all three are equivalent. The result is not true in general if p is not strictly positive.

Example 4.12. Let X_3 and X_4 be independent Bernoulli variables with $P(X_3 = 1) = P(X_4 = 1) = \frac{1}{2}$, and $P(X_1 = X_2 = X_4) = 1$. Then $X_4 \perp\!\!\!\perp X_1 \mid X_2, X_3$ and $X_4 \perp\!\!\!\perp X_2 \mid X_1, X_3$, but $X_4 \not\perp\!\!\!\perp X_1, X_2 \mid X_3$.

Hence, P satisfies the pairwise Markov property with respect to Figure 4.2, but not the global Markov property.

It is important to note that one can define models of the form (1) that are not graphical, if the sets $\mathcal{C}$ do not correspond to the cliques of a graph. See the Examples Sheet.

4.4 Decomposability

Given the discussion in Section 2.3 we might wonder whether we can always perform inference on cliques separately in graphical models? The answer turns out to be that, in general, we can't—at least not without being more careful. However, for a particularly important subclass known as *decomposable models*, we can.

Definition 4.13. Let $\mathcal{G}$ be an undirected graph with vertices $V = A \cup S \cup B$, where A, B, S are disjoint sets. We say that (A, S, B) constitutes a *decomposition* of $\mathcal{G}$ if:

- $\mathcal{G}_S$ is complete;
- A and B are separated by S in $\mathcal{G}$.

If A and B are both non-empty we say the decomposition is *proper*.

Example 4.14. Consider the graph in Figure 4.1(a). Here $\{1, 2\}$ is separated from $\{4, 5\}$ by $\{3\}$, and $\{3\}$ is trivially complete so $(\{1, 2\}, \{3\}, \{4, 5\})$ is a decomposition. Note that $(\{2\}, \{1, 3\}, \{4, 5\})$ is also a decomposition, for example. We say that a decomposition is *minimal* if there is no subset of S that can be used to separate (some supersets of) A and B.

The graph in Figure 4.1(b) cannot be decomposed, since the only possible separating sets are $\{1, 3\}$ and $\{2, 4\}$, which are not complete. A graph which cannot be (properly) decomposed is called *prime*.

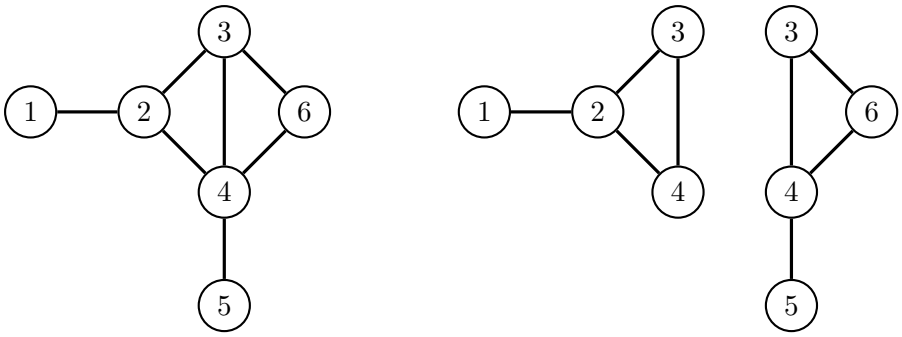


Figure 4.3: Left: a decomposable graph. Right: the results of a possible decomposition of the graph, $(\{1,2\},\{3,4\},\{5,6\})$.

Definition 4.15. Let $\mathcal{G}$ be a graph. We say that $\mathcal{G}$ is *decomposable* if it is complete, or there is a proper decomposition (A,S,B) and both $\mathcal{G}_{A\cup S}$ and $\mathcal{G}_{B\cup S}$ are also decomposable.

The graph in Figure 4.1(a) is decomposable, because using the decomposition $(\{1,2\},\{3\},\{4,5\})$ we can see that $\mathcal{G}_{\{1,2,3\}}$ and $\mathcal{G}_{\{3,4,5\}}$ are complete (and therefore decomposable by definition).

The graph in Figure 4.3 can be decomposed as shown, into $\mathcal{G}_{\{1,2,3,4\}}$ and $\mathcal{G}_{\{3,4,5,6\}}$, both of which are themselves decomposable.

Definition 4.16. Let $\mathcal{C}$ be a collection of subsets of V. We say that the sets $\mathcal{C}$ satisfy the *running intersection property* if there is an ordering $C_1,\dots,C_k$, such that for every $j=2,\dots,k$ there exists $\sigma(j)<j$ with

$$C_j \cap \bigcup_{i=1}^{j-1} C_i = C_j \cap C_{\sigma(j)}.$$

In other words, the intersection of each set with all the previously seen objects is contained in a single set.

Example 4.17. The sets $\{1,2,3\}$, $\{3,4\}$, $\{2,3,5\}$, $\{3,5,6\}$ satisfy the running intersection property, under that ordering.

The sets $\{1,2\}$, $\{2,3\}$, $\{3,4\}$, $\{1,4\}$ cannot be ordered in such a way.

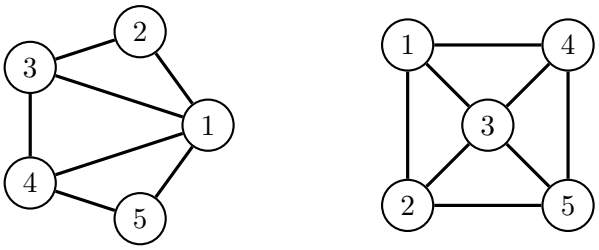
Proposition 4.18. *If $C_1,\dots,C_k$ satisfy the running intersection property, then there is a graph whose cliques are precisely (the inclusion maximal elements of) $\mathcal{C}=\{C_1,\dots,C_k\}$.*

Proof. This is left as an exercise for the interested reader. □

Definition 4.19. Let $\mathcal{G}$ be an undirected graph. A *cycle* is a sequence of vertices $\langle v_1,\dots,v_k\rangle$ for $k\geq 3$, such that there is a path $v_1-\dots-v_k$ and an edge v_k-v_1.

A *chord* on a cycle is any edge between two vertices not adjacent on the cycle. We say that a graph is *chordal* or *triangulated* if whenever there is a cycle of length ≥ 4, it contains a chord.

Beware of taking the word 'triangulated' at face value: the graph in Figure 4.4(b) is *not* triangulated because of the cycle $1-2-5-4$, which contains no chords.



(a) (b)

Figure 4.4: Two undirected graphs: (a) is chordal, (b) is not.

Theorem 4.20. *Let $\mathcal{G}$ be an undirected graph. The following are equivalent:*

(i) $\mathcal{G}$ is decomposable;

(ii) $\mathcal{G}$ is triangulated;

(iii) every minimal a, b-separator is complete;

(iv) the cliques of $\mathcal{G}$ satisfy the running intersection property, starting with C.

Proof. (i) $\implies$ (ii). We proceed by induction on p, the number of vertices in the graph. Let $\mathcal{G}$ be decomposable; if it is complete then it is clearly triangulated, so the result holds for $p = 1$. Otherwise, let (A, S, B) be a proper decomposition, so that $\mathcal{G}_{A\cup S}$ and $\mathcal{G}_{B\cup S}$ are both have strictly fewer vertices and are decomposable. By the induction hypothesis, there are no chordless cycles entirely contained in $A \cup S$ or $B \cup S$, so any such cycle must contain a vertex $a \in A$ and $b \in B$. Then the cycle must pass through S twice, and since S is complete this means there is a chord on the cycle.

(ii) $\implies$ (iii). Suppose there is a minimal a, b-separator, say S, which is not complete; let $s_1, s_2 \in S$ be non-adjacent. Since the separator is minimal there is a path π_1 from a to b via $s_1 \in S$, and another path π_2 from a to b via $s_2 \in S$, and neither of these paths intersects any other element of S. By concatenating the paths we obtain a closed walk; by shrinking the end of the paths to any vertices which are common to both we obtain a cycle. Make the cycle of minimal length by traversing chords, and we end up with a chordless cycle of length ≥ 4.

(iii) $\implies$ (iv). If the graph is complete there is nothing to prove, otherwise pick a, b not adjacent and let S be a minimal separator. As in Theorem 4.10, let $\tilde{A}$ be the connected component of a in $\mathcal{G}_{V\setminus S}$, and $\tilde{B}$ the rest. Then apply the result by induction to the strictly smaller graphs $\mathcal{G}_{\tilde{A}\cup S}$ and $\mathcal{G}_{\tilde{B}\cup S}$. Then claim that this gives a series of cliques that satisfies the RIP. [See Examples Sheet 2.]

(iv) $\implies$ (i). We proceed by induction, on the number of cliques. If $k = 1$ there is nothing to prove. Let $H_{k-1} = C_1 \cup \cdots \cup C_{k-1}$, $S_k = C_k \cap H_{k-1}$, and $R_k = C_k \setminus S_k$; we claim that $(H_{k-1} \setminus S_k, S_k, R_k)$ is a proper decomposition, and that the graph $\mathcal{G}_{H_{k-1}}$ has $k-1$ cliques that also satisfy the running intersection property. □

Corollary 4.21. *Let $\mathcal{G}$ be decomposable and (A, S, B) be a proper decomposition. Then $\mathcal{G}_{A\cup S}$ and $\mathcal{G}_{B\cup S}$ are also decomposable.*

Proof. If $\mathcal{G}$ is triangulated then so are any induced subgraphs of $\mathcal{G}$. □

This corollary reassures us that to check if a graph is decomposable we can just go ahead and start decomposing, and we will never have to 'back track'.

Definition 4.22. A *forest* is a graph that contains no cycles. If a forest is connected we call it a *tree*.

All forests (and hence trees) are decomposable, since they are clearly triangulated. In fact, the relationship between trees and connected decomposable graphs is more fundamental than this. Decomposable graphs are 'tree-like', in a sense we will make precise later in the course (Section 7). This turns out to be extremely useful for computational reasons.

4.5 Separator Sets

Let $\mathcal{G}$ be a decomposable graph, and let $C_1, \ldots, C_k$ be an ordering of the cliques which satisfies running intersection. Define the jth *separator set* for $j \geq 2$ as

$$S_j \equiv C_j \cap \bigcup_{i=1}^{j-1} C_i = C_j \cap C_{\sigma(j)}.$$

By convention $S_1 = \emptyset$.

Lemma 4.23. *Let $\mathcal{G}$ be a graph with decomposition (A, S, B), and let p be a distribution; then p factorizes with respect to $\mathcal{G}$ if and only if its marginals $p(x_{A\cup S})$ and $p(x_{B\cup S})$ factorize according to $\mathcal{G}_{A\cup S}$ and $\mathcal{G}_{B\cup S}$ respectively, and*

$$p(x_V) \cdot p(x_S) = p(x_{A\cup S}) \cdot p(x_{B\cup S}). \tag{2}$$

Proof. Note that, as observed in the proof of Theorem 4.10, every clique in $\mathcal{G}_{A\cup S}$ is a (subset of a) clique in $\mathcal{G}$. Hence if (2) and the factorizations with respect to those subgraphs hold, then we can see that p factorizes with respect to $\mathcal{G}$.

Now suppose that p factorizes with respect to $\mathcal{G}$, and note that this implies that p obeys the global Markov property with respect to $\mathcal{G}$. From the decomposition, we have $A \perp_s B \mid S$ in $\mathcal{G}$, and so by the global Markov property applied to $\mathcal{G}$ we obtain the independence $X_A \perp\!\!\!\perp X_B \mid X_S\,[p]$; this gives us the equation (2) by Theorem 2.4. Since this is a decomposition, all cliques of $\mathcal{G}$ are contained either within $A \cup S$ or $B \cup S$ (or both). Let $\mathcal{A}$ be the cliques contained in $A \cup S$, and $\mathcal{B}$ the rest.

Then $p(x_V) = \prod_{C\in\mathcal{A}} \psi_C(x_C) \cdot \prod_{C\in\mathcal{B}} \psi_C(x_C) = h(x_A, x_S) \cdot k(x_B, x_S)$. Substituting $p(x_V)$ into (2) and integrating both sides with respect to x_A gives

$$p(x_S) \cdot k(x_B, x_S) \int h(x_A, x_S)\, dx_A = p(x_S) \cdot p(x_B, x_S)$$
$$p(x_S) \cdot k(x_B, x_S) \cdot \tilde{h}(x_S) = p(x_S) \cdot p(x_B, x_S),$$

which shows that $p(x_B, x_S) = \psi'_S(x_S) \prod_{C\in\mathcal{B}} \psi_C$ as required. □

Theorem 4.24. *Let $\mathcal{G}$ be a decomposable graph with cliques $C_1, \ldots, C_k$. Then p factorizes with respect to $\mathcal{G}$ if and only if*

$$p(x_V) = \prod_{i=1}^{k} p(x_{C_i\setminus S_i} \mid x_{S_i}) = \prod_{i=1}^{k} \frac{p(x_{C_i})}{p(x_{S_i})}.$$

Further, the quantities $p(x_{C_i\setminus S_i} \mid x_{S_i})$ are variation independent (i.e. they may jointly take any set of values that would be valid individually), so inference for $p(x_V)$ can be based on separate inferences for each $p(x_{C_i})$.

Proof. If p factorizes in the manner suggested then it satisfies the factorization property for $\mathcal{G}$.

For the converse we proceed by induction on k. If $k = 1$ the result is trivial. Otherwise, let $H_{k-1} \equiv \bigcup_{i<k} C_i$, and note that $C_k \setminus S_k$ is separated from $H_{k-1} \setminus S_k$ by S_k, so we have a decomposition $(H_{k-1} \setminus S_k, S_k, C_k \setminus S_k)$, and hence applying Lemma 4.23,

$$p(x_{S_k}) \cdot p(x_V) = p(x_{C_k}) \cdot p(x_{H_{k-1}})$$

where $p(x_{H_{k-1}})$ factorizes according to $\mathcal{G}_{H_{k-1}}$. This is the graph with cliques $C_1, \ldots, C_{k-1}$, which trivially also satisfy running intersection. Hence, by the induction hypothesis

$$p(x_{S_k}) \cdot p(x_V) = p(x_{C_k}) \cdot \prod_{i=1}^{k-1} \frac{p(x_{C_i})}{p(x_{S_i})},$$

giving the required result.

The variation independence follows from the fact that $p(x_{C_k \setminus S_k} \mid x_{S_k})$ can take the form of any valid probability distribution. □

This result is extremely useful for statistical inference, since we only need to consider the margins of variables corresponding to cliques. Suppose we have a contingency table with counts $n(x_V)$. The likelihood for a decomposable graph is

$$\begin{aligned} l(p; n) &= \sum_{x_V} n(x_V) \log p(x_V) \\ &= \sum_{x_V} n(x_V) \sum_{i=1}^{k} \log p(x_{C_i \setminus S_i} \mid x_{S_i}) \\ &= \sum_{i=1}^{k} \sum_{x_{C_i}} n(x_{C_i}) \log p(x_{C_i \setminus S_i} \mid x_{S_i}), \end{aligned}$$

so inference about $p(x_{C_i \setminus S_i} \mid x_{S_i})$ should be based entirely upon $n(x_{C_i})$. Using Lagrange multipliers (see also Sheet 0, Question 4) we can see that the likelihood is maximized by choosing

$$\hat{p}(x_{C_i \setminus S_i} \mid x_{S_i}) = \frac{n(x_{C_i})}{n(x_{S_i})}, \qquad \text{i.e. } \hat{p}(x_{C_i}) = \frac{n(x_{C_i})}{n},$$

using the empirical distribution for each clique.

4.6 Non-Decomposable Models

It would be natural to ask at this point whether the closed-form results for decomposable models also hold for general undirected graph models; unfortunately they do not. However, from our discussion about exponential families we can say the following:

Theorem 4.25. *Let $\mathcal{G}$ be an undirected graph, and suppose we have counts $n(x_V)$. Then the maximum likelihood estimate $\hat{p}$ under the set of distributions that are Markov to $\mathcal{G}$ is the unique element in which*

$$n \cdot \hat{p}(x_C) = n(x_C).$$

(a) (b)

Figure 4.5: (a) A non-decomposable graph and (b) one possible triangulation of it.

The *iterative proportional fitting* (IPF) algorithm, also sometimes called the *iterative proportional scaling* (IPS) algorithm, starts with a discrete distribution that satisfies the Markov property for the graph $\mathcal{G}$ (usually we pick the uniform distribution, so that everything is independent), and then iteratively fixes each margin $p(x_C)$ to match the required distribution using the update step:

$$\begin{aligned} p^{(t+1)}(x_V) &= p^{(t)}(x_V) \cdot \frac{p(x_C)}{p^{(t)}(x_C)} \\ &= p^{(t)}(x_{V \setminus C} \mid x_C) \cdot p(x_C). \end{aligned} \tag{3}$$

Note that this is closely related to the message passing algorithm in Section 7.

Algorithm 1 Iterative Proportional Fitting (IPF) algorithm.

function IPF(collection of consistent margins $q(x_{C_i})$ for sets $C_1, \ldots, C_k$)
  set $p(x_V)$ to uniform distribution;
  while $\max_i \max_{x_{C_i}} |p(x_{C_i}) - q(x_{C_i})| >$ tol **do**
    for i in $1, \ldots, k$ **do**
      update $p(x_V)$ to $p(x_{V \setminus C_i} \mid x_{C_i}) \cdot q(x_{C_i})$;
    end for
  end while
  return distribution p with margins $p(x_{C_i}) = q(x_{C_i})$.
end function

The sequence of distributions in IPF converges to the MLE $\hat{p}(x_V)$. To see this, first note that the update (3) ensures that the moments for the sufficient statistics involving the clique C are matched. Second, after each update step the joint distribution remains Markov with respect to $\mathcal{G}$: this can be seen easily by considering the factorization. Performing each step increases the likelihood, and since the log-likelihood is strictly concave, this sort of co-ordinate based iterative updating scheme will converge to the global maximum.

Example 4.26. Consider the 4-cycle in Figure 4.5(a), with cliques $\{1,2\}, \{2,3\}, \{3,4\}, \{1,4\}$.

Suppose we have data from $n = 96$ observations as shown in the table below (the column 'count').

X_1	X_2	X_3	X_4	count
0	0	0	0	5
1	0	0	0	10
0	1	0	0	20
1	1	0	0	1
0	0	1	0	0
1	0	1	0	3
0	1	1	0	4
1	1	1	0	0
0	0	0	1	24
1	0	0	1	0
0	1	0	1	9
1	1	0	1	3
0	0	1	1	1
1	0	1	1	2
0	1	1	1	4
1	1	1	1	10

step 0	step 1	step 2	step 3	step 4	$\hat{n}$
6	7.5	13	13	12.59	12.6
6	3.75	6.5	6.5	6.97	6.95
6	9.25	11.97	11.97	11.59	11.58
6	3.5	4.53	4.53	4.86	4.87
6	7.5	2	1.17	1.13	1.13
6	3.75	1	0.58	0.63	0.63
6	9.25	6.53	3.81	3.69	3.69
6	3.5	2.47	1.44	1.55	1.55
6	7.5	13	13	13.33	13.35
6	3.75	6.5	6.5	6.11	6.1
6	9.25	11.97	11.97	12.28	12.27
6	3.5	4.53	4.53	4.26	4.28
6	7.5	2	2.83	2.91	2.91
6	3.75	1	1.42	1.33	1.33
6	9.25	6.53	9.25	9.49	9.46
6	3.5	2.47	3.5	3.29	3.3

The marginals over the cliques are:

$n(x_{12})$	$X_2=0$	1
$X_1=0$	30	37
1	15	14

$n(x_{23})$	$X_3=0$	1
$X_2=0$	39	6
1	33	18

$n(x_{34})$	$X_4=0$	1
$X_3=0$	36	36
1	7	17

$n(x_{14})$	$X_4=0$	1
$X_1=0$	29	38
1	14	15

To implement IPF, we start with a uniform table, given in the column 'step 0'. We then scale the entries so as to match the X_1, X_2 margin above. For instance, the four entries corresponding to $X_1 = X_2 = 0$ are scaled to add up to 30; this gives the column 'step 1'. This is repeated for each of the other cliques, giving steps 2–4. By the fourth step the distribution of all cliques has been updated, but note that the margin over X_1, X_2 is now 29.96, 15.04, 37.04, 13.96. We keep cycling until the process converges to the final column, which matches all four margins.

5 Gaussian Graphical Models

Recall that X_V has a **multivariate Gaussian distribution** with parameters μ and Σ if the joint density is

$$f(x_V) = \frac{1}{(2\pi)^{p/2}|\Sigma|^{1/2}} \exp\left\{-\frac{1}{2}(x_V - \mu)^T \Sigma^{-1}(x_V - \mu)\right\}, \qquad x_V \in \mathbb{R}^p.$$

Proposition 5.1. *Let $X_V \sim N_p(\mu, \Sigma)$, and let A be a $q \times p$ matrix of full rank q. Then*

$$AX_V \sim N_q(A\mu, A\Sigma A^T).$$

In particular, for any $U \subseteq V$ we have $X_U \sim N_q(\mu_U, \Sigma_{UU})$.

Proof sketch (you should fill in the gaps). For $q = p$ this just follows from applying the transformation $Z = AX_V$ to the density of X_V. If $q < p$ then since Σ is positive definite we can write $\Sigma = LL^T$ for a non-singular lower triangular matrix L; then construct a non-singular $p \times p$ matrix

$$\tilde{A} = \begin{pmatrix} A \\ B \end{pmatrix}$$

whose first q rows are A, and such that $\tilde{A}L$ has its first q rows orthogonal to its last $p - q$ rows. Then

$$\tilde{A}\Sigma\tilde{A}^T = \begin{pmatrix} A\Sigma A^T & 0 \\ 0 & B\Sigma B^T \end{pmatrix}$$

and the first q components have the desired marginal distribution. □

For simplicity of notation, we will assume throughout that $\mu = 0$. Note that the dependence structure is entirely determined by Σ, and μ is an orthogonal parameter to Σ.

5.1 Gaussian Graphical Models

We only consider cases in which Σ is positive definite, so all our density functions are strictly positive. Hence, by the Hammersley-Clifford Theorem, the pairwise and global Markov properties, and the factorization criterion all lead to the same conditional independence restrictions. If any of these hold, we will say that Σ 'is Markov with respect to' a graph, without ambiguity.

Recall that $X_A \perp\!\!\!\perp X_B$ if and only if $\Sigma_{AB} = 0$, and note that a corollary of this is that $X \perp\!\!\!\perp Y$ and $X \perp\!\!\!\perp Z$ *does* imply $X \perp\!\!\!\perp Y, Z$ for jointly Gaussian random variables.

Theorem 5.2. *Let $X_V \sim N_p(\mu, \Sigma)$ for positive definite Σ, with $K = \Sigma^{-1}$. Then the distribution of X_V is Markov with respect to $\mathcal{G}$ if and only if $k_{ab} = 0$ whenever $a \not\sim b$ in $\mathcal{G}$.*

Proof. This follows immediately from Proposition 3.3. □

We introduce some notation for convenience. If M is a matrix whose rows and columns are indexed by $A \subseteq V$, we write $\{M\}_{A,A}$ to indicate the matrix indexed by V (i.e. it has $|V|$ rows and columns) whose A, A-entries are M and with zeroes elsewhere.

For example, if $|V| = 3$ then

$$M = \begin{pmatrix} a & b \\ b & c \end{pmatrix} \qquad\qquad \{M\}_{12,12} = \begin{pmatrix} a & b & 0 \\ b & c & 0 \\ 0 & 0 & 0 \end{pmatrix},$$

where 12 is used as an abbreviation for $\{1, 2\}$ in the subscript.

Lemma 5.3. *Let $\mathcal{G}$ be a graph with decomposition (A, S, B), and $X_V \sim N_p(0, \Sigma)$. Then $p(x_V)$ is Markov with respect to $\mathcal{G}$ if and only if*

$$\Sigma^{-1} = \left\{(\Sigma_{A\cup S, A\cup S})^{-1}\right\}_{A\cup S, A\cup S} + \left\{(\Sigma_{B\cup S, B\cup S})^{-1}\right\}_{B\cup S, B\cup S} - \left\{(\Sigma_{S,S})^{-1}\right\}_{S,S},$$

and $\Sigma_{A\cup S, A\cup S}$ and $\Sigma_{B\cup S, B\cup S}$ are Markov with respect to $\mathcal{G}_{A\cup S}$ and $\mathcal{G}_{B\cup S}$ respectively.

Proof. We know from Lemma 4.23 that

$$p(x_V) \cdot p(x_S) = p(x_A, x_S) \cdot p(x_B, x_S).$$

where $p(x_A, x_S)$ and $p(x_B, x_S)$ are Markov with respect to $\mathcal{G}_{A\cup S}$ and $\mathcal{G}_{B\cup S}$ respectively. Since margins of multivariate Gaussians are also multivariate Gaussian, we can insert the appropriate density for each term, take logs and rearrange to see that:

$$x_V^T \Sigma^{-1} x_V + x_S^T (\Sigma_{SS})^{-1} x_S = x_{A\cup S}^T (\Sigma_{A\cup S, A\cup S})^{-1} x_{A\cup S} + x_{B\cup S}^T (\Sigma_{B\cup S, B\cup S})^{-1} x_{B\cup S} + \text{const.}$$

which is a quadratic polynomial in the variables x_v. By, comparing coefficients for each term we obtain that

$$\Sigma^{-1} = \left\{(\Sigma_{A\cup S, A\cup S})^{-1}\right\}_{A\cup S, A\cup S} + \left\{(\Sigma_{B\cup S, B\cup S})^{-1}\right\}_{B\cup S, B\cup S} - \left\{(\Sigma_{S,S})^{-1}\right\}_{S,S}.$$

This gives the result. □

Applying the previous result to a decomposable graph repeatedly we see that X_V is Markov with respect to $\mathcal{G}$ if and only if

$$\Sigma^{-1} = \sum_{i=1}^{k} \left\{(\Sigma_{C_i, C_i})^{-1}\right\}_{C_i, C_i} - \sum_{i=2}^{k} \left\{(\Sigma_{S_i, S_i})^{-1}\right\}_{S_i, S_i}.$$

5.2 Maximum Likelihood Estimation

Let $X_V^{(1)}, \ldots, X_V^{(n)}$ be i.i.d. $N_p(0, \Sigma)$; then from Section 3 the sufficient statistic for Σ is the sample covariance matrix:

$$W \equiv \frac{1}{n} \sum_{i=1}^{n} X_V^{(i)} X_V^{(i)T}.$$

In addition, $\hat{\Sigma} = W$ is also the MLE for Σ under the unrestricted model (i.e. when all edges are present in the graph). Let $\hat{\Sigma}^{\mathcal{G}}$ denote the MLE for Σ under the restriction that the distribution satisfies the Markov property for $\mathcal{G}$, and $\hat{K}^{\mathcal{G}}$ its inverse.

Recall that if $i \not\sim j$ then $k_{ij} = 0$, so the sufficient statistics for a graph $\mathcal{G}$ reduce to the entries in W that correspond to edges in the graph. The MLE involves picking $\hat{K}$ such that:

$$\begin{aligned} \hat{k}_{ij} &= 0 && \text{whenever } i \not\sim j \\ \hat{\sigma}_{ij} &= W_{ij} && i \sim j; \end{aligned}$$

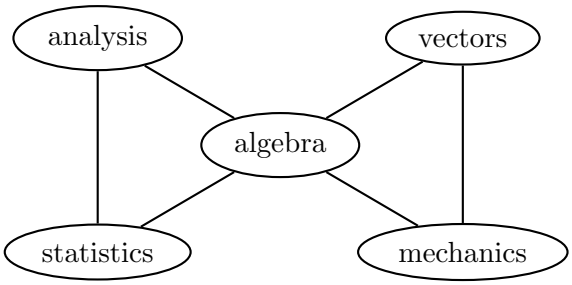


Figure 5.1: A graph for the maths test data.

(here $\hat{\sigma}_{ij}$ is the (i,j) entry of the inverse of $\hat{K}$).

For a decomposable graph $\mathcal{G}$ with cliques $C_1, \ldots, C_k$ this means that the MLE can be written in the form

$$\left(\hat{\Sigma}^{\mathcal{G}}\right)^{-1} = \sum_{i=1}^{k} \left\{(W_{C_i,C_i})^{-1}\right\}_{C_i,C_i} - \sum_{i=2}^{k} \left\{(W_{S_i,S_i})^{-1}\right\}_{S_i,S_i}.$$

This matches the sufficient statistics so that $\Sigma_{C_i,C_i} = W_{C_i,C_i}$ for each i.

5.3 Data Examples

Example 5.4. Whittaker (1990) analyses data on five maths test results administered to 88 students, in analysis, algebra, vectors, mechanics and statistics. The empirical concentration matrix (i.e. S^{-1}) is given by the following table (entries multiplied by 10^3)

	mechanics	vectors	algebra	analysis	statistics
mechanics	5.24	−2.43	−2.72	0.01	−0.15
vectors	−2.43	10.42	−4.72	−0.79	−0.16
algebra	−2.72	−4.72	26.94	−7.05	−4.70
analysis	0.01	−0.79	−7.05	9.88	−2.02
statistics	−0.15	−0.16	−4.70	−2.02	6.45

Notice that some of the entries in the concentration matrix are quite small, suggesting that conditional independence holds. Indeed, fitting the graphical model in Figure 5.1 gives an excellent fit (see Examples Sheet 2). The model suggests that abilities in analysis and statistics are independent of that in mechanics and vector calculus, conditional on one's fundamental skill at algebra.

6 Directed Graphical Models

Undirected graphs represent symmetrical relationships between random variables: the vertices in an undirected graph are not typically ordered. However, in many realistic situations the relationships we wish to model are not symmetric: for example, in regression we have a outcome that is modelled as a function of covariates, and implicitly this suggests that the covariates are 'prior' to the outcome (in a temporal sense or otherwise).

A further limitation of undirected graphs is that they are only able to represent conditional independences; they can only represent marginal independences if the relevant variables are in disconnected components. In practice, marginal independences arise very naturally if we have independent inputs to a system, and an output that is a (random) function of the inputs.

An example is given in Figure 6.1. Suppose that within the general population acamdeic and sporting abilities are uncorrelated, but that either may be sufficient to gain admission to the elite Yarvard University. Then—as we will see—*conditional* upon admission to Yarvard we would expect academic and sporting abilities to be *negatively* associated.

Such situations are naturally represented by a directed graph.

Definition 6.1. A *directed graph* $\mathcal{G}$ is a pair (V, D), where

- V is a finite set of *vertices*; and
- $D \subseteq V \times V$ is a collection of *edges*, which are *ordered* pairs of vertices. Loops (i.e. edges of the form (v, v)) are not allowed.

If $(v, w) \in D$ we write $v \to w$, and say that v is a *parent* of w, and conversely w a *child* of v. Examples are given in Figures 6.1 and 6.2(a).

We still say that v and w are *adjacent* if $v \to w$ or $w \to v$. A *path* in $\mathcal{G}$ is a sequence of distinct vertices such that each adjacent pair in the sequence is adjacent in $\mathcal{G}$. The path is *directed* if all the edges point away from the beginning of the path.

For example, in the graph in Figure 6.2(a), 1 and 2 are parents of 3. There is a path $1 \to 3 \leftarrow 2 \to 5$, and there is a directed path $1 \to 3 \to 5$ from 1 to 5.

The set of parents of w is $\mathrm{pa}_{\mathcal{G}}(w)$, and the set of children of v is $\mathrm{ch}_{\mathcal{G}}(v)$.

Definition 6.2. A graph contains a *directed cycle* if there is a directed path from v to w together with an edge $w \to v$. A directed graph is *acyclic* if it contains no directed cycles. We call such graphs *directed acyclic graphs* (DAGs).

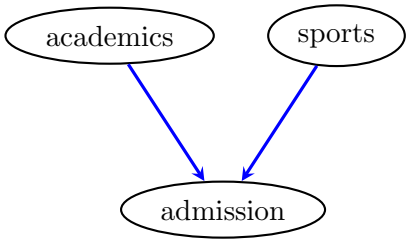


Figure 6.1: A directed graph with vertices representing abilities in academic disciplines and sports, and an indicator of admission to Yarvard, an elite US university.

All the directed graphs considered in this course are acyclic.

A *topological ordering* of the vertices of the graph is an ordering $1, \ldots, k$ such that $i \in \mathrm{pa}_{\mathcal{G}}(j)$ implies that $i < j$. That is, vertices at the 'top' of the graph come earlier in the ordering. Acyclicity ensures that a topological ordering always exists.

We say that a is an *ancestor* of v if *either* $a = v$, or there is a directed path $a \to \cdots \to v$. The set of ancestors of v is denoted by $\mathrm{an}_{\mathcal{G}}(v)$. The ancestors of 4 in the DAG in Figure 6.2(a) are $\mathrm{an}_{\mathcal{G}}(4) = \{2, 4\}$. The *descendants* of v are defined analogously and denoted $\mathrm{de}_{\mathcal{G}}(v)$; the *non-descendants* of v are $\mathrm{nd}_{\mathcal{G}}(v) \equiv V \setminus \mathrm{de}_{\mathcal{G}}(v)$. The non-descendants of 4 in Figure 6.2(a) are $\{1, 2, 3\}$.

6.1 Markov Properties

As with undirected graphs, we will associate a model with each DAG via various Markov properties. The most natural way to describe the model associated with a DAG is via a factorization criterion, so this is where we begin.

For any multivariate probability distribution $p(x_V)$, given an arbitrary ordering of the variables $x_1, \ldots, x_k$, we can iteratively use the definition of conditional distributions to see that

$$p(x_V) = \prod_{i=1}^{k} p(x_i \mid x_1, \ldots, x_{i-1}).$$

A directed acyclic graph model uses this form with a topological ordering of the graph, and states that the right-hand side of each factor only depends upon the parents of i.

Definition 6.3 (Factorization Property)**.** Let $\mathcal{G}$ be a directed acyclic graph with vertices V. We say that a probability distribution $p(x_V)$ *factorizes with respect to* $\mathcal{G}$ if

$$p(x_V) = \prod_{v \in V} p(x_v \mid x_{\mathrm{pa}_{\mathcal{G}}(v)}), \qquad\qquad x_V \in \mathcal{X}_V.$$

This is clearly a conditional independence model; given a total ordering on the vertices V, let $\mathrm{pre}_{<}(v) = \{w \mid w < v\}$ denote all the vertices that precede v according to the ordering. It is not hard to see that we are requiring

$$p(x_v \mid x_{\mathrm{pre}_{<}(v)}) = p(x_v \mid x_{\mathrm{pa}_{\mathcal{G}}(v)}), \qquad\qquad v \in V$$

for an arbitrary topological ordering of the vertices $<$. That is,

$$X_v \perp\!\!\!\perp X_{\mathrm{pre}_{<}(v) \setminus \mathrm{pa}_{\mathcal{G}}(v)} \mid X_{\mathrm{pa}_{\mathcal{G}}(v)} \, [p]. \tag{4}$$

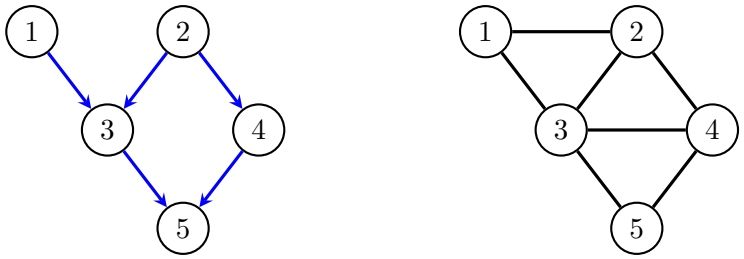
Since the ordering is arbitrary provided that it is topological, we can pick $<$ so that as many vertices come before v as possible; then we see that (4) implies

$$X_v \perp\!\!\!\perp X_{\mathrm{nd}_{\mathcal{G}}(v) \setminus \mathrm{pa}_{\mathcal{G}}(v)} \mid X_{\mathrm{pa}_{\mathcal{G}}(v)} \, [p]. \tag{5}$$

Distributions are said to obey the *local Markov property* with respect to $\mathcal{G}$ if they satisfy (5) for every $v \in V$.

For example, the local Markov property applied to each vertex in Figure 6.2(a) would require that

$$X_1 \perp\!\!\!\perp X_2, X_4 \qquad X_2 \perp\!\!\!\perp X_1 \qquad X_3 \perp\!\!\!\perp X_4 \mid X_1, X_2$$
$$X_4 \perp\!\!\!\perp X_1, X_3 \mid X_2 \qquad X_5 \perp\!\!\!\perp X_1, X_2 \mid X_3, X_4$$



(a) (b)

Figure 6.2: (a) A directed graph and (b) its moral graph.

There is some redundancy here, but not all independences that hold are given directly. For example, using Theorem 2.6 we can deduce that $X_4, X_5 \perp\!\!\!\perp X_1 \mid X_2, X_3$, but we might wonder if there is a way to tell this immediately from the graph. For such a 'global Markov property' we need to do a bit more work.

6.2 Ancestrality

We say that a set of vertices A is *ancestral* if it contains all its own ancestors. So, for example, the set $\{1, 2, 4\}$ is ancestral in Figure 6.2(a); however $\{1, 3\}$ is not, because $\{2\}$ is an ancestor of $\{3\}$ but it not included.

Ancestral sets play an important role in directed graphs because of the following proposition.

Proposition 6.4. *Let A be an ancestral set in $\mathcal{G}$. Then $p(x_V)$ factorizes with respect to $\mathcal{G}$ only if $p(x_A)$ factorizes with respect to $\mathcal{G}_A$.*

Proof. See Examples Sheet 3. □

Now suppose we wish to interrogate whether a conditional independence $X_A \perp\!\!\!\perp X_B \mid X_C$ holds under a DAG model. From the previous result, we can restrict ourselves to asking if this independence holds in the induced subgraph over the ancestral set $\mathrm{an}_{\mathcal{G}}(A \cup B \cup C)$.

Definition 6.5. A *v-structure* is a triple $i \to k \leftarrow j$ such that $i \not\sim j$.

Let $\mathcal{G}$ be a directed acyclic graph; the *moral graph* $\mathcal{G}^m$ is formed from $\mathcal{G}$ by joining any non-adjacent parents and dropping the direction of edges.

In other words, the moral graph removes any 'v-structures' by filling in the missing edge, and then drops the direction of edges. An example is given in Figure 6.2.

Proposition 6.6. *If p_V factorizes with respect to a DAG $\mathcal{G}$, then it also factorizes with respect to the undirected graph $\mathcal{G}^m$.*

Proof. This follows from an inspection of the factorization and checking the cliques from $\mathcal{G}^m$. □

Using this proposition, we see that the DAG in Figure 6.2(a) implies $X_1 \perp\!\!\!\perp X_4, X_5 \mid X_2, X_3$, by using the global Markov property applied to the moral graph in Figure 6.2(b). In fact, moral graphs are used to define the global Markov property for DAGs.

Definition 6.7. We say that $p(x_V)$ satisfies the *global Markov property* with respect to $\mathcal{G}$ if whenever A and B are separated by C in $(\mathcal{G}_{\mathrm{an}(A\cup B\cup C)})^m$ we have $X_A \perp\!\!\!\perp X_B \mid X_C\,[p]$.

The global Markov property is *complete* in the sense that any independence not exhibited by a separation will not generally hold in distributions Markov to $\mathcal{G}$. We state the result formally here, but the proof is not given in this course.

Theorem 6.8 (Completeness of global Markov property.)**.** *Let $\mathcal{G}$ be a DAG. There exists a probability distribution p such that $X_A \perp\!\!\!\perp X_B \mid X_C\ [p]$ if and only if $A \perp_s B \mid C$ in $(\mathcal{G}_{\mathrm{an}(A\cup B\cup C)})^m$.*

In other words, the global Markov property gives all conditional independences that are implied by the DAG model.

We now give the main result concerning equivalence of these three definitions, which says that each of our properties give precisely equivalent models.

Theorem 6.9. *Let $\mathcal{G}$ be a DAG and p a probability density. Then the following are equivalent:*

(i) p factorizes according to $\mathcal{G}$;

(ii) p is globally Markov with respect to $\mathcal{G}$;

(iii) p is locally Markov with respect to $\mathcal{G}$.

Notice that, unlike for undirected graphs, there is no requirement of positivity on p: it is true even for degenerate distributions. There is also a 'pairwise' Markov property for directed graphs, which we will not cover; see Lauritzen's book for interest.

Proof. (i) $\implies$ (ii). Let $W = \mathrm{an}_{\mathcal{G}}(A \cup B \cup C)$, and suppose that there is a separation between A and B given C in $(\mathcal{G}_W)^m$. The distribution $p(x_W)$ can be written as

$$p(x_W) = \prod_{v\in W} p(x_v \mid x_{\mathrm{pa}(v)}),$$

so in other words it is Markov w.r.t. $\mathcal{G}_W$ and hence to $(\mathcal{G}_W)^m$ (see Propositions 6.6 and 6.4). But if p factorizes according to the undirected graph $(\mathcal{G}_W)^m$ then it is also globally Markov with respect to it by Theorem 4.10, and hence the separation implies $X_A \perp\!\!\!\perp X_B \mid X_C\ [p]$.

(ii) $\implies$ (iii). Note that moralizing only adds edges adjacent to vertices that have a child in the graph, and also that $\{v\} \cup \mathrm{nd}_{\mathcal{G}}(v)$ is an ancestral set. It follows that in the moral graph $(\mathcal{G}_{\{v\}\cup\mathrm{nd}_{\mathcal{G}}(v)})^m$, there is a separation between v and $\mathrm{nd}_{\mathcal{G}}(v) \setminus \mathrm{pa}_{\mathcal{G}}(v)$ given $\mathrm{pa}_{\mathcal{G}}(v)$.

(iii) $\implies$ (i). Let $<$ be a topological ordering of the vertices in $\mathcal{G}$. The local Markov property implies that X_v is independent of $X_{\mathrm{nd}(v)\setminus\mathrm{pa}(v)}$ given $X_{\mathrm{pa}(v)}$, so in particular it is independent of $X_{\mathrm{pre}_<(v)\setminus\mathrm{pa}(v)}$ given $X_{\mathrm{pa}(v)}$. Hence

$$p(x_V) = \prod_v p(x_v \mid x_{\mathrm{pre}_<(v)}) = \prod_v p(x_v \mid x_{\mathrm{pa}(v)})$$

as required. □

6.3 Statistical Inference

The factorization of distributions that are Markov with respect to a DAG is particularly attractive statistically because, as with the decomposable models in Theorem 4.24, the conditional distributions can all be dealt with entirely separately.

Consider again the example of a contingency table with counts $n(x_V)$. The likelihood for a DAG model is

$$\begin{aligned} l(p; n) &= \sum_{x_V} n(x_V) \log p(x_V) \\ &= \sum_{x_V} n(x_V) \sum_{v \in V} \log p(x_v \mid x_{\mathrm{pa}(v)}) \\ &= \sum_{v \in V} \sum_{x_v, x_{\mathrm{pa}(v)}} n(x_v, x_{\mathrm{pa}(v)}) \log p(x_v \mid x_{\mathrm{pa}(v)}) \\ &= \sum_{v \in V} \sum_{x_{\mathrm{pa}(v)}} \sum_{x_v} n(x_v, x_{\mathrm{pa}(v)}) \log p(x_v \mid x_{\mathrm{pa}(v)}), \end{aligned}$$

where each of the conditional distributions $p(x_v \mid x_{\mathrm{pa}(v)})$ can be dealt with entirely separately. That is, we can separately maximize each inner sum $\sum_{x_v} n(x_v, x_{\mathrm{pa}(v)}) \log p(x_v \mid x_{\mathrm{pa}(v)})$ subject to the restriction that $\sum_{x_v} p(x_v \mid x_{\mathrm{pa}(v)}) = 1$, and hence obtain the MLE

$$\hat{p}(x_v \mid x_{\mathrm{pa}(v)}) = \frac{n(x_v, x_{\mathrm{pa}(v)})}{n(x_{\mathrm{pa}(v)})};$$

$$\text{hence} \quad \hat{p}(x_V) = \prod_{v \in V} \hat{p}(x_v \mid x_{\mathrm{pa}(v)}) = \prod_{v \in V} \frac{n(x_v, x_{\mathrm{pa}(v)})}{n(x_{\mathrm{pa}(v)})}.$$

This looks rather like the result we obtained for decomposable models, and indeed we will see that there is an important connection.

A slightly more general result is to say that if we have a separate parametric model defined by some parameter θ_v for each conditional distribution $p(x_v \mid x_{\mathrm{pa}(v)}; \theta_v)$, then we can perform our inference on each θ_v separately.

Formally: the MLE for θ satisfies

$$p(x_V; \hat{\theta}) = \prod_{v \in V} p(x_v \mid x_{\mathrm{pa}(v)}; \hat{\theta}_v), \qquad\qquad x_V \in \mathcal{X}_V.$$

In addition, if we have independent priors $\pi(\theta) = \prod_v \pi(\theta_v)$, then

$$\begin{aligned} \pi(\theta \mid x_V) &\propto \pi(\theta) \cdot p(x_V \mid \theta) \\ &= \prod_v \pi(\theta_v) \cdot p(x_v \mid x_{\mathrm{pa}(v)}, \theta_v), \end{aligned}$$

which factorizes into separate functions for each θ_v, showing that the θ_v are independent conditional on X_V. Hence

$$\pi(\theta_v \mid x_V) \propto \pi(\theta_v) \cdot p(x_v \mid x_{\mathrm{pa}(v)}, \theta_v),$$

so $\pi(\theta_v \mid x_V) = \pi(\theta_v \mid x_v, x_{\mathrm{pa}(v)})$, and θ_v only depends upon X_v and $X_{\mathrm{pa}(v)}$.

In other words, the data from $X_v, X_{\mathrm{pa}(v)}$ are sufficient for each θ_v. This means that if no vertex has many parents, even very large graphs represent manageable models. For a Gaussian distribution we can use our results about conditional distributions to obtain closed form expressions for the covariance matrices that are Markov with respect to a graph (see Examples Sheet 3).

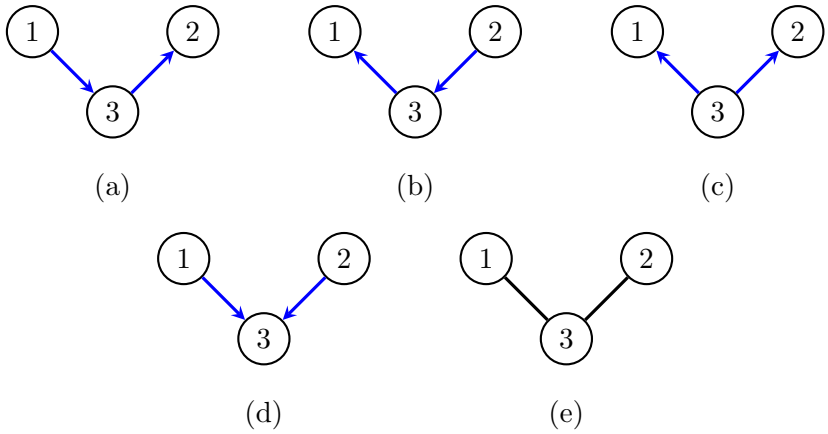


Figure 6.3: (a)-(c) Three directed graphs, and (e) an undirected graph to which they are all Markov equivalent; (d) a graph which is not Markov equivalent to the others.

6.4 Markov Equivalence

For undirected graphs, the independence $X_a \perp\!\!\!\perp X_b \mid X_{V\setminus\{a,b\}}$ is implied by the graphical model if and only if the edge $a - b$ is not present in the graph. This shows that (under any choice of Markov property) each undirected graphical model is distinct.

For directed graphs this is not the case. The graphs in Figures 6.3 (a), (b) and (c) are all different, but all imply precisely the independence $X_1 \perp\!\!\!\perp X_2 \mid X_3$.

Definition 6.10. We say that two graphs $\mathcal{G}$ and $\mathcal{G}'$ are *Markov equivalent* if any p which is Markov with respect to $\mathcal{G}$ is also Markov with respect to $\mathcal{G}'$, and vice-versa. This is an equivalence relation, so we can partition graphs into sets we call *Markov equivalence classes*.

In model selection problems we are not trying to learn the graph itself, but rather the Markov equivalence class of indistinguishable models. The presence or absence of edges induces all conditional independences, so unsurprisingly the graph of adjacencies is very important.

Definition 6.11. Given a DAG $\mathcal{G} = (V, D)$, define the *skeleton* of $\mathcal{G}$ as the undirected graph $\text{skel}(\mathcal{G}) = (V, E)$, where $\{i, j\} \in E$ if and only if either $(i, j) \in D$ or $(j, i) \in D$. In other words, we drop the orientations of edges in $\mathcal{G}$.

For example, the skeleton of the graphs in Figures 6.3(a)–(d) is the graph in Figure 6.3(e).

Lemma 6.12. *Let $\mathcal{G}$ and $\mathcal{G}'$ be graphs with different skeletons. Then $\mathcal{G}$ and $\mathcal{G}'$ are not Markov equivalent.*

Proof. Suppose without loss of generality that $i \to j$ in $\mathcal{G}$ but that $i \not\sim j$ in $\mathcal{G}'$. Then let p be any distribution in which $X_v \perp\!\!\!\perp X_{V\setminus\{v\}}$ for each $v \in V \setminus \{i, j\}$, but that X_i and X_j are dependent.

The local Markov property for $\mathcal{G}$ is clearly satisfied, since each variable is independent of its non-descendants given its parents. For $\mathcal{G}'$, however, we claim that the global Markov property is not satisfied. By Sheet 2 Question 5, there is some set C such that the GMP requires $X_i \perp\!\!\!\perp X_j \mid X_C$.

Let $c \in C$; under p we have $X_c \perp\!\!\!\perp X_{V\setminus\{c\}}$, so by applying property 2 of the graphoid axioms, $X_c \perp\!\!\!\perp X_j, X_{C\setminus\{c\}}$. Then using properties 3 and 4 we see that $X_i \perp\!\!\!\perp X_j \mid X_C$ is equivalent to $X_i \perp\!\!\!\perp X_j \mid X_{C\setminus\{c\}}$. Repeating this we end up with a requirement that $X_i \perp\!\!\!\perp X_j$, which does not hold by construction. Hence p is not Markov with respect to $\mathcal{G}'$, and the graphs are not Markov equivalent. □

Theorem 6.13. *Directed graphs $\mathcal{G}$ and $\mathcal{G}'$ are Markov equivalent if and only if they have the same skeletons and v-structures.*

Proof. We will prove the 'only if' direction for now: the converse is harder.

If $\mathcal{G}$ and $\mathcal{G}'$ have different skeletons then the induced models are different by the previous Lemma. Otherwise, suppose that $a \to c \leftarrow b$ is a v-structure in $\mathcal{G}$ but not in $\mathcal{G}'$.

Let p be a distribution in which all variables other than X_a, X_b, X_c are independent of all other variables. By the factorization property, we can then pick an arbitrary

$$p(x_V) = p(x_c \mid x_a, x_b) \prod_{v \in V\setminus\{c\}} p(x_v)$$

and obtain a distribution that is Markov with respect to $\mathcal{G}$.

In $\mathcal{G}'$ there is no v-structure, so either $a \to c \to b$, $a \leftarrow c \to b$, or $a \leftarrow c \leftarrow b$. In particular, either a or b is a child of c. Now let $A = \mathrm{an}_{\mathcal{G}}(\{a, b, c\})$; we claim that there is no $d \in A$ such that $a \to d \leftarrow b$. To see this, note that if this is true, then d is a descendant of each of a, b and c, and if $d \in A$ it is also an ancestor of one a, b and c, so the graph is cyclic.

Now, it follows that in the moral graph $(\mathcal{G}'_A)^m$, there is no edge between a and b, so $a \perp_s b \mid A \setminus \{a, b\}$ in $(\mathcal{G}'_A)^m$. But by a similar argument to the previous Lemma, the corresponding independence does not hold in p, and therefore p is not Markov with respect to $\mathcal{G}'$ if $p(x_c \mid x_a, x_b)$ is chosen not to factorize. □

6.5 Directed Graphs, Undirected Graphs, and Decomposability

Closely related to the previous point is whether an undirected graph can represent the same conditional independences as a directed one. The undirected graph in Figure 6.3(e) represents the same model as each of the directed graphs in Figures 6.3(a)–(c), so clearly in some cases this occurs.

However the graph in Figure 6.3(d) does not induce the same model as any undirected graph. Indeed, it is again this 'v-structure' that is the important factor in determining whether the models are the same.

Theorem 6.14. *A DAG $\mathcal{G}$ is Markov equivalent to an undirected graph if and only if it contains no v-structures. In this case the equivalent undirected graph is the skeleton of $\mathcal{G}$.*

Proof. We proceed by induction on the number of vertices; the result is clearly true for graphs of size $|V| \leq 1$, since there are no constraints on any such graphs.

First, if $\mathcal{G}$ has a v-structure $i \to k \leftarrow j$, note that there is an independence between X_i and X_j by the local Markov property; hence if we add the edge $i \sim j$ then the graph will not be Markov equivalent to $\mathcal{G}$. However, since $i \sim j$ in $\mathcal{G}^m$, we also know that there is a distribution, Markov with respect to $\mathcal{G}$, for which $X_i \not\perp\!\!\!\perp X_j \mid X_{V\setminus\{i,j\}}$ by Theorem 6.8. Thus, if we fail to add this edge then we also will not obtain a Markov equivalent graph. Hence no undirected graph can be Markov equivalent to $\mathcal{G}$.

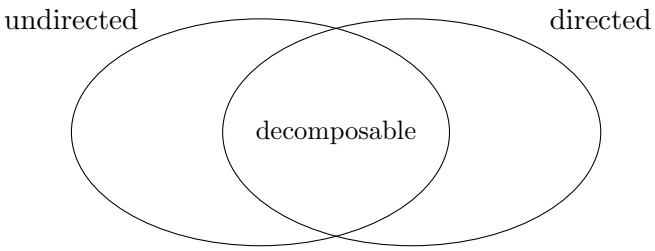


Figure 6.4: Venn diagram of model classes introduced by directed and undirected graphs.

Otherwise, suppose that $\mathcal{G}$ has no v-structures, so that $\mathcal{G}^m = \text{skel}(\mathcal{G})$. We have already established in Proposition 6.6 that if $\mathcal{G}$ is a DAG, then p being Markov with respect to $\mathcal{G}$ implies that it is also Markov with respect to $\mathcal{G}^m$.

Now suppose that p is Markov with respect to $\mathcal{G}^m$, and let v be a vertex in $\mathcal{G}$ without children. We will show that $p(x_{V\setminus\{v\}})$ is Markov with respect to $\mathcal{G}_{V\setminus\{v\}}$ and that $X_v \perp\!\!\!\perp X_{V\setminus(\text{pa}(v)\cup\{v\})} \mid X_{\text{pa}(v)}$ under p, and hence that p satisfies the local Markov property with respect to $\mathcal{G}$.

The neighbours of v in $\mathcal{G}^m$ are its parents in $\mathcal{G}$, and in the moral graph $\mathcal{G}^m$ these are all adjacent, so there is a decomposition $(\{v\}, \text{pa}_{\mathcal{G}}(v), W)$ in $\mathcal{G}^m$, where $W = V\setminus(\{v\}\cup\text{pa}_{\mathcal{G}}(v))$. By Lemma 4.23, we have $X_v \perp\!\!\!\perp X_W \mid X_{\text{pa}(v)}$, and that $p(x_{V\setminus\{v\}})$ is Markov with respect to $(\mathcal{G}^m)_{V\setminus\{v\}}$. Now, since $\mathcal{G}$ has no v-structures neither does $\mathcal{G}_{V\setminus\{v\}}$, and so $(\mathcal{G}^m)_{V\setminus\{v\}} = (\mathcal{G}_{V\setminus\{v\}})^m$; since this graph also has $|V|-1$ vertices, by the induction hypothesis, $p(x_{V\setminus\{v\}})$ is Markov with respect to $\mathcal{G}_{V\setminus\{v\}}$. Hence, the result holds. □

Corollary 6.15. *A undirected graph is Markov equivalent to a directed graph if and only if it is decomposable.*

Proof. This can be seen by the same decomposition and induction as in the proof of the Theorem above. □

This shows that decomposable models represent the intersection of undirected and directed graphical models.

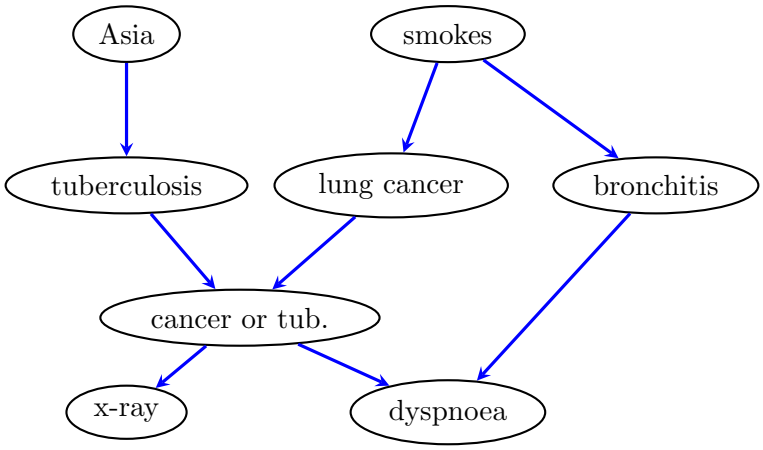


Figure 7.1: The 'Chest Clinic' network, a fictitious diagnostic model.

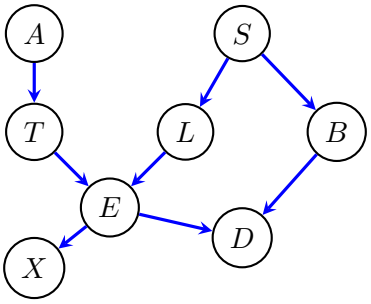
7 Junction Trees and Message Passing

In this chapter we answer some of the problems mentioned in the introduction: given a large network of variables, how can we efficiently evaluate conditional and marginal probabilities? And how should we update our beliefs given new information?

Consider the graph in Figure 7.1, which is a simplified diagnostic model, containing patient background, diseases, and symptoms. The variables represent the following indicators:

- Asia (A): the patient recently visited parts of Asia with endemic tuberculosis;
- smokes (S): the patient smokes;
- tuberculosis (T), lung cancer (L), bronchitis (B): the patient has each of these respective diseases;
- either (E): logical indicator of having either lung cancer or tuberculosis;
- x-ray (X): there is a shadow on the patient's chest x-ray;
- dyspnoea (D): the patient suffers from the sleeping disorder dyspnoea.

In practice, we observe the background and symptoms and with to infer the probability of disease given this 'evidence'. Of course, to calculate the updated probability we just need to use Bayes' formula, but for large networks this is computationally infeasible. Instead we will develop an algorithm that exploits the structure of the graph to simplify the calculations.



For this discussion we will abuse notation mildly and use capital letters $A, S, X, \ldots$ to represent both the random variables and the vertices, and lower case letters for states of the random variables. From the DAG factorization, we have

$$p(a, s, t, \ell, b, e, x, d) = p(a) \cdot p(s) \cdot p(t \mid a) \cdot p(\ell \mid s) \cdot p(b \mid s) \cdot p(e \mid t, \ell) \cdot p(x \mid e) \cdot p(d \mid e, b).$$

Suppose we wish to know the probability of lung cancer give a patient's smoking status, whether or not he or she has visited Asia (tuberculosis is endemic in some South Asian countries), their x-ray, and whether they have dyspnoea. To work out the probability of lung cancer:

$$p(\ell \mid x, d, a, s) = \frac{p(\ell, x, d \mid a, s)}{\sum_{l'} p(\ell', x, d \mid a, s)} \tag{6}$$

The quantity we need can be obtained from the factorization of the directed graph as

$$p(\ell, x, d \mid a, s) = \sum_{t,e,b} p(t \mid a) \cdot p(\ell \mid s) \cdot p(b \mid s) \cdot p(e \mid t, \ell) \cdot p(x \mid e) \cdot p(d \mid e, b). \tag{7}$$

There is more than one way to evaluate this quantity, because some of the summations can be 'pushed in' past terms that do not depend upon them. So, for example,

$$\begin{aligned} &p(\ell, x, d \mid a, s) \\ &= p(\ell \mid s) \sum_{e} p(x \mid e) \left(\sum_{b} p(b \mid s) \cdot p(d \mid e, b) \right) \left(\sum_{t} p(t \mid a) \cdot p(e \mid t, \ell) \right). \end{aligned}$$

How computationally difficult is this to calculate? A common metric is just to total the number of additions, subtractions, multiplications and divisions required. In our case, start with the expression in the sum $\sum_t p(t \mid a) \cdot p(e \mid t, \ell)$. This has to be calculated for each of the 16 values of t, a, e, ℓ, and involves a single multiplication. The summation involves adding pairs of these expressions, so this gives 8 separate additions, and leaves an expression depending on a, e, ℓ. The other expression in brackets is calculated in exactly the same way, so there are another 24 operations and expression depending on s, d, e.

Now, the outer sum is over expressions depending on a, e, ℓ, s, d, x, and involves two multiplications; this gives a total of $2 \times 2^6 = 128$. The sum itself is over 32 pairs of numbers, and each of the 32 results must be multiplied by one number. So, in total we have $24 + 24 + 128 + 32 + 32 = 240$ operations.

The naïve way implied by (6) and (7) requires rather more effort: each term in the summand of (7) involves five multiplications, and there are $2^8 = 256$ different terms. Each of the 2^5 sums is then over 8 terms (i.e. requires 7 additions). Hence we get $5 \times 2^8 + 7 \times 2^5 =$ 1,504 operations; a factor of over six times as many as our more careful approach. Over larger networks with dozens or hundreds of variables these differences are very substantial.

This section provides a method for systematically arranging calculations of this sort in an efficient way, using the structure of a graph.

7.1 Junction Trees

We have already seen that we can write distributions that are Markov with respect to an undirected graph as a product of 'potentials', which are functions only of a few variables. A junction tree is a way of arranging these potentials that is computationally convenient.

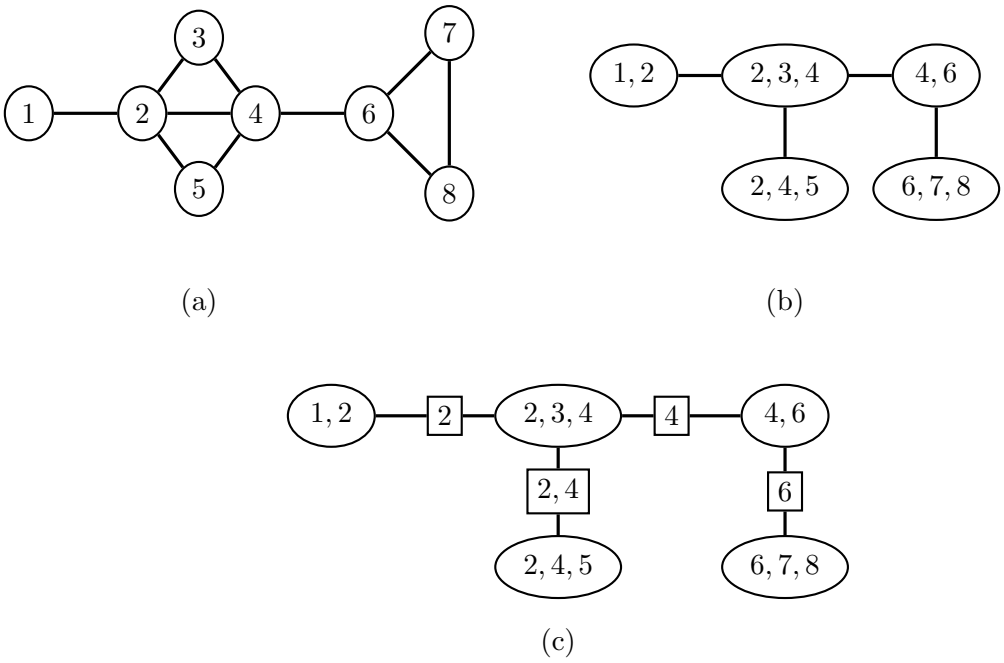


Figure 7.2: (a) A decomposable graph and (b) a possible junction tree of its cliques. (c) The same junction tree with separator sets explicitly marked.

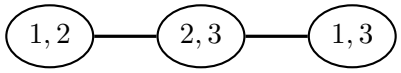


Figure 7.3: A tree of sets that is not a junction tree.

Let $\mathcal{T}$ be a tree (i.e. a connected, undirected graph without any cycles) with vertices $\mathcal{V}$ contained in the power set of V; that is, each vertex of $\mathcal{T}$ is a subset of V. We say that $\mathcal{T}$ is a *junction tree* if whenever we have $C_i, C_j \in \mathcal{V}$ with $C_i \cap C_j \neq \emptyset$, there is a (unique) path π in $\mathcal{T}$ from C_i to C_j such that for every vertex C on the path, $C_i \cap C_j \subseteq C$.

Example 7.1. The graph in Figure 7.2(b) is a junction tree. Note that, for example, $\{2, 4, 5\}$ and $\{4, 6\}$ have a non-zero intersection $\{4\}$, and that indeed 4 is contained on the intermediate vertex $\{2, 3, 4\}$.

The graph in Figure 7.3 is not a junction tree, because the sets $\{1, 2\}$ and $\{1, 3\}$ have the non-empty intersection $\{1\}$, but the intermediate sets in the tree (i.e. $\{2, 3\}$) do not contain $\{1\}$; this more general object is sometimes called a *clique tree*. The fact that these sets cannot be arranged in a junction tree is a consequence of them not satisfying the running intersection property (under any ordering), as the next result shows.

Proposition 7.2. *If $\mathcal{T}$ is a junction tree then its vertices $\mathcal{V}$ can be ordered to satisfy the running intersection property. Conversely, if a collection of sets satisfies the running intersection property they can be arranged into a junction tree.*

Proof. We proceed by induction on $k = |\mathcal{V}|$. If $k \leq 2$ then both the junction tree and running intersection conditions are always satisfied. Otherwise, since $\mathcal{T}$ is a tree it contains a leaf (i.e. a vertex joined to exactly one other), say C_k which is adjacent to $C_{\sigma(k)}$.

Consider $\mathcal{T}^{-k}$, the graph obtained by removing C_k from $\mathcal{T}$. The set of paths between C_i and C_j vertices in $\mathcal{T}^{-k}$ is the same as the set of such paths in $\mathcal{T}$: we cannot have paths via C_k because it would require repetition of $C_{\sigma(k)}$. Hence $\mathcal{T}^{-k}$ is still a junction tree, and by induction its elements $C_1, \dots, C_{k-1}$ satisfy the RIP.

But then by the definition of a junction tree, $C_k \cap \bigcup_{i<k} C_i = C_k \cap C_{\sigma(k)}$, so $C_1, \dots, C_k$ satisfies the RIP.

For the converse result, again by induction just join the final set C_k to $C_{\sigma(k)}$ and it is clear that we obtain a junction tree by definition of running intersection. □

In other words, this result shows that junction trees are available for the cliques of decomposable graphs. The graph in Figure 7.2(a) for example has cliques $\{1,2\}$, $\{2,3,4\}$, $\{2,4,5\}$, $\{4,6\}$ and $\{6,7,8\}$. Since it is a decomposable graph, these satisfy the running intersection property, and can be arranged in a junction tree such as the one in Figure 7.2(b). Notice that this is not unique, since we could join either (or both) of $\{1,2\}$ or $\{4,6\}$ to $\{2,4,5\}$ instead of $\{2,3,4\}$.

We can explicitly add in the separator sets as nodes in our tree, so that each edge contains an additional node, as shown in Figure 7.2(c).

Definition 7.3. We will associate each node C in our junction tree with a *potential* $\psi_C(x_C) \geq 0$, which is a function over the variables in the corresponding set. We say that two potentials ψ_C, ψ_D are *consistent* if

$$\sum_{x_{C \setminus D}} \psi_C(x_C) = f(x_{C \cap D}) = \sum_{x_{D \setminus C}} \psi_D(x_D).$$

That is, the margins of ψ_C and ψ_D over $C \cap D$ are the same.

Of course, the standard example of when we would have consistent margins comes when each potential is the margin of a probability distribution. Indeed, this relationship turns out to be quite fundamental.

Proposition 7.4. *Let $C_1, \dots, C_k$ satisfy the running intersection property with separator sets $S_2, \dots, S_k$, and let*

$$p(x_V) = \prod_{i=1}^{k} \frac{\psi_{C_i}(x_{C_i})}{\psi_{S_i}(x_{S_i})}$$

(where $S_1 = \emptyset$ and $\psi_\emptyset = 1$ by convention). Then each $\psi_{C_i}(x_{C_i}) = p(x_{C_i})$ and $\psi_{S_i}(x_{S_i}) = p(x_{S_i})$ if (and only if) each pair of potentials is consistent.

Proof. The only if is clear, since margins of a distribution are indeed consistent in this way.

For the converse we proceed by induction on k; for $k = 1$ there is nothing to prove. Otherwise, let $R_k = C_k \setminus S_k \left(= C_k \setminus \bigcup_{i<k} C_i\right)$, so

$$p(x_{V \setminus R_k}) = \sum_{x_{R_k}} p(x_V) = \prod_{i=1}^{k-1} \frac{\psi_{C_i}(x_{C_i})}{\psi_{S_i}(x_{S_i})} \times \frac{1}{\psi_{S_k}(x_{S_k})} \sum_{x_{R_k}} \psi_{C_k}(x_{C_k})$$

Since the cliques are consistent, we have

$$\frac{\sum_{x_{R_k}} \psi_{C_k}(x_{C_k})}{\psi_{S_k}(x_{S_k})} = \frac{\psi_{S_k}(x_{S_k})}{\psi_{S_k}(x_{S_k})} = 1,$$

so

$$p(x_{V\setminus R_k}) = \prod_{i=1}^{k-1} \frac{\psi_{C_i}(x_{C_i})}{\psi_{S_i}(x_{S_i})}. \tag{8}$$

By the induction hypothesis, we have that $\psi_{C_i}(x_{C_i}) = p(x_{C_i})$ for $i \leq k-1$. In addition, by the RIP $S_k = C_k \cap C_j$ for some $j < k$, and hence by consistency

$$\psi_{S_k}(x_{S_k}) = \sum_{x_{C_j \setminus S_k}} \psi_{C_j}(x_{C_j}) = \sum_{x_{C_j \setminus S_k}} p(x_{C_j}) = p(x_{S_k}).$$

Finally, substituting (8) into our original expression, we have

$$p(x_V) = p(x_{V\setminus R_k}) \frac{\psi_{C_k}(x_{C_k})}{\psi_{S_k}(x_{S_k})} = p(x_{V\setminus R_k}) \frac{\psi_{C_k}(x_{C_k})}{p(x_{S_k})},$$

and so $p(x_{R_k} \mid x_{V\setminus R_k}) = \frac{\psi_{C_k}(x_{C_k})}{p(x_{S_k})}$ by definition of conditional probabilities. Since this only depends upon x_{C_k}, this is also $p(x_{R_k} \mid x_{S_k})$. Hence,

$$\psi_{C_k}(x_{C_k}) = p(x_{R_k} \mid x_{S_k}) \cdot p(x_{S_k}) = p(x_{C_k})$$

as required. □

If a graph is not decomposable then we can *triangulate* it by adding edges. We discuss will this further later on.

7.2 Message Passing and the Junction Tree Algorithm

We have seen that having locally consistent potentials is enough to deduce that we have correctly calculated marginal probabilities. The obvious question now is how we arrive at consistent margins in the first place. In fact we shall do this with 'local' update steps, that alter potentials to become consistent without altering the overall distribution. We will show that this leads to consistency in a finite number of steps.

Suppose that two cliques C and D are adjacent in the junction tree, with a separator set $S = C \cap D$. An *update* from C to D consists of replacing ψ_S and ψ_D with the following:

$$\psi'_S(x_S) = \sum_{x_{C\setminus S}} \psi_C(x_C), \qquad \psi'_D(x_D) = \frac{\psi'_S(x_S)}{\psi_S(x_S)} \psi_D(x_D).$$

This operation is also known as *message passing*, with the 'message' $\psi'_S(x_S)$ being passed from C to D. We note three important points about this updating step:

- after updating, ψ_C and ψ'_S are consistent;
- if ψ_D and ψ_S are consistent, then so are ψ'_D and ψ'_S: to see this, note that

$$\begin{aligned} \sum_{x_{D\setminus S}} \psi'_D(x_D) &= \sum_{x_{D\setminus S}} \frac{\psi'_S(x_S)}{\psi_S(x_S)} \psi_D(x_D) \\ &= \frac{\psi'_S(x_S)}{\psi_S(x_S)} \sum_{x_{D\setminus S}} \psi_D(x_D), \end{aligned}$$

  so if ψ_S and ψ_D are consistent then $\psi_S(x_S) = \sum_{x_{D\setminus S}} \psi_D(x_D)$ and we are left with ψ'_S.

- the product over all clique potentials

$$\frac{\prod_{C\in\mathcal{C}}\psi_C(x_C)}{\prod_{S\in\mathcal{S}}\psi_S(x_S)}$$

  is unchanged: the only altered terms are ψ_D and ψ_S, and by definition of ψ'_D we have

$$\frac{\psi'_D(x_D)}{\psi'_S(x_S)} = \frac{\psi_D(x_D)}{\psi_S(x_S)}.$$

Hence, updating preserves the joint distribution and does not upset margins that are already consistent. The junction tree algorithm is a way of updating all the margins such that, when it is complete, they are all consistent.

Let $\mathcal{T}$ be a tree. Given any node $t \in \mathcal{T}$, we can 'root' the tree at t, and replace it with a directed graph in which all the edges point away from t.[3] The *junction tree algorithm* involves messages being passed from the edge of the junction tree (the leaves) towards a chosen root (the *collection* phase), and then being sent away from that root back down to the leaves (the *distribution* phase). Once these steps are completed, the potentials will all be consistent. This process is also called *belief propagation.*

Algorithm 2 Collect and distribute steps of the junction tree algorithm.

```
function COLLECT(rooted tree T, potentials ψ_t)
    let 1 < ... < k be a topological ordering of T
    for t in k, ..., 2 do
        send message from ψ_t to ψ_σ(t);
    end for
    return updated potentials ψ_t
end function
function DISTRIBUTE(rooted tree T, potentials ψ_t)
    let 1 < ... < k be a topological ordering of T
    for t in 2, ..., k do
        send message from ψ_σ(t) to ψ_t;
    end for
    return updated potentials ψ_t
end function
```

The *junction tree algorithm* consists of running $\textsc{Collect}(\mathcal{T}, \psi_t)$ and $\textsc{Distribute}(\mathcal{T}, \psi'_t)$, as given in Algorithm 2.

Theorem 7.5. *Let $\mathcal{T}$ be a junction tree with potentials $\psi_{C_i}(x_{C_i})$. After running the junction tree algorithm, all pairs of potentials will be consistent.*

Proof. We have already seen that each message passing step will make the separator node consistent with the child node. It follows that each pair ψ_{C_i} and ψ_{S_i} are consistent after the collection step. We also know that this consistency will be preserved after future updates from $\psi_{C_{\sigma(i)}}$. Hence, after the distribution step, each ψ_{C_i} and ψ_{S_i} remain consistent, and $\psi_{C_{\sigma(i)}}$ and ψ_{S_i} become consistent for each i. Hence, every adjacent pair of cliques is now consistent.

[3]This process always gives a Markov equivalent graph although, of course, we are not really applying the Markov property to our junction tree. The directions are just for convenience.

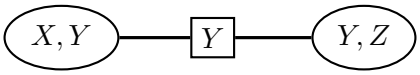
(a) (b)

Figure 7.4: Illustration of the junction tree algorithm with $\{2, 3, 4\}$ chosen as the root. (a) Collect steps towards the root: note that the $\{4, 6\}$ to $\{2, 3, 4\}$ step must happen after the $\{6, 7, 8\}$ to $\{4, 6\}$ update. (b) Distribute steps away from the root and towards the leaves: this time the constraint on the ordering is reversed.

But whenever $C_i \cap C_j \neq \emptyset$ there is a path in the junction tree such that every intermediate clique also contains $C_i \cap C_j$, so this local consistency implies global consistency of the tree. □

Remark 7.6. In practice, message passing is often done in parallel, and it is not hard to prove that if all potentials update simultaneously then the potentials will converge to a consistent solution in at most d steps, where d is the width (i.e. the length of the longest path) of the tree.

Example 7.7. Suppose we have just two tables, ψ_{XY} and ψ_{YZ} arranged in the junction tree:



representing a distribution in which $X \perp\!\!\!\perp Z \mid Y$. We can initialize by setting

$$\psi_{XY}(x, y) = p(x \mid y) \qquad \psi_{YZ}(y, z) = p(y, z) \qquad \psi_Y(y) = 1,$$

so that $p(x, y, z) = p(y, z) \cdot p(x \mid y) = \psi_{YZ}\psi_{XY}/\psi_Y$.

Now, we could pick YZ as the root node of our tree, so the collection step consists of replacing

$$\psi'_Y(y) = \sum_x \psi_{XY}(x, y) = \sum_x p(x \mid y) = 1;$$

so ψ'_Y and ψ_Y are the same; hence the collection step leaves ψ_Y and ψ_{YZ} unchanged.

The distribution step consists of

$$\psi''_Y(y) = \sum_z \psi_{YZ}(y, z) = \sum_z p(y, z) = p(y);$$

$$\psi'_{XY}(x, y) = \frac{\psi''_Y(y)}{\psi_Y(y)}\psi_{XY}(x, y) = \frac{p(y)}{1}p(x \mid y) = p(x, y);$$

hence, after performing both steps, each potential is the marginal distribution corresponding to those variables.

In junction graphs that are not trees it is still possible to perform message passing, but convergence is not guaranteed. This is known as 'loopy belief propagation, and is a topic of current research.

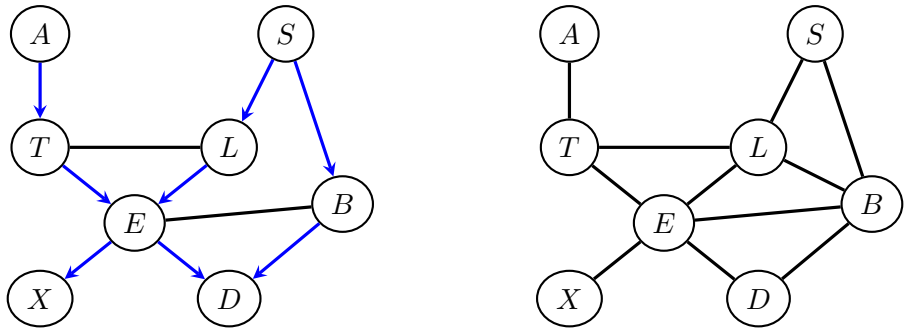


Figure 7.5: The moral graph of the Chest Clinic network, and a possible triangulation.

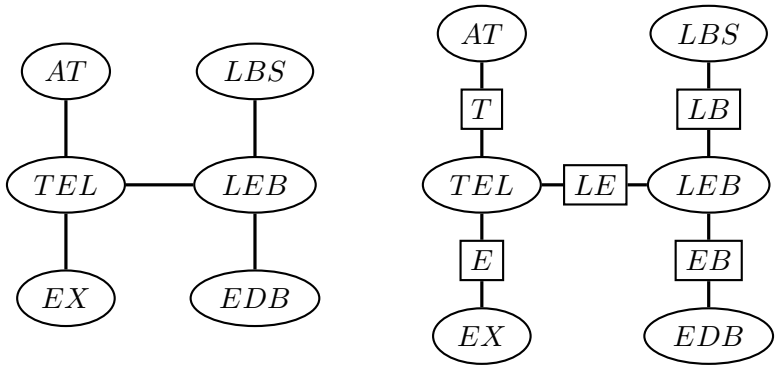


Figure 7.6: A possible junction tree for the Chest Clinic network, and (right) with separator sets drawn on.

7.3 Directed Graphs and Triangulation

How does any of this relate to directed graphs? And what should we do if our model is *not* decomposable? In this case we cannot immediately form a junction tree. However, all is not lost, since we can always embed our model in a larger model which *is* decomposable.

For a directed graph, we start by taking the moral graph, so that we obtain an undirected model. If the directed model is decomposable then so is the moral graph. If the moral graph is still not decomposable, then we can *triangulate* it by adding edges to obtain a decomposable graph. Figure 7.5(b) contains a triangulation of the moral graph of Figure 7.1. We can arrange the cliques as

$$\{L, E, B\}, \qquad \{T, E, L\}, \qquad \{L, B, S\}, \qquad \{E, D, B\}, \qquad \{A, T\}, \qquad \{E, X\},$$

giving rise to the junction tree in Figure 7.6

Taking the 4-cycle in Figure 4.5(a) as an example, we can add chords to the cycle until we obtain a graph that is triangulated; a resulting graph is called a *triangulation*. This process is not unique, as is obvious from this example. Given the new graph we can form a junction tree for the larger model.

Naturally, to keep our computations efficient we want the cliques in the model to remain small when we triangulate: after all, we could always embed our graph in the complete model! Finding a triangulation that is 'optimal'—in the sense of giving the smallest cliques—is a very hard problem in general. Some approximate and heuristic methods exist. A simple method, *Tarjan elimination*, is given on Examples Sheet 3.

Suppose we have a directed graphical model embedded within a decomposable model $C_1, \ldots, C_k$. For each vertex v, the set $\{v\} \cup \mathrm{pa}_{\mathcal{G}}(v)$ is contained within at least one of these cliques. Assigning each vertex arbitrarily to one such clique, let $v(C)$ be the vertices assigned to C. Then we can set $\psi_C(x_C) = \prod_{v \in v(C)} p(x_v \mid x_{\mathrm{pa}(v)})$ and $\psi_S(x_S) = 1$, and we have

$$\prod_{i=1}^{k} \frac{\psi_{C_i}(x_{C_i})}{\psi_{S_i}(x_{S_i})} = \prod_{v \in V} p(x_v \mid x_{\mathrm{pa}(v)}) = p(x_V).$$

This is called *initialization*. Now if we run the junction tree algorithm to obtain consistent potentials, then these will just be the marginal probabilities for each clique.

7.4 Evidence

The junction tree gives us a mechanism for calculating marginal distributions for quantities that are contained in the same clique. How should we deal with queries about conditional distributions for quantities that may not be adjacent? For example, what difference does it make to our chest clinic network if a patient smokes?

We can answer this by introducing 'evidence' into our tables, and then propagating it through the tree. The new evidence corresponds to replacing an existing marginal table with one in which the event that occurred has probability 1: for example,

$$p(s) = \begin{array}{c|c} \text{smokes} & \text{doesn't smoke} \\ \hline 0.25 & 0.75 \end{array} \quad \text{becomes} \quad \tilde{p}(s) = \begin{array}{c|c} \text{smokes} & \text{doesn't smoke} \\ \hline 1 & 0 \end{array}.$$

Let our evidence be the event $\{X_e = y_e\}$ for some relevant node e; we can write the new joint distribution as

$$p(x_V \mid X_e = y_e) = p(x_V, x_e) \frac{\mathbb{1}_{\{x_e = y_e\}}}{p(x_e)}.$$

Thus, replacing

$$\psi'_C(x_C) \leftarrow \psi_C(x_C) \cdot \frac{\mathbb{1}_{\{x_e = y_e\}}}{p(y_e)}$$

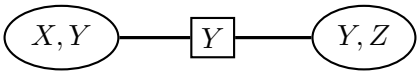
for one potential with $C \ni e$ will alter the joint distribution in the required way (note that we should not do this in more than one place, even if e appears in multiple cliques). If the potentials are already consistent then $p(y_e)$ can be calculated from ψ_C directly.

Of course, after replacing ψ_C the potentials will no longer be consistent, and therefore the junction tree algorithm needs to be run again. In fact, only a distribution step with ψ_C chosen as the root node is needed.

Proposition 7.8. *Suppose that potentials Ψ for a junction tree $\mathcal{T}$ with root C are all consistent, except for ψ_C. Then after running* DISTRIBUTE*$(\mathcal{T}, \Psi)$, all potentials are consistent.*

Proof. Each separator set potential is already consistent with the clique potential(s) 'away' from C in the graph. This consistency is preserved, and distribution will ensure that each separator set is consistent with the clique potentials 'towards' C. Hence, all clique potentials and separator sets are now consistent. □

If we try to introduce evidence in two different places without propagating in between then we may not obtain the conditional distribution that we want. To see this, consider again our very simple example with two cliques:



If the potentials are already consistent, then $\psi_{XY} = p(x, y)$ and $\psi_{YZ} = p(y, z)$ with $\psi_Y = p(y)$. Now suppose we want to introduce two pieces of evidence: $\{X = x^*\}$ and $\{Z = z^*\}$. To introduce the first, we replace ψ_{XY} with

$$\psi'_{XY} = \psi_{XY} \frac{\mathbb{1}_{\{x=x^*\}}}{p(x^*)} = p(y \mid x^*)\mathbb{1}_{\{x=x^*\}}.$$

This means that the potentials are jointly representing the distribution q in which

$$q(x, y, z) = \frac{\psi'_{XY}(x, y)\psi_{YZ}(y, z)}{\psi_Y(y)} = \frac{p(y \mid x^*) \cdot p(y, z)}{p(y)} \mathbb{1}_{\{x=x^*\}} = p(y, z \mid x^*)\mathbb{1}_{\{x=x^*\}},$$

as required.

Now, the second would be introduced by replacing ψ_{YZ} with

$$\psi'_{YZ} = p(y \mid z^*)\mathbb{1}_{\{z=z^*\}}.$$

But now this gives

$$\begin{aligned} r(x, y, z) = \frac{\psi'_{XY}(x, y)\psi'_{YZ}(y, z)}{\psi_Y(y)} &= \frac{p(y \mid x^*) \cdot p(y \mid z^*)}{p(y)} \mathbb{1}_{\{x=x^*, z=z^*\}} \\ &= \frac{p(y, x^*) \cdot p(y, z^*)}{p(y)p(x^*)p(y^*)} \mathbb{1}_{\{x=x^*, z=z^*\}} \\ &= p(y \mid x^*, z^*) \frac{p(x^*, z^*)}{p(x^*)p(z^*)} \mathbb{1}_{\{x=x^*, z=z^*\}}, \end{aligned}$$

where the last equality holds from applying Theorem 2.4(iv) to $X \perp\!\!\!\perp Z \mid Y$. Now since $X \not\perp\!\!\!\perp Z$ in general, this final expression is not equal to $p(y \mid x^*, z^*)$.

This is because we failed to update ψ_{YZ} with the new information about $X = x^*$ *before* introducing information about Z. If we first run a distribution step rooted at XY, then all potentials will be consistent and contain margins of $p(z, y \mid X = x^*)$. In particular, if $\psi_{ZY} = p(z, y \mid X = x^*)$ then introducing $Z = z^*$ amounts to

$$\psi''_{YZ}(y, z) = \psi'_{YZ}(y, z) \frac{\mathbb{1}_{\{z=z^*\}}}{\psi'_{YZ}(z)} = p(z, y \mid x^*) \frac{\mathbb{1}_{\{z=z^*\}}}{p(z^* \mid x^*)} = p(y \mid x^*, z^*) \cdot \mathbb{1}_{\{z=z^*\}}.$$

8 Causal Inference

In most statistical prediction problems we simply use conditional distributions, without regard to the reason that some varibles are correlated. Causal inference asks *why* some variables are correlated, and in particular whether such a correlation would endure if we were to perform an experiment in the system.

Example 8.1. Taking the Chest Clinic in Figure 7.1 as an example, suppose the probabilities for smoking and lung cancer are:

$$p(s) = \begin{array}{c|c} \text{smokes} & \text{doesn't smoke} \\ \hline 0.2 & 0.8 \end{array} \qquad p(\ell \mid s) = \begin{array}{r\|c|c} \text{smoker} & \text{cancer} & \text{no cancer} \\ \hline \text{yes} & 0.1 & 0.9 \\ \text{no} & 0.01 & 0.99 \end{array}.$$

Here we see that the probability of developing lung cancer is about 1% for non-smokers, and 10% for smokers. Clearly then smoking status is a useful predictor of whether someone will get lung cancer (though far from a perfect one). Does this mean that smoking is bad for you? On its own, no—we are often reminded that 'correlation does not imply causation': even though smoking and cancer are correlated, we cannot deduce that smoking is the *cause* of the cancer.

To illustrate, consider the relationship in reverse. Using Bayes' rule, one can check that a lung cancer sufferer has about a 71% chance of being a smoker, compared to 19% for a non-sufferer; in this sense lung cancer can be used to 'predict' whether or not someone smokes. But does this mean that having lung cancer causes people to smoke? Manifestly not![4]

To settle the argument we can imagine performing an experiment, in which we stop everyone smoking and observe what happens to the lung cancer rates. If smoking is the (only) cause of the difference in the probabilities above, then we would expect that modifying smoking status would also change the lung cancer rates: in other words the rate of lung cancer would eventually drop from 2.8% to 1%. On the other hand, if people smoke because of their lung cancer, then the rate of lung cancer will not change at all by stopping people from smoking!

The asymmetry in the previous example is an example of a *causal relationship*. Ordinary prediction is, in some sense, symmetric: if the smoking predicts cancer, then cancer predicts smoking. However, causal prediction is not symmetric: if I make someone smoke then that will make it more likely that they get cancer, but if I give someone cancer by exposing them to radiation, for example, it will not cause them to start smoking.

The scenarios of preventing someone from smoking, or of giving them cancer, are examples of *interventions* or *treatments*. These affect both the values of variables in the system *and* some of the relationships between them. If we intervene in a system in such a way as to set a variable such as $X = x$, we denote the resulting distribution of other variables as

$$P(Y = y \mid do(T = t)).$$

Note that, as shown in the example above, this is not generally the same as $P(Y = y \mid T = t)$: there is a difference between *observing* that $\{T = t\}$ and *intervening* to set $\{T = t\}$. If

[4] In fact, the idea that lung cancer was a cause of smoking was really posited—likely with his tongue firmly in his cheek—by Fisher as a possible explanation for the correlation between smoking and cancer.

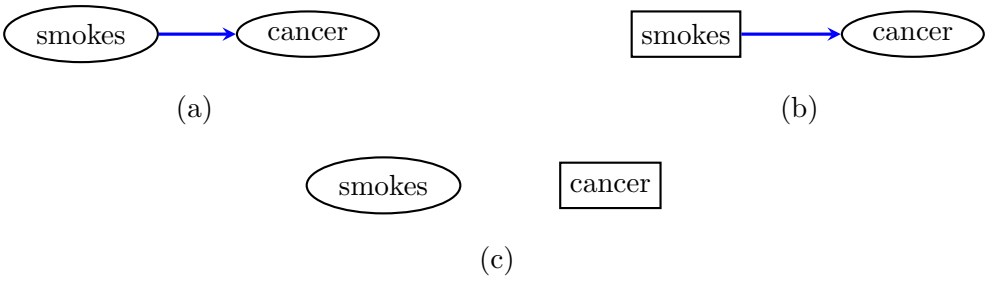


Figure 8.1: (a) A causal DAG on two vertices; (b) after intervening on 'smokes' we assume that the dependence of cancer on smoking status is preserved; (c) after intervening on 'cancer', this will no longer depend upon smoking status, so the relationship disappears.

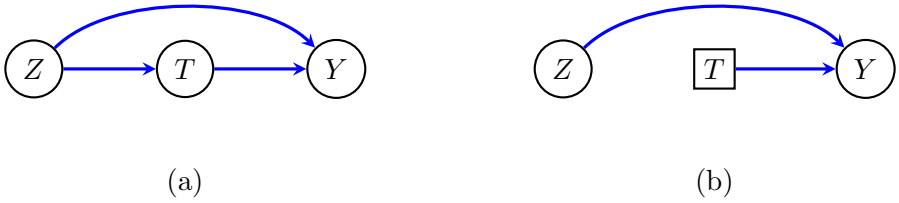


Figure 8.2: (a) A causal DAG on three vertices, and (b) after intervening on T.

we assume that smoking does cause cancer but not the other way around, we might then have:

$$P(\{\text{cancer}\} \mid do(\{\text{smokes}\})) = P(\{\text{cancer}\} \mid \{\text{smokes}\})$$
$$P(\{\text{smokes}\} \mid do(\{\text{cancer}\})) = P(\{\text{smokes}\}).$$

Directed graphs provide a convenient framework for representing the structural assumptions underlying a causal system, and the asymmetry in interventions. We can think of each edge $t \to y$ as saying that X_t is a 'direct cause' of X_y; i.e. that it affects it in a way that is not mediated by any of the other variables. In our example, the system could be represented by the graph in Figure 8.1(a).

8.1 Interventions

Definition 8.2. Let $\mathcal{G}$ be a directed acyclic graph representing a causal system, and let p be a probability distribution over the variables X_V. An *intervention* on a variable X_t (for $t \in V$) does two things:

- *graphically* we represent this by removing edges pointing into t (i.e. of the form $v \to t$);
- *probabilistically*, we replace our usual factorization

$$p(x_V) = \prod_{v \in V} p(x_v \mid x_{\text{pa}(v)})$$

with

$$p(x_{V\setminus\{t\}} \mid do(x_t)) = \frac{p(x_V)}{p(x_t \mid x_{\mathrm{pa}(t)})} = \prod_{v\in V\setminus\{t\}} p(x_v \mid x_{\mathrm{pa}(v)}).$$

In words, we are assuming that X_t no longer depends upon its parents, but has been fixed to x_t. We can think of this as replacing the factor $p(x_t \mid x_{\mathrm{pa}(t)})$ with an indicator function that assigns probability 1 to the event that $\{X_t = x_t\}$. Other variables will continue to depend upon their parents according to the same conditionals $p(x_v \mid x_{\mathrm{pa}(v)})$.

When we say a graph and its associated probability distribution is *causal*, we mean that we are making the assumption that, if we were to intervene on a variable X_v via some experiment, then the distribution would change in the way described above. This assumption is something that has to be justified in specific applied examples.

Example 8.3 (Confounding)**.** Consider the graph in Figure 8.2(a); here Z causally affects both T and Y, so some of the observed correlation between T and Y will be due to this 'common cause' Z. We say that T and Y are 'confounded' by Z. Suppose we intervene to fix $T = t$, so that it is no longer causally affected by Z. Hence, we go from

$$p(z, t, y) = p(z) \cdot p(t \mid z) \cdot p(y \mid z, t)$$

to

$$p(z, y \mid do(t)) = p(z) \cdot p(y \mid z, t) \cdot \mathbb{1}_{\{T=t\}} = p(z) \cdot p(y \mid z, t).$$

Note that this last object is not the same as the *ordinary* conditional distribution

$$p(z, y \mid t) = p(z \mid t) \cdot p(y \mid z, t)$$

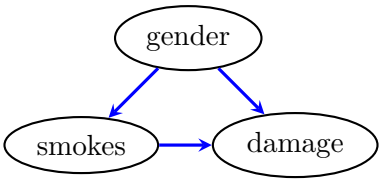
unless $p(z \mid t) = p(z)$; in general this would happen if $T \perp\!\!\!\perp Z$, in which case Z is not really a confounder.

Example 8.4. Suppose we have a group of 64 people, half men and half women. We ask them whether they smoke, and test them for lung damage. The results are given by the following table.

	women			men	
	not smoke	smoke		not smoke	smoke
no damage	21	6		6	6
damage	3	2		2	18

Given that a person smokes, the probability that they have lung damage is $P(D = 1 \mid S = 1) = \frac{20}{32} = \frac{5}{8}$. If someone doesn't smoke the probability is $P(D = 1 \mid S = 0) = \frac{5}{32}$.

What happens if we had prevented everyone from smoking? Would this mean that only $\frac{5}{32} \times 64 = 10$ of our participants showed lung damage? If we assume the following causal model, then the answer is no.



We have (taking $G = 0$ to represent male) that

$$\begin{aligned}
&P(D = 1 \mid do(S = 0)) \\
&= \sum_g P(D = 1 \mid S = 0, G = g) \cdot P(G = g) \\
&= P(D = 1 \mid S = 0, G = 0) \cdot P(G = 0) + P(D = 1 \mid S = 0, G = 1) \cdot P(G = 1) \\
&= \frac{2}{8} \cdot \frac{1}{2} + \frac{3}{24} \cdot \frac{1}{2} \\
&= \frac{3}{16} > \frac{5}{32}.
\end{aligned}$$

So in fact, we would expect $\frac{3}{16} \times 64 = 12$ people to have damage if no-one was able to smoke.

The difference can be accounted for by the fact that some of the chance of getting lung damage is determined by gender. If we 'observe' that someone does not smoke then they are more likely to be female; but forcing someone not to smoke does *not* make them more likely to be female!

8.2 Adjustment Sets and Causal Paths

From herein we will consider two special variables: the *treatment*, T, and the outcome, Y. They will correspond to vertices labelled t and y respectively. We correspondingly identify $T \equiv X_t$ and $Y \equiv X_y$.

For this section we will assume we are interested in the distribution of Y after intervening on T. The method given above for finding $p(y \mid do(t))$ appears to involve summing over all the other variables in the graph:

$$p(y \mid do(t)) = \sum_{x_W} \frac{p(y, t, x_W)}{p(t \mid x_{\mathrm{pa}(t)})}$$

Here we present some methods for 'adjusting' by only a small number of variables.

Lemma 8.5. *Let $\mathcal{G}$ be a causal DAG. Then*

$$p(y \mid do(t)) = \sum_{x_{\mathrm{pa}(t)}} p(y \mid t, x_{\mathrm{pa}(t)}) \cdot p(x_{\mathrm{pa}(t)}).$$

Proof. Let $X_V := (Y, T, X_{\mathrm{pa}(t)}, X_W)$, where X_W contains any other variables (that is, not Y, T, nor a parent of T). Then

$$p(y, x_{\mathrm{pa}(t)}, x_W \mid do(t)) = \frac{p(y, t, x_{\mathrm{pa}(t)}, x_W)}{p(t \mid x_{\mathrm{pa}(t)})} = p(y, x_W \mid t, x_{\mathrm{pa}(t)}) \cdot p(x_{\mathrm{pa}(t)}).$$

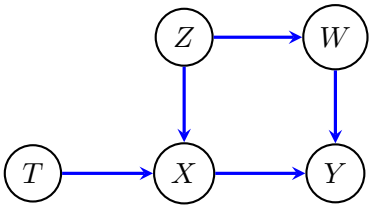


Figure 8.3: A causal directed graph.

Then

$$\begin{aligned} p(y \mid do(t)) &= \sum_{x_W, x_{\mathrm{pa}(t)}} p(y, x_W \mid t, x_{\mathrm{pa}(t)}) \cdot p(x_{\mathrm{pa}(t)}) \\ &= \sum_{x_{\mathrm{pa}(t)}} p(x_{\mathrm{pa}(t)}) \sum_{x_W} p(y, x_W \mid t, x_{\mathrm{pa}(t)}) \\ &= \sum_{x_{\mathrm{pa}(t)}} p(x_{\mathrm{pa}(t)}) p(y \mid t, x_{\mathrm{pa}(t)}) \end{aligned}$$

as required. □

This result is called an 'adjustment' formula. Applied to the graph in Figure 8.3, for example, it would tell us that $p(y \mid do(x)) = \sum_{z,t} p(y \mid x, z, t) \cdot p(z, t)$, so, for example, we do not need to consider W. In fact, though, you might notice that $Y \perp\!\!\!\perp T \mid X, Z$, so we can write

$$\begin{aligned} p(y \mid do(x)) &= \sum_{z,t} p(y \mid x, z) \cdot p(z, t) \\ &= \sum_{z} p(y \mid x, z) \cdot p(z), \end{aligned}$$

and we only need to adjust for Z. Further,

$$\begin{aligned} p(y \mid do(x)) = \sum_{z} p(y \mid x, z) \cdot p(z) &= \sum_{z,w} p(y, w \mid x, z) \cdot p(z) \\ &= \sum_{z,w} p(y \mid x, w, z) \cdot p(w \mid x, z) \cdot p(z) \\ &= \sum_{z,w} p(y \mid x, w) \cdot p(w \mid z) \cdot p(z) \\ &= \sum_{z,w} p(y \mid x, w) \cdot p(w, z) \\ &= \sum_{w} p(y \mid x, w) \cdot p(w); \end{aligned}$$

the fourth equality here uses the fact that $W \perp\!\!\!\perp X \mid Z$ and $Y \perp\!\!\!\perp Z \mid W, X$, which can be seen from the graph.

So, in other words, we could adjust by W instead of Z. This illustrates that there are often multiple equivalent ways of obtaining the same causal quantity. We will give a criterion for *valid* adjustment sets, but we first need an a few definitions and results to be able to prove this criterion correct.

8.3 Paths and d-separation

Definition 8.6. Let $\mathcal{G}$ be a directed graph and π a path in $\mathcal{G}$. We say that an internal vertex t on π is a *collider* if the edges adjacent to t meet as $\rightarrow t \leftarrow$. Otherwise (i.e. we have $\rightarrow t \rightarrow$, $\leftarrow t \leftarrow$, or $\leftarrow t \rightarrow$) we say t is a *non-collider*.

Definition 8.7. Let π be a path from a to b. We say that π is *open* given (or conditional on) $C \subseteq V \setminus \{a, b\}$ if

- all colliders on π are in $\mathrm{an}_{\mathcal{G}}(C)$;
- all non-colliders are outside C.

(Recall that $C \subseteq \mathrm{an}_{\mathcal{G}}(C)$.) A path which is not open given C is said to be *blocked* by C.

Example 8.8. Consider the graph in Figure 8.4. There are three paths from T to W:

$$T \rightarrow X \leftarrow Z \rightarrow W, \qquad T \rightarrow X \rightarrow Y \leftarrow W, \qquad \text{and} \qquad T \rightarrow Y \leftarrow W.$$

Without conditioning on any variable, all three paths are both blocked, since they contain colliders. Given $\{Y\}$, however, all paths are open, because Y is the only collider on the second and third path, and the only collider on the first is X, which is an ancestor of Y. Given $\{Z, Y\}$, the first path is blocked because Z is a non-collider, but the second and third are open.

Definition 8.9 (d-separation)**.** Let A, B, C be disjoint sets of vertices in a directed graph $\mathcal{G}$ (C may be empty). We say that A and B are *d-separated* given C in $\mathcal{G}$ (and write $A \perp_d B \mid C\ [\mathcal{G}]$) if every path from $a \in A$ to $b \in B$ is blocked by C.

We now introduce a theorem that shows d-separation can be used to evaluate the global Markov property. In other words, instead of being based on paths in moral graphs, we can use paths in the original DAG.

Theorem 8.10. *Let $\mathcal{G}$ be a DAG and let A, B, C be disjoint subsets of $\mathcal{G}$. Then A is d-separated from B by C in $\mathcal{G}$ if and only if A is separated from B by C in $(\mathcal{G}_{\mathrm{an}(A \cup B \cup C)})^m$.*

Proof (not examinable). Suppose A is not d-separated from B by C in $\mathcal{G}$, so there is an open path π in $\mathcal{G}$ from some $a \in A$ to some $b \in B$. Dividing the path up into sections of the form $\leftarrow \cdots \leftarrow\!\!\rightarrow \cdots \rightarrow$, we see that π must lie within $\mathrm{an}_{\mathcal{G}}(A \cup B \cup C)$, because every collider must be an ancestor of C, and the extreme vertices are in A and B. Each of the colliders $i \rightarrow k \leftarrow j$ gives an additional edge $i - j$ in the moral graph and so can be avoided; all the other vertices are not in C since the path is open. Hence we obtain a path from $a \in A$ to $b \in B$ in the moral graph that avoids C.

Conversely, suppose A is not separated from B by C in $(\mathcal{G}_{\mathrm{an}(A \cup B \cup C)})^m$, so there is a path π in $(\mathcal{G}_{\mathrm{an}(A \cup B \cup C)})^m$ from some $a \in A$ to some $b \in B$ that does not traverse any element of C. Each such path is made up of edges in the original graph and edges added over v-structures. Suppose an edge corresponds to a v-structure over k; then k is in $\mathrm{an}_{\mathcal{G}}(A \cup B \cup C)$. If k is an ancestor of C then the path remains open; otherwise, if k is an ancestor of A then there is a directed path from k to $a' \in A$, and every vertex on it is a non-collider that is not contained in C. Hence we can obtain a path with fewer edges over v-structures from a' to b. Repeating this process we obtain a path from A to B in which every edge is either in $\mathcal{G}$ or is a v-structure over an ancestor of C. Hence the path is open. □

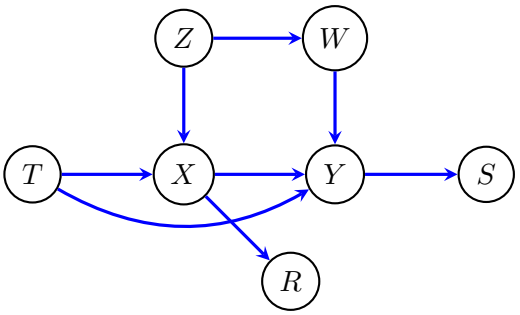


Figure 8.4: A causal directed graph.

We also obtain the following useful characterization of d-open paths.

Proposition 8.11. *If π is a d-open path between a, b given C in $\mathcal{G}$, then every vertex on π is in* $\mathrm{an}_{\mathcal{G}}(\{a, b\} \cup C)$.

Proof. Consider a path from a to b, and divide it into *treks*. That is, segments separated by a collider vertex. In general, these segments look like a pair of directed paths $\leftarrow \cdots \leftarrow\rightarrow \cdots \rightarrow$. Now, we know that if a path is open, then every collider vertex is an ancestor of something in C. Hence everything on the path is an ancestor of C, apart from possibly the extreme directed paths that lead to a and b, which are themselves ancestors of a or b. □

8.4 Adjustment Sets

Given the addition of d-separation to our toolkit, we are now in a position to consider more general adjustment sets than simply the parents of the variable intervened on.

Definition 8.12. Suppose that we are interested in the total effect of T on Y. We define the *causal nodes* as all vertices on a causal path from T to Y, other than T itself. We write this set as $\mathrm{cn}_{\mathcal{G}}(T \to Y)$.

We also define the *forbidden nodes* as consisting of T or any descendants of causal nodes

$$\mathrm{forb}_{\mathcal{G}}(T \to Y) = \mathrm{de}_{\mathcal{G}}(\mathrm{cn}_{\mathcal{G}}(T \to Y)) \cup \{T\}.$$

Note that strict descendants of T are generally *not* forbidden nodes, as we will see presently.

Example 8.13. Consider the graph in Figure 8.4; we have

$$\mathrm{cn}_{\mathcal{G}}(X \to Y) = \{Y\} \qquad \mathrm{cn}_{\mathcal{G}}(T \to Y) = \{X, Y\},$$

and

$$\mathrm{forb}_{\mathcal{G}}(X \to Y) = \{S, X, Y\} \qquad \mathrm{forb}_{\mathcal{G}}(T \to Y) = \{R, S, T, X, Y\},$$

Definition 8.14. We say that C is a *valid adjustment set* for the ordered pair (t, y) if

- no vertex in C is in $\mathrm{forb}_{\mathcal{G}}(t \to y)$;
- every non-causal path from t to y is blocked by C.

We can divide a valid adjustment set C into two components, $B = C \cap \mathrm{nd}_{\mathcal{G}}(v)$ and $D = C \setminus \mathrm{nd}_{\mathcal{G}}(v)$. We first show the following result.

Proposition 8.15. *If $C = B \dot{\cup} D$ is a valid adjustment set for (t, y) then so is B.*

In addition, for any $d \in \mathrm{de}_{\mathcal{G}}(t)$ either $d \perp_d t \mid C \setminus \mathrm{de}_{\mathcal{G}}(d)$ or $d \perp_d y \mid \{t\} \cup C \setminus \mathrm{de}_{\mathcal{G}}(d)$.

Proof. Clearly if C does not contain a vertex in $\mathrm{forb}_{\mathcal{G}}(t \to y)$ then neither does $B \subseteq C$.

Consider the possible paths from t to y. Any paths that begin with an edge $t \to$ are either causal, or will meet a collider that is not conditioned upon in B. Hence this path will be blocked. Any paths that begin with an edge $t \leftarrow$ must be blocked by C. If this is blocked at a collider, then it will also be blocked at that collider by $B \subseteq C$. If it is blocked at a non-collider in $\mathrm{de}_{\mathcal{G}}(t)$, then (by the same reasoning as above) there must also be a collider on the path within those descendants at which the path is blocked by B. Hence B satisfies the criteria to be a valid adjustment set as well.

Note that this proof also applies to any superset of B that removes a set closed under taking descendants.

For the d-separation statements, suppose for contradiction there is a d for which this does not hold. Note that both the d-separation statements apply to moral graphs over the sets $\{d, t, y\} \cup (C \setminus \mathrm{de}_{\mathcal{G}}(d))$, so we can just consider this moral graph, and therefore there are undirected paths from t and y to d that do not intersect $\{d\} \cup (C \setminus \mathrm{de}_{\mathcal{G}}(d))$. We can concatenate these (shortening if necessary) to obtain a path from t to y that is open given $C \setminus \mathrm{de}_{\mathcal{G}}(d)$, which contradicts the comment in the previous paragraph. Hence the d-separation statements also hold. □

We refer to a valid adjustment set such as B as a *back-door* adjustment set, since it blocks all non-causal paths from t to y, but does not contain descendants of t.

Lemma 8.16. *If $C = B \dot{\cup} D$ is a valid adjustment set for (t, y) and $B = C \cap \mathrm{nd}_{\mathcal{G}}(t)$, then*

$$\sum_{x_C} p(x_C) \cdot p(y \mid t, x_C) = \sum_{x_B} p(x_B) \cdot p(y \mid t, x_B).$$

Proof. We proceed by a simple induction. Consider the collection of d-separation statements in Proposition 8.15, and take some d that has no descendants in $C \setminus \{d\}$. Then either $d \perp_d y \mid \{t\} \cup C \setminus \{d\}$, in which case we have

$$\begin{aligned}\sum_{x_C} p(x_C) \cdot p(y \mid t, x_C) &= \sum_{x_{C\setminus\{d\}}, x_d} p(x_C) \cdot p(y \mid t, x_{C\setminus\{d\}}) \\ &= \sum_{x_{C\setminus\{d\}}} p(x_{C\setminus\{d\}}) \cdot p(y \mid t, x_{C\setminus\{d\}}),\end{aligned}$$

or $d \perp_d t \mid C \setminus \{d\}$, and so

$$\begin{aligned}&\sum_{x_C} p(x_{C\setminus\{d\}}) \cdot p(x_d \mid x_{C\setminus\{d\}}) \cdot p(y \mid t, x_C) \\ &= \sum_{x_{C\setminus\{d\}}, x_d} p(x_{C\setminus\{d\}}) \cdot p(x_d \mid x_{C\setminus\{d\}}, t) \cdot p(y \mid t, x_C) \\ &= \sum_{x_{C\setminus\{d\}}} p(x_{C\setminus\{d\}}) \sum_{x_d} p(x_d, y \mid t, x_{C\setminus\{d\}}) \\ &= \sum_{x_{C\setminus\{d\}}} p(x_{C\setminus\{d\}}) \cdot p(y \mid t, x_{C\setminus\{d\}}).\end{aligned}$$

Then, by a clear inductive argument, the result holds. □

The main result of this subsection justifies the name 'valid' being applied to these adjustment sets.

Theorem 8.17. *Let C be a valid adjustment set for (t, y). Then*

$$p(y \mid do(t)) = \sum_{x_C} p(x_C) \cdot p(y \mid t, x_C).$$

Proof. By Lemma 8.16 we have that

$$\sum_{x_C} p(x_C) \cdot p(y \mid t, x_C) = \sum_{x_B} p(x_B) \cdot p(y \mid t, x_B).$$

Hence the associated back-door set can be used to adjust for confounding if and only if C can be used, and hence we assume that C contains no descendants of v.

Now, since no vertex in C is a descendant of t, we have that $T \perp\!\!\!\perp X_C \mid X_{\mathrm{pa}(t)}$ using the local Markov property. We also claim that y is d-separated from $\mathrm{pa}_{\mathcal{G}}(t)$ by $C \cup \{t\}$.

To see this, suppose for contradiction that there is an open path π from y to some $s \in \mathrm{pa}_{\mathcal{G}}(t)$ given $C \cup \{t\}$. If this path passes through t then this vertex is clearly a collider, and we can shorten it to give an open path from t to y that begins $t \leftarrow$. This contradicts C being a back-door adjustment set. If π is also open given C, then we can add the edge $s \to v$ to find an open path from y to t. If π is not open given C, this can only be because there is a collider r on π that is an ancestor of t but not of C; hence there is a directed path from r to t that does not contain any element of C. In this case, simply concatenate the path from y to r with this directed path (shortening if necessary) to obtain an open path from t to y. Either way we obtain a path from t to y that is open given C and begins $t \leftarrow$, which contradicts our assumptions.

We conclude that y is d-separated from $\mathrm{pa}_{\mathcal{G}}(t)$ by $C \cup \{t\}$, and hence the global Markov property implies that $Y \perp\!\!\!\perp X_{\mathrm{pa}(t)} \mid T, X_C$. Then:

$$\begin{aligned}
p(y \mid do(t)) &= \sum_{x_{\mathrm{pa}(t)}} p(x_{\mathrm{pa}(t)}) \cdot p(y \mid t, x_{\mathrm{pa}(t)}) \\
&= \sum_{x_{\mathrm{pa}(t)}} p(x_{\mathrm{pa}(t)}) \sum_{x_C} p(y, x_C \mid t, x_{\mathrm{pa}(t)}) \\
&= \sum_{x_{\mathrm{pa}(t)}} p(x_{\mathrm{pa}(t)}) \sum_{x_C} p(y \mid x_C, t, x_{\mathrm{pa}(t)}) \cdot p(x_C \mid t, x_{\mathrm{pa}(t)}) \\
&= \sum_{x_{\mathrm{pa}(t)}} p(x_{\mathrm{pa}(t)}) \sum_{x_C} p(y \mid x_C, t) \cdot p(x_C \mid x_{\mathrm{pa}(t)}) \\
&= \sum_{x_C} p(y \mid x_C, t) \sum_{x_{\mathrm{pa}(t)}} p(x_{\mathrm{pa}(t)}) \cdot p(x_C \mid x_{\mathrm{pa}(t)}) \\
&= \sum_{x_C} p(x_C) \cdot p(y \mid t, x_C),
\end{aligned}$$

where the fourth equality makes use of the two independences. □

We note that the proof above implicitly assumes that $\mathrm{pa}_{\mathcal{G}}(t) \cap C = \emptyset$, which of course need not be the case. The extension to the case with an intersection is straightforward, and we leave it as an exercise for the interested reader.

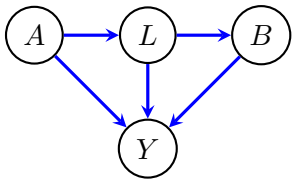


Figure 8.5: Causal diagram representing treatment for HIV patients. A is treatment with AZT (an anti-retroviral drug), L represents infection with pneumonia, B treatment with antibiotics, and Y survival.

Proposition 8.18. *Let $\mathcal{G}$ be a causal DAG. The set $\mathrm{pa}_{\mathcal{G}}(t)$ is a valid adjustment set for (t, y).*

Proof. Any non-causal path from t to y either (i) contains a collider or (ii) begins $t \leftarrow$. Hence, clearly $\mathrm{pa}_{\mathcal{G}}(t)$ blocks all non-causal paths from t to y. □

We now give a result to show that our definition of a valid adjustment set is as broad as it can be.

Proposition 8.19. *If $v \in \mathrm{forb}_{\mathcal{G}}(T \to Y)$ then v is not contained in any valid adjustment set for the total effect of T on Y.*

Proof. See Examples Sheet 4. □

Example 8.20 (HIV Treatment)**.** Figure 8.5 depicts a situation that arises in HIV treatment, and more generally in the treatment of chronic diseases. A doctor prescribes patients with AZT (A), which is known to reduce AIDS-related mortality, but also harms the immune system of the patient, increasing the risk of opportunistic infections such as pneumonia (L). If pneumonia arises, patients are generally treated with antibiotics (B), and the outcome of interest is 5 year survival (Y).

An epidemiologist might ask what the effect on survival would be if we treated all patients with antibiotics and AZT from the start, without waiting for an infection to present. What would this do to survival?

Well,

$$p(y \mid do(a, b)) = \sum_{\ell} p(y \mid a, \ell, b) \cdot p(\ell \mid a),$$

so the answer can be determined directly from observed data without having to perform an experiment. Note that, in this case, there is no valid adjustment set, because L is a descendant of A so it is a forbidden node for adjustment, but without including L the non-causal path $B \leftarrow L \to Y$ will induce spurious dependence.

8.5 Gaussian Causal Models

Definition 8.21. Given a multivariate system X_V with mean vector zero and covariance matrix Σ, we denote the *regression coefficients* for the least squares regression of X_y on X_C (where $C \subseteq V \setminus \{y\}$) by $\beta_{C,y}$. We furthermore denote each individual regression coefficient by $\beta_{t,v \cdot C'}$, where $C' = C \setminus \{t\}$.

In practice, if there are only two symbols before the dot, we will omit the comma from the notation and write, for example, β_{Cy} or $\beta_{ty\cdot C'}$.

As a simple example, considering the graph in Figure 8.4, the coefficients being estimated when we regress Y on X and W are

$$\beta_{xw,y} = (\beta_{xy\cdot w}, \beta_{wy\cdot x})^T.$$

The adjustment formula can be thought of as averaging the conditional distribution over a portion of the population:

$$\mathbb{E}[Y \mid do(z)] = \sum_{x_C} p(x_C) \cdot \mathbb{E}[Y \mid z, x_C].$$

If the variables we are dealing with are multivariate Gaussian, then conditional means such as $\mathbb{E}[Y \mid z, x_C]$ are determined by regressing Y on Z, X_C using a simple linear model. That is,

$$\mathbb{E}[Y \mid z, x_C] = z\beta_{zy\cdot C} + \sum_{c \in C} x_c \beta_{cy\cdot zC'}$$

for some $\beta_{zy\cdot C}$ and vector of regression coefficients $\beta_{Cy\cdot z} = (\beta_{cy\cdot zC'} : c \in C; C' = C \setminus \{c\})$. Then

$$\begin{aligned}
\mathbb{E}[Y \mid do(z)] &= \int_{\mathcal{X}_C} p(x_C) \cdot \left(z\beta_{zy\cdot C} + \sum_{c \in C} x_c \beta_{cy\cdot zC'} \right) dx_C \\
&= z\beta_{zy\cdot C} + \sum_{c \in C} \beta_{cy\cdot zC'} \mathbb{E}X_c \\
&= z\beta_{zy\cdot C},
\end{aligned}$$

since we chose the means to be zero:[5] $\mathbb{E}X_c = 0$. In other words, the causal effect for Z on Y is obtained by regressing Y on Z *and* the variables in the adjustment set X_C.

Note that regression coefficient between Z and Y in this model is the same for all values of $X_C = x_C$. This means that we can forget the averaging in the adjustment formula and just look at a suitable regression to obtain the causal effect. Note that this is quite different to what happened in the discrete case (or what happens in general): recall that the effects of smoking on lung damage were different for men and women in Example 8.4, and we had to weight the sexes in the correct proportions to obtain an unbiased estimate of the average causal effect.

8.6 Structural Equation Models

You showed on Problem Sheet 3 that $X_V \sim N_p(0, \Sigma)$ is Markov with respect to a DAG $\mathcal{G}$ if and only if we can recursively generate the model as

$$X_i = \sum_{j \in \mathrm{pa}_{\mathcal{G}}(i)} b_{ij} X_j + \varepsilon_i, \qquad \forall i \in V, \tag{9}$$

where $\varepsilon_i \sim N(0, d_{ii})$ are independent Gaussians.

[5] Note that, if the mean were not zero, it would only affect the intercept of this regression, not the slope.

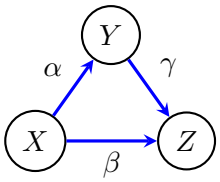


Figure 8.6: A directed graph with edge coefficients.

Definition 8.22. If $(\mathcal{G}, p)$ is causal and p is a multivariate Gaussian distribution, we call $(\mathcal{G}, p)$ a *structural equation model*.

In this case, by writing (9) as a matrix equation, we obtain

$$\Sigma = \operatorname{Var} X = (I - B)^{-1} D (I - B)^{-T},$$

where B is lower triangular and D is diagonal; each entry b_{ij} in B is non-zero only if $j \to i$ in $\mathcal{G}$. To work out the covariance between two variables in our graph, we can expand the matrix $(I - B)^{-1} D (I - B)^{-T}$ using the fact that for a nilpotent[6] matrix B of dimension p,

$$(I - B)^{-1} = I + B + B^2 + \cdots + B^{p-1}. \tag{10}$$

Note that, for example,

$$(B^2)_{ij} = \sum_k b_{ik} b_{kj}$$

and that $b_{ik} b_{kj} \neq 0$ only if $j \to k \to i$ is a directed path in $\mathcal{G}$. Similarly

$$(B^3)_{ij} = \sum_k \sum_l b_{ik} b_{kl} b_{lj}$$

and $b_{ik} b_{kl} b_{lj} \neq 0$ only if $j \to l \to k \to i$ is a directed path in $\mathcal{G}$. In fact, the (i, j)-term of B^d consists of a sum over all directed paths from j to i with length exactly d.

Example 8.23. Suppose we have the model in Figure 8.6 generated by the following structural equations:

$$X = \varepsilon_x, \qquad Y = \alpha X + \varepsilon_y, \qquad Z = \beta X + \gamma Y + \varepsilon_z$$

for $(\varepsilon_x, \varepsilon_y, \varepsilon_z)^T \sim N_3(0, I)$.

This gives

$$\begin{pmatrix} X \\ Y \\ Z \end{pmatrix} = \begin{pmatrix} 0 & 0 & 0 \\ \alpha & 0 & 0 \\ \beta & \gamma & 0 \end{pmatrix} \begin{pmatrix} X \\ Y \\ Z \end{pmatrix} + \begin{pmatrix} \varepsilon_x \\ \varepsilon_y \\ \varepsilon_z \end{pmatrix}$$

$$\begin{pmatrix} 1 & 0 & 0 \\ -\alpha & 1 & 0 \\ -\beta & -\gamma & 1 \end{pmatrix} \begin{pmatrix} X \\ Y \\ Z \end{pmatrix} = \begin{pmatrix} \varepsilon_x \\ \varepsilon_y \\ \varepsilon_z \end{pmatrix}.$$

[6]Recall that a $p \times p$ matrix is nilpotent if $B^p = B \cdots B = 0$.

Now, you can check that:

$$\begin{pmatrix} 1 & 0 & 0 \\ -\alpha & 1 & 0 \\ -\beta & -\gamma & 1 \end{pmatrix}^{-1} = \begin{pmatrix} 1 & 0 & 0 \\ \alpha & 1 & 0 \\ \beta + \alpha\gamma & \gamma & 1 \end{pmatrix}.$$

The entry $\beta + \alpha\gamma$ corresponds to the sum of the two paths $Z \leftarrow X$ and $Z \leftarrow Y \leftarrow X$.

It is not too hard to see then that the i, j entry of the right-hand side of (10) will give all directed paths of any length from i to j. The transpose $(I - B)^{-T}$ will give the same paths in the other direction, and so multiplying will lead to entries consisting of pairs of directed paths. This motivates the idea of a trek.

Definition 8.24. A *trek* from i to j, with *source* k, is a pair of paths, (π_l, π_r), where π_l is a directed path from k to i, and π_r is a directed path from k to j. The two paths are known as the left and right *side* of the trek.

Thus a trek is essentially a path without colliders, except that we do allow repetition of vertices. Looking at the graph in Figure 8.6 again, we find the following treks from Y to Z:

$$Y \to Z \qquad Y \leftarrow X \to Z \qquad Y \leftarrow X \to Y \to Z.$$

and from Z to Z:

$$\begin{array}{lll} Z & Z \leftarrow Y \to Z & Z \leftarrow X \to Z \\ Z \leftarrow Y \leftarrow X \to Z & Z \leftarrow X \to Y \to Z & Z \leftarrow Y \leftarrow X \to Y \to Z. \end{array} \tag{11}$$

Note that $Y \to Z$ shows that the left side can be empty, and Z shows that both sides can be empty. Unsurprisingly, it is also possible for the right side to be empty, since $Z \leftarrow Y$ is a trek from Z to Y.

Example 8.25. Continuing Example 8.23, for the graph in Figure 8.6 we have

$$\begin{aligned} \Sigma &= (I - B)^{-1}(I - B)^{-T} \\ &= \begin{pmatrix} 1 & 0 & 0 \\ \alpha & 1 & 0 \\ \beta + \alpha\gamma & \gamma & 1 \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 \\ \alpha & 1 & 0 \\ \beta + \alpha\gamma & \gamma & 1 \end{pmatrix}^T \\ &= \begin{pmatrix} 1 & 0 & 0 \\ \alpha & 1 & 0 \\ \beta + \alpha\gamma & \gamma & 1 \end{pmatrix} \begin{pmatrix} 1 & \alpha & \beta + \alpha\gamma \\ 0 & 1 & \gamma \\ 0 & 0 & 1 \end{pmatrix} \\ &= \begin{pmatrix} 1 & \alpha & \beta + \alpha\gamma \\ \alpha & 1 + \alpha^2 & \alpha\beta + \gamma + \alpha^2\gamma \\ \beta + \alpha\gamma & \alpha\beta + \gamma + \alpha^2\gamma & 1 + \gamma^2 + \beta^2 + 2\alpha\beta\gamma + \alpha^2\gamma^2 \end{pmatrix}. \end{aligned}$$

Now, notice that

$$\sigma_{zz} = 1 + \gamma^2 + \beta^2 + 2\alpha\beta\gamma + \alpha^2\gamma^2.$$

consists of a sum of the edge coefficents over the six treks in (11).

Definition 8.26. Given a trek $\tau = (\pi_l, \pi_r)$ with source k, define the *trek covariance* as

$$c(\tau) = d_{kk} \prod_{i \to j \in \pi_l} b_{ji} \prod_{i \to j \in \pi_r} b_{ji}.$$

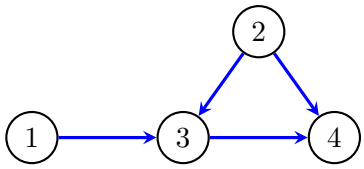


Figure 8.7: A directed graph.

Example 8.27. For the trek $Z \leftarrow X \rightarrow Y$ from Z to Y with source X, we obtain $c(\tau) = d_{xx}b_{yx}b_{zx} = 1 \cdot \alpha \cdot \beta$. In this model $D = I$, but in general the d_{kk} factors may not be equal to 1.

We will show the following general rule.

Theorem 8.28 (Trek Rule)**.** *Let $\Sigma = (I - B)^{-1}D(I - B)^{-T}$ be a covariance matrix that is Markov with respect to a DAG $\mathcal{G}$. Then*

$$\sigma_{ij} = \sum_{\tau \in \mathcal{T}_{ij}} c(\tau)$$

where $\mathcal{T}_{ij}$ is the set of treks *from i to j.*

Proof. We proceed by induction on the number of variables p. The result holds for one vertex since $\mathrm{Cov}(X_1, X_1) = d_{11}$ which is the trek covariance for the trivial trek 1. Assume the result holds for $|V| < p$, so in particular it holds on any ancestral subgraph. Let X_p be a random variable associated with a vertex p that has no children in $\mathcal{G}$. By the induction hypothesis, $\mathrm{Cov}(X_i, X_j)$ is of the required form for $i, j < p$.

We have $X_p = \sum_{j \in \mathrm{pa}_\mathcal{G}(p)} b_{pj}X_j + \varepsilon_p$, where ε_p is independent of $X_1, \ldots, X_{p-1}$. Hence, for any $i < p$:

$$\mathrm{Cov}(X_i, X_p) = \sum_{j \in \mathrm{pa}_\mathcal{G}(p)} b_{pj} \mathrm{Cov}(X_i, X_j).$$

Now, note that any trek from i to p must consist of the combination of $j \rightarrow p$ for some parent j of p, and a trek from i to j. This establishes the result for $i \neq p$.

If $i = p$, we have

$$\mathrm{Cov}(X_p, X_p) = \sum_{j \in \mathrm{pa}_\mathcal{G}(p)} b_{pj} \mathrm{Cov}(X_p, X_j) + \mathrm{Cov}(X_p, \varepsilon_p).$$

Note that, by the part already established, any trek from p to p of length ≥ 1 is included in the first sum, and the final term is $\mathrm{Cov}(X_p, \varepsilon_p) = \mathrm{Var}\, \varepsilon_p = d_{pp}$. This is the trek covariance for the trek p of length 0. □

Example 8.29. Consider the graph in Figure 8.7.

The set of treks from 3 to 3 is:

$$3 \qquad 3 \leftarrow 2 \rightarrow 3 \qquad 3 \leftarrow 1 \rightarrow 3. \tag{12}$$

In the trek 3, both the left and right-hand sides have length zero, and again the source is 3 itself. The respective trek covariances are

$$d_{33} \qquad\qquad d_{22}b_{32}^2 \qquad\qquad d_{11}b_{31}^2$$

(note the trivial trek 3 has trek covariance d_{33}). It follows from Theorem 8.28 that

$$\mathrm{Var}(X_3) = \sigma_{33} = d_{33} + d_{22}b_{32}^2 + d_{11}b_{31}^2.$$

The treks from 3 to 4 are:

$$\begin{array}{ll} 3 \to 4 & 3 \leftarrow 2 \to 4 \\ 3 \leftarrow 2 \to 3 \to 4 & 3 \leftarrow 1 \to 3 \to 4. \end{array} \tag{13}$$

The associated trek covariances are

$$\begin{array}{ll} d_{33}b_{43} & d_{22}b_{32}b_{42} \\ d_{22}b_{32}^2b_{43} & d_{11}b_{31}^2b_{43}. \end{array}$$

It follows from Theorem 8.28 that

$$\begin{aligned} \mathrm{Cov}(X_3, X_4) = \sigma_{34} &= d_{33}b_{43} + d_{22}b_{32}b_{42} + d_{22}b_{32}^2b_{43} + d_{11}b_{31}^2b_{43} \\ &= (d_{33} + d_{22}b_{32}^2 + d_{11}b_{31}^2)b_{43} + d_{22}b_{32}b_{42} \\ &= \mathrm{Var}(X_3)b_{43} + \mathrm{Var}(X_2)b_{32}b_{42}. \end{aligned}$$

Thus, we can decompose the covariance into parts due to the causal path $3 \to 4$ and the back-door path $3 \leftarrow 2 \to 4$.

8.7 Optimal Adjustment Sets

One can show that when all variables are observed, there is an *optimal adjustment set*; that is, one which is minimal, and gives an estimate of the causal parameter that has the smallest possible variance. We will prove this in the case of linear causal models, but note that the same result applies to any system of (nonparametric) structural equations with all the variables observed.

[TO BE CONTINUED...]