DTU

Model-based Machine Learning

PGM foundations I

Outline

Representation

The concept of inference

Conditional Probability Tables (CPTs)

D-separation

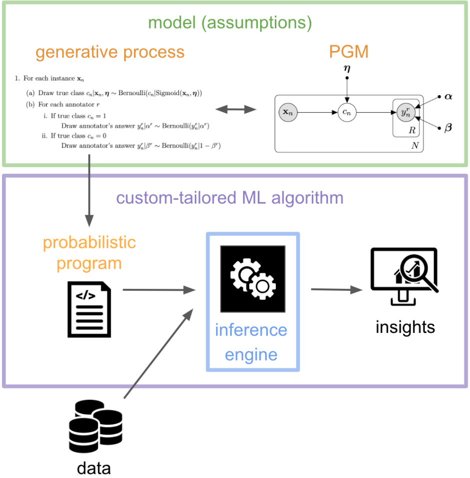
(Based on Michael Jordan, David Blei)

Road to MBML: where are we?

Foundations of PGMs and probabilistic programming
Probabilistic modelling in various contexts - your modelling toolbox
Bayesian inference (exact and approximate)

Week	Topic
1	Intro to the course + Prob. review
2	PGM foundations
3	PGM foundations II
4	Freq. vs Bayesian + Prob. Prog. + Mixture models
5	Regression models
6	Classification and Hierarchical models
7	Temporal models
8	Topic Models
9	Markov-chain Monte Carlo (MCMC)
10	Variational inference
11	Generative models
12	Gaussian processes
13	Project support

Model-based Machine Learning



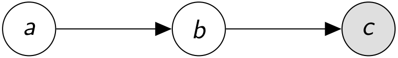
Learning objectives

At the end of this lecture, you should be able to:

- Explain the mathematical notation and representation conventions of directed graphical models
- Factorize the joint distribution that the PGM represents, taking advantage of conditional independence
- Perform exact inference in basic discrete PGMs represented with their Conditional Probability Tables (CPTs)
- Explain the concept of D-separation and prove conditional independence through the D-separation algorithm

PGM representation

- An example graphical model



- **Nodes** represent random variables
  - shaded nodes correspond to observed variables
  - unshaded nodes denote unobserved variables (also known as hidden or latent variables)
- **Edges** express probabilistic relationships between the variables

PGM representation

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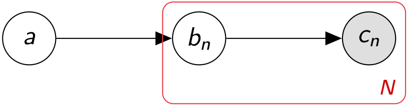

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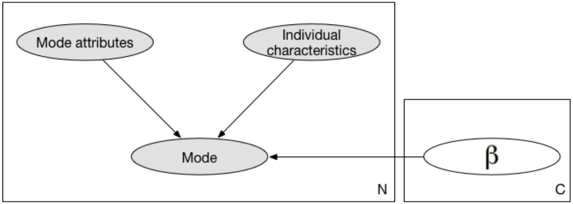
- **Edges** express probabilistic relationships between the variables
- **Plates** indicate repetition

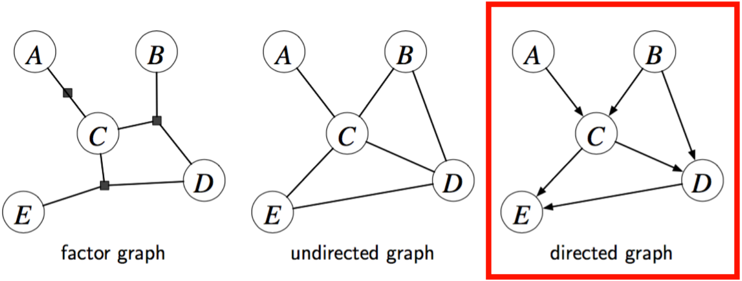
PGM representation

- A practical example



PGM representation

- There are other kinds of graphical models...

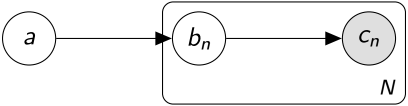


  - Each has different properties and expressiveness
- We will mainly consider **directed** graphical models in this and coming lectures!

Recall our notation

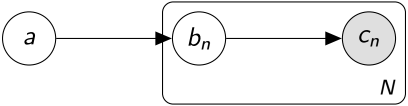
- Unlike in the "standard" statistics notation, where:
  - X is a random variable and x is atom/event
  - We write e.g. $p(X = x)$
- In the machine learning literature, this notation is typically simplified
  - Lowercase letters, such as x, represent random variables
  - We simply write $p(x)$. Everything else should be clear from the context!
- This allows us to have
  - Bold letters denote vectors (e.g. $\mathbf{x}$, where the i^{th} element is referred as x_i)
  - Matrices are represented by bold uppercase letters such as $\mathbf{X}$
  - Roman letters, such as N, denote constants
- This is the notation that we will adopt from now on!

PGM representation



- PGMs represent a set of **conditional independence** relationships

PGM representation



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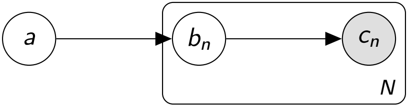
$$c_n \perp\!\!\!\perp a \mid b_n \quad (c_n \text{ is conditionally independent of } a \text{ given } b_n)$$

  - if we observed b_n, then observing a tell us nothing about c_n

PGM representation



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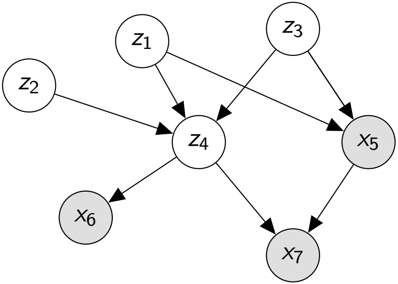
- A PGM specifies a **joint distribution** over variables and how it factorizes:

$$p(a, \mathbf{b}, \mathbf{c}) = p(a) \prod_{n=1}^{N} p(b_n|a)\, p(c_n|b_n)$$

where $\mathbf{b} = \{b_n\}_{n=1}^{N}$ and $\mathbf{c} = \{c_n\}_{n=1}^{N}$

From PGMs to joint distributions

- Another example



- Corresponding factorization of the joint distribution:

$$p(z_1, z_2, z_3, z_4, x_5, x_6, x_7) = ?$$

From PGMs to joint distributions

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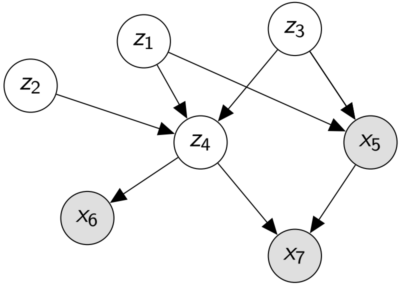

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$$p(z_1, z_2, z_3, z_4, x_5, x_6, x_7) = p(z_1)\, p(z_2)\, p(z_3)\, p(z_4|z_1, z_2, z_3) \\ \times\, p(x_5|z_1, z_3)\, p(x_6|z_4)\, p(x_7|z_4, x_5)$$

Why are factorizations so important?

- Consider the joint distribution $p(z_1, z_2, z_3, z_4, x_5, x_6, x_7)$
- Assume each variable is binary
- How many parameters do we need to represent $p(z_1, z_2, z_3, z_4, x_5, x_6, x_7)$? You can think of it as a huge table...

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  - You need $2^7 - 1 = 127$ parameters (entries in that table)!
- How about for the factorized version?

$$p(z_1)\, p(z_2)\, p(z_3)\, p(z_4|z_1, z_2, z_3)\, p(x_5|z_1, z_3)\, p(x_6|z_4)\, p(x_7|z_4, x_5)$$

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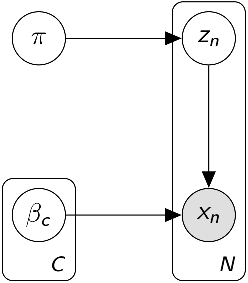
  - Just $1 + 1 + 1 + 2^3 + 2^2 + 2 + 2^2 = 21$ parameters!
  - Much more efficient, right?
    We are exploiting the **conditional independencies** between the variables

Playtime

- What is the factorization of the joint distribution corresponding to this PGM?



$$p(\pi, \beta, \mathbf{z}, \mathbf{x}) = ?$$

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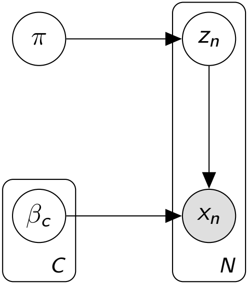

$$p(\pi, \beta, \mathbf{z}, \mathbf{x}) = p(\pi) \left(\prod_{c=1}^{C} p(\beta_c) \right) \prod_{n=1}^{N} p(z_n|\pi)\, p(x_n|z_n, \beta)$$

Careful with the parenthesis!

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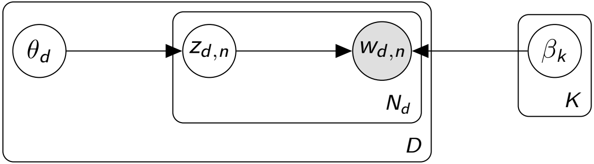

$$p(\boldsymbol{\theta}, \boldsymbol{\beta}, \mathbf{z}, \mathbf{w}) = ?$$

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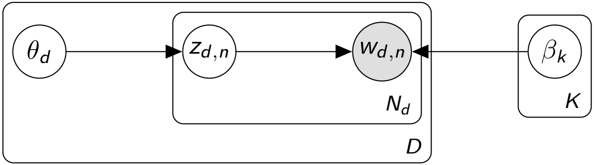
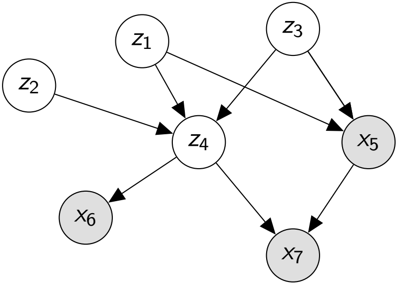


$$p(\boldsymbol{\theta}, \boldsymbol{\beta}, \mathbf{z}, \mathbf{w}) = \left(\prod_{k=1}^{K} p(\beta_k) \right) \prod_{d=1}^{D} p(\theta_d) \prod_{n=1}^{N_d} p(z_{d,n}|\theta_d)\, p(w_{d,n}|z_{d,n}, \boldsymbol{\beta})$$

Inference

- **Model + Data $\rightarrow$ Insights**
- Answer various types of questions about the data by computing the posterior distribution of the latent variables given the observed ones



- Example: $p(z_2 | x_5, x_6, x_7) = ?$

Two fundamental rules that you should always remember..

- Product rule of probability (or chain rule)

$$p(x, z) = p(x|z)\, p(z)$$

- Sum rule of probability (or marginalization rule)

$$p(x) = \sum_z p(x, z)$$

...or, if z is continuous

$$p(x) = \int p(x, z)\, dz$$

- This is also called *marginalizing over z*. But more on that later... :-)

Inference

- **Exact** inference
  - Set of latent variables $\mathbf{z} = \{z_m\}_{m=1}^{M}$
  - Observed variables $\mathbf{x} = \{x_n\}_{n=1}^{N}$
  - Using Bayes' theorem, the **posterior distribution** of $\mathbf{z}$ can be computed as

$$\overbrace{p(\mathbf{z}|\mathbf{x})}^{\text{posterior}} = \frac{\overbrace{p(\mathbf{x},\mathbf{z})}^{\text{joint}}}{p(\mathbf{x})} = \frac{\overbrace{p(\mathbf{x}|\mathbf{z})}^{\text{likelihood}}\ \overbrace{p(\mathbf{z})}^{\text{prior}}}{\underbrace{p(\mathbf{x})}_{\text{evidence}}}$$

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  - The **model evidence** , or marginal likelihood, can be computed by making use of the sum rule of probability to give

$$p(\mathbf{x}) = \sum_{\mathbf{z}} p(\mathbf{x}|\mathbf{z})\, p(\mathbf{z})$$

Bayes update = reweight + renormalize

$$p(\mathbf{z}|\mathbf{x}) = \frac{p(\mathbf{x}|\mathbf{z})\, p(\mathbf{z})}{p(\mathbf{x})} \qquad \text{with } p(\mathbf{x}) = \sum_{\mathbf{z}} p(\mathbf{x}|\mathbf{z}) p(\mathbf{z})$$

Interpretation:

- Start with prior weights $p(\mathbf{z})$.
- **Reweight** each hypothesis by how well it predicts the observation: multiply by $p(\mathbf{x}|\mathbf{z})$.
- **Renormalize** so the weights sum to 1: divide by $p(\mathbf{x})$.

Key idea: Posterior is the prior *tilted* toward hypotheses that make the observed data more likely.

Tiny discrete example: compute the posterior in 2 steps

- **Setup.** Hypotheses $z \in \{z_1, z_2, z_3\}$. We observe x.

	z_1	z_2	z_3
Prior $p(z)$	0.60	0.30	0.10
Likelihood $p(x\|z)$	0.10	0.50	0.90
Unnorm. weight $p(x\|z)p(z)$	0.06	0.15	0.09

- **Step 1 (reweight):** $w(z) = p(x|z)p(z)$

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$$p(x) = \sum_i w(z_i) = 0.06 + 0.15 + 0.09 = 0.30, \quad p(z_i|x) = \frac{w(z_i)}{p(x)}$$

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- **Posterior:**

$$p(z_1|x) = 0.20, \quad p(z_2|x) = 0.50, \quad p(z_3|x) = 0.30$$

Why the evidence term is not scary

$$p(z|x) \propto p(x|z)p(z) \quad \Longrightarrow \quad p(z|x) = \frac{p(x|z)p(z)}{\sum_{z'} p(x|z')p(z')}$$

- Notice the "proportional to" sign $\propto$)
- Important to note:
  1. **Evidence is just a normalizer:** it ensures $\sum_z p(z|x) = 1$

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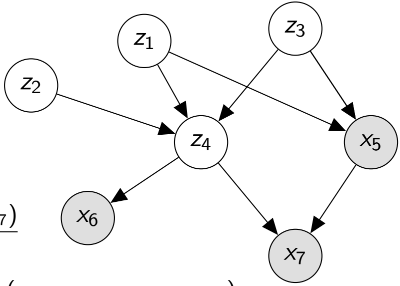
- Important to note:
  1. **Evidence is just a normalizer:** it ensures $\sum_z p(z|x) = 1$
  2. **Comparisons don't need it:** for any two hypotheses,

$$\frac{p(z_a|x)}{p(z_b|x)} = \frac{p(x|z_a)p(z_a)}{p(x|z_b)p(z_b)} \quad \text{(evidence cancels)}$$

- **Takeaway:** Bayesian updating is "prior odds $\times$ likelihood ratio"

Inference

- Returning to the previous example...

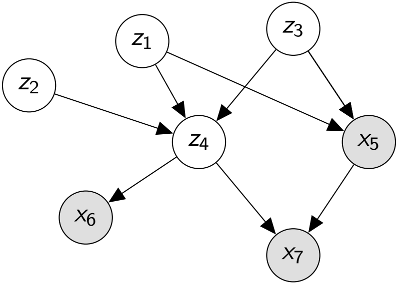


- Assuming discrete variables:

$$p(z_2|x_5, x_6, x_7) = \frac{p(z_2, x_5, x_6, x_7)}{p(x_5, x_6, x_7)}$$
$$\propto \sum_{z_1} \sum_{z_3} \sum_{z_4} p(z_1, z_2, z_3, z_4, x_5, x_6, x_7)$$

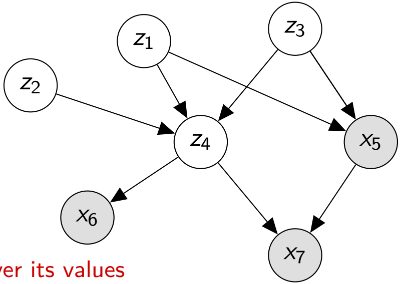
- In this case, it can be computed exactly (using the sum rule of probability)!
- Notice that, in this case, we don't need to compute $p(x_5, x_6, x_7)$!
  We can just renormalize the numerator in the end
  (hence the "proportional to" sign)

Inference



- What if x_6 is missing?

Inference



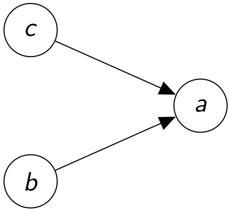
- What if x_6 is missing?
  - No problem! Just marginalize over its values

$$p(z_2|x_5, x_7) = \frac{p(z_2, x_5, x_7)}{p(x_5, x_7)}$$
$$\propto \sum_{z_1}\sum_{z_3}\sum_{z_4}\sum_{x_6} p(z_1, z_2, z_3, z_4, x_5, x_6, x_7)$$

  - Corresponds to considering all possible values of x_6 and averaging over them (weighted by their respective probabilities)
- PGMs provide a consistent way of handling **missing data**

Conditional Probability Tables (CPTs)

- For now, our PGMs have only discrete random variables
- Each node has associated a **Conditional Probability Table**
  - It maps all possible values of its incoming set of arcs...
  - ...to all possible values of the node itself
- For example



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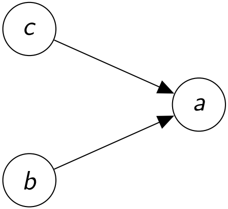


- This relationship could be defined by:

	$a=0$	$a=1$
$b=0, c=0$	0.7	0.3
$b=0, c=1$	0.3	0.7
$b=1, c=0$	0.5	0.5
$b=1, c=1$	0.1	0.9

Table: $p(a|b,c)$

- It factorizes as:

$$p(a,b,c) = p(a|b,c)\,p(b)\,p(c)$$

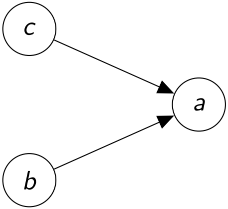
$b=0$	$b=1$
0.4	0.6

Table: $p(b)$

$c=0$	$c=1$
0.7	0.3

Table: $p(c)$

Conditional Probability Tables (CPTs)



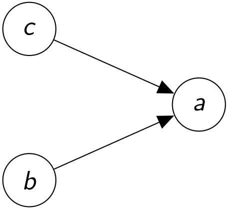
- Joint distribution factorizes as:

$$p(a, b, c) = p(a|b, c)\, p(b)\, p(c)$$

- Imagine we observe $b = 1$. Let's calculate $p(a|b = 1)$

$$p(a|b = 1) =$$

Conditional Probability Tables (CPTs)



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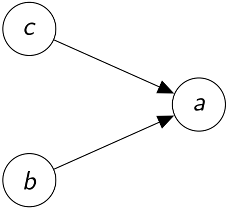

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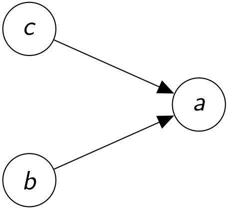

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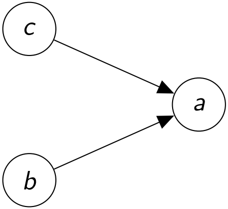

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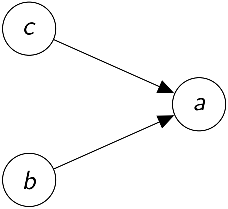
$$= \sum_c p(a|b = 1, c)\, p(c)$$

$$= p(a|b = 1, c = 0)\, p(c = 0) + p(a|b = 1, c = 1)\, p(c = 1)$$

Conditional Probability Tables (CPTs)



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$$
\begin{aligned}
p(a|b=1) &= \frac{\sum_c p(a, b=1, c)}{p(b=1)} = \frac{\sum_c p(a|b=1, c)\, \cancel{p(b=1)}\, p(c)}{\cancel{p(b=1)}} \\
&= \sum_c p(a|b=1, c)\, p(c) \\
&= p(a|b=1, c=0)\, p(c=0) + p(a|b=1, c=1)\, p(c=1) \\
&= p(a|b=1, c=0) \times 0.7 + p(a|b=1, c=1) \times 0.3
\end{aligned}
$$

Conditional Probability Tables (CPTs)

$$p(a|b=1) = p(a|b=1, c=0) \times 0.7 + p(a|b=1, c=1) \times 0.3$$

- Considering $p(a|b,c)$:

	$a=0$	$a=1$
$b=0, c=0$	0.7	0.3
$b=0, c=1$	0.3	0.7
$b=1, c=0$	0.5	0.5
$b=1, c=1$	0.1	0.9

- We have:

$$p(a=1|b=1) = 0.5 \times 0.7 + 0.9 \times 0.3 = 0.62$$
$$p(a=0|b=1) = 0.5 \times 0.7 + 0.1 \times 0.3 = 0.38$$

- Thus $p(a|b=1)$ will be:

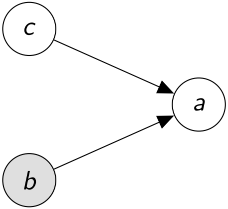
$a=0$	$a=1$
0.38	0.62

Playtime!

- Solve $p(c|b=1)$
- Estimated time: 20 min

Conditional Probability Tables (CPTs)

- Indeed, b and c are independent.
  Just look at the factorization...



$$p(a, b, c) = p(a|b, c)\, p(b)\, p(c)$$

Conditional Probability Tables (CPTs)

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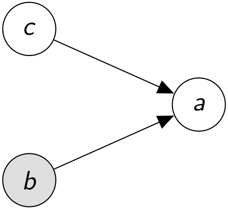
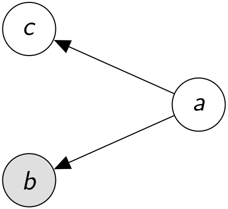


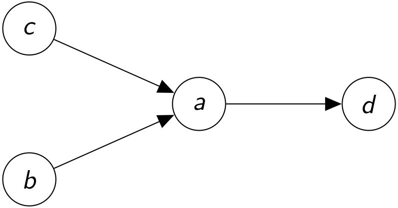
$$p(a, b, c) = p(a|b, c)\, p(b)\, p(c)$$

- What if we had this instead?



$$p(a, b, c) = p(b|a)\, p(c|a)\, p(a)$$

Conditional Probability Tables (CPTs)

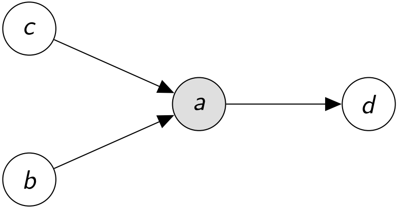


- Another relationship, another CPT:

	$d=0$	$d=1$
$a=0$	0.6	0.4
$a=1$	0.2	0.8

Table: $p(d|a)$

Conditional Probability Tables (CPTs)



- Another relationship, another CPT:

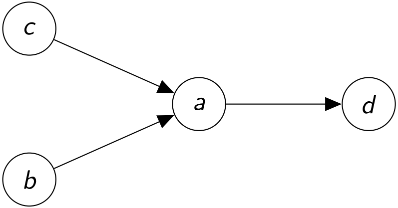
	$d = 0$	$d = 1$
$a = 0$	0.6	0.4
$a = 1$	0.2	0.8

Table: $p(d|a)$

- If a is observed, then we can get the distribution of d directly
- We can conclude that $d \perp\!\!\!\perp b, c \mid a$
- And also $p(a, b, c, d) = p(a|b, c)\, p(d|a)\, p(b)\, p(c)$

Conditional Probability Tables (CPTs)

- Full PGM:



- Of course, if we do **not** observe a, then d will depend on the values of b and c

- Another relationship, another CPT:

	$d = 0$	$d = 1$
$a = 0$	0.6	0.4
$a = 10$	0.2	0.8

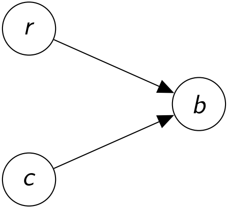
Table: $p(d|a)$

Some useful rules

	We want	We have	We do
1.	$p(a, b)$	$p(a, b, c)$	$p(a, b) = \sum_c p(a, b, c)$
2.	$p(a\|b, c)$	$p(a, b, c)$	$p(a\|b, c) = \frac{p(a,b,c)}{\sum_a p(a,b,c)}$
3.	$p(a\|b)$	$p(a, b, c)$	$p(a\|b) = \frac{\sum_c p(a,b,c)}{\sum_c \sum_a p(a,b,c)}$
4.	$p(a\|b)$	$p(b\|a), p(a)$	$p(a\|b) = \frac{p(b\|a)\, p(a)}{\sum_a p(b\|a)\, p(a)}$
5.	$p(a\|b)$	$p(a\|b, c), p(c)$	$p(a\|b) = \sum_c p(a\|b, c)\, p(c)$

- Note that these are just applications of the sum and product rules of probability!

Travel mode choice - a possible story



	$r=1$	$r=0$
	0.7	0.3

Table: $p(r)$

	$c=1$	$c=0$
	0.3	0.7

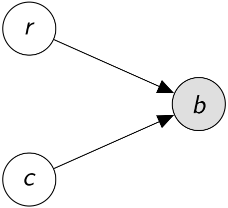
Table: p(c)

- Every day, John needs to decide whether to go to work by bike ($b=1$), or just take his car ($b=0$)?
  - It depends on whether he has schedule constraints ($c=1$): e.g. a meeting far away may imply the need for a car
  - It depends on whether it rains ($r=1$), or not ($r=0$)

	$b=1$	$b=0$
$c=1, r=1$	0.1	0.9
$c=1, r=0$	0.2	0.8
$c=0, r=1$	0.3	0.7
$c=0, r=0$	0.8	0.2

Table: $p(b|c,r)$

Mode choice - a possible story



- We observe that he took his car ($b = 0$)
- What is the probability that it is raining?
  - $p(r = 1 | b = 0) = ?$
- Notice that we have $p(b, r, c) = p(b|r, c)\, p(r)\, p(c)$

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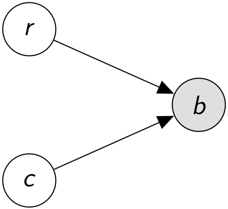

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$$p(r = 1 | b = 0) \overset{1,2}{=} \frac{\sum_{c \in \{0,1\}} p(b = 0, r = 1, c)}{p(b = 0)} =$$

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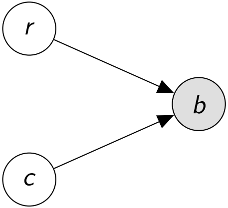

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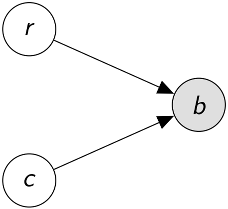
$$\overset{3}{=} \frac{\sum_{c\in\{0,1\}} p(b = 0|r = 1, c)\, p(r = 1)\, p(c)}{\sum_{r\in\{0,1\}} \sum_{c\in\{0,1\}} p(b = 0, r, c)} =$$

Mode choice - a possible story



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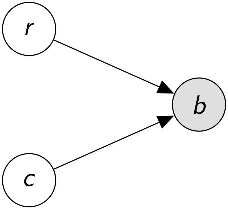

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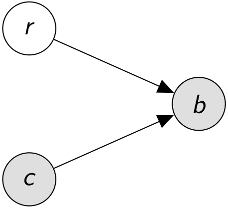
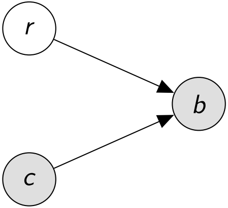
$$= \frac{(0.9 \times 0.3 + 0.7 \times 0.7) \times 0.7}{(0.9 \times 0.3 + 0.7 \times 0.7) \times 0.7 + (0.8 \times 0.3 + 0.2 \times 0.7) \times 0.3} = \frac{0.532}{0.646} = 0.824$$

Explaining away



- What if we **also** observe that the schedule is constrained, $c = 1$
- Should the probability that it is raining change?...
  - $p(r = 1 | b = 0, c = 1) = ?$

Explaining away



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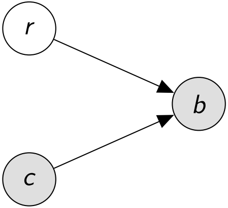

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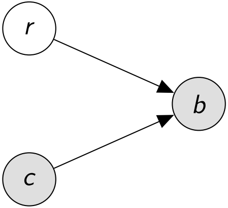
Explaining away



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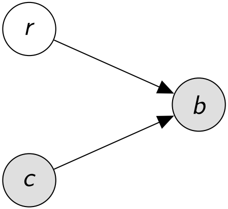
$$= \frac{p(b = 0 | r = 1, c = 1)\, p(r = 1)}{\sum_r p(b = 0 | r, c = 1)\, p(r)} = \frac{0.9 \times 0.7}{(0.9 \times 0.7) + (0.8 \times 0.3)} = \frac{0.63}{0.87} = 0.72$$

Explaining away



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- What happened is that knowing the choice of car (b=0) was **explained away** by the fact that the schedule is constrained/tight
- As if you believe less that John does not pick the bike due to the rain

Independence properties

- Just by analysing the representation, we simplify the calculations!
  - Observed data vs Latent variables (color of node)
  - Arrow directions
  - Conditional independence rules (D-separation)
- The Bayesian network assumption says:

  "Each variable is conditionally independent of its non-descendants, given its parents"

D-separation

- When does x influence y?

D-separation

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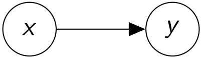
- Direct connection:



D-separation

- When does x influence y?
- Direct connection:

$$x \longrightarrow y$$

- Indirect connection:

Causal effect: $x \longrightarrow z \longrightarrow y$

D-separation

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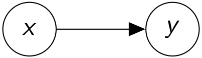

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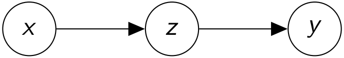
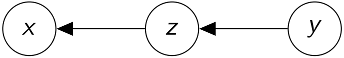


Evidential effect:



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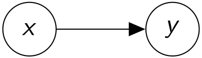

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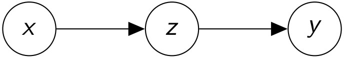

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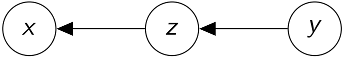
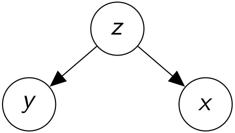


Common (latent) cause:



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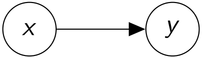

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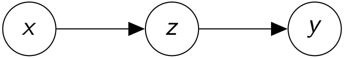

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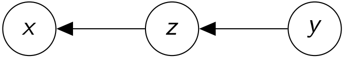

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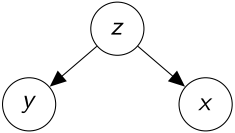
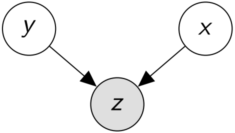


Common (observed) effect:



D-separation

- When influence can flow from x to y via z, we say that the trail x, y, z is *active* (otherwise, it is *blocked*)

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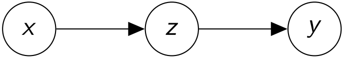
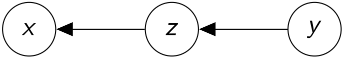
Causal trail:



Active iff z is not observed

Evidential trail:



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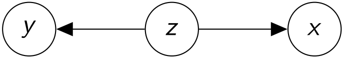

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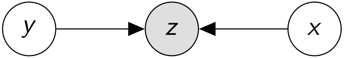


Active iff z **or one of its descendants are observed**

D-separation: a simple(r) algorithm

For any expression "is $\mathbf{x}$ independent of $\mathbf{y}$ given $\mathbf{z}$" (formally, $\mathbf{x} \perp\!\!\!\perp \mathbf{y} | \mathbf{z}$)[1]

1. Draw the *ancestral graph*
   - It is the part of the original graph that has only the variable sets $\mathbf{x}$, $\mathbf{y}$ and $\mathbf{z}$, and all their ancestors among them
2. *Moralize* the graph by *marrying* the parents
   - For each pair of variables with a common child, draw an undirected edge (line) between them (if a variable has more than two parents, draw lines between every pair of parents)
3. *Disorient* the graph by replacing all edges for undirected ones
4. Delete the variables $\mathbf{z}$ (and any other observed variables not explicitly included in $\mathbf{z}$), and their edges

[1] Note that $\mathbf{x}$, $\mathbf{y}$ and $\mathbf{z}$ can themselves be sets of variables!

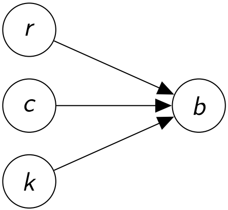
D-separation: a simple(r) algorithm (cont.)

Analysis of the result

- If $\mathbf{x}$ and $\mathbf{y}$ are **disconnected**, then they are conditionally independent given $\mathbf{z}$!
    - Being disconnected means that there is no possible path between $\mathbf{x}$ and $\mathbf{y}$ in the resulting graph
- Otherwise, they are not proven to be independent

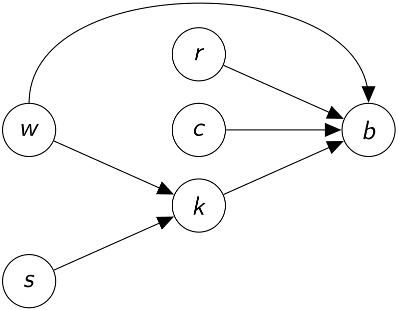
Mode choice - a possible story

- Every day, John needs to decide whether to go to work by bike ($b = 1$), or to just take his car ($b = 0$)?
  - It depends on whether he has schedule constraints ($c = 1$): e.g. a meeting far away may imply the need for a car
  - It depends on whether it rains ($r = 1$), or not ($r = 0$)
  - It also depends on whether he needs to pickup and drop off his kids, k

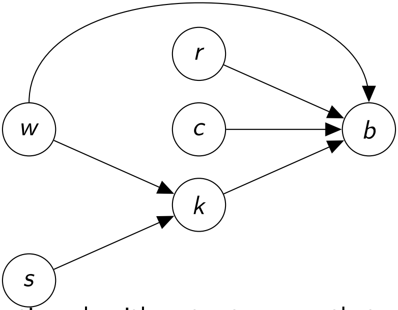


Mode choice - a possible story

- We can dig further in this problem...
  - If there is no school on that day ($s = 0$), he probably won't need to bring his kids at all
  - His wife w, may bring the kids
  - His wife may need to take the car (in which case, he has to take the kids by bike)



Playtime!



- Using the D-separation algorithm, try to prove that:

$$s \perp\!\!\!\perp b \mid k$$

$$s \perp\!\!\!\perp b \mid \{k, w\}$$

$$\{r, c\} \perp\!\!\!\perp k$$

$$\{r, c\} \perp\!\!\!\perp s \mid \{k, b\}$$

- Estimated time: 20 min

Readings

- **Main reading**: Chapter 8: “Graphical Models”, pages 359-366 and pages 372-379 of Chris Bishop’s book, “Pattern Recognition and Machine Learning” (PRML) URL: https://www.microsoft.com/en-us/research/uploads/prod/2006/01/Bishop-Pattern-Recognition-and-Machine-Learning-2006.pdf)
- “D-separation: How to determine which variables are independent in a Bayes net”. Jessica Noss. EECS MIT. http://web.mit.edu/jmn/www/6.034/d-separation.pdf
- Chapter 10: “Directed graphical models”, pages 307-311 and pages 324-327 of Kevin Murphy’s book “Machine Learning: A Probabilistic Perspective”
- Koller, D., and Friedman, N. (2009). Probabilistic graphical models: principles and techniques. MIT press.