From Independencies to Directed Graphs

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Recap

- We talked about reasonably weak assumption to facilitate the efficient representation of a probabilistic model
- Independence assumptions reduce the number of interacting variables
- Parametric assumptions restrict the way the variables may interact.
- (Conditional) independence assumptions lead to a factorisation of the pdf/pmf, e.g.
  - $p(\mathbf{x}, \mathbf{y}, \mathbf{z}) = p(\mathbf{x})p(\mathbf{y})p(\mathbf{z})$
  - $p(x_1, \ldots, x_d) = p(x_d | x_{d-3}, x_{d-2}, x_{d-1})p(x_1, \ldots, x_{d-1})$

Program

1. Equivalence of factorisation and ordered Markov property
2. Understanding models from their factorisation

Program

1. Equivalence of factorisation and ordered Markov property
   - Chain rule
   - Ordered Markov property implies factorisation
   - Factorisation implies ordered Markov property
2. Understanding models from their factorisation

Chain rule

Iteratively applying the product rule allows us to factorise any joint pdf (pmf) $p(\mathbf{x}) = p(x_1, x_2, \ldots, x_d)$ into product of conditional pdfs.

$$\begin{aligned}
p(\mathbf{x}) &= p(x_1)p(x_2, \ldots, x_d|x_1) \\
&= p(x_1)p(x_2|x_1)p(x_3, \ldots, x_d|x_1, x_2) \\
&= p(x_1)p(x_2|x_1)p(x_3|x_1, x_2)p(x_4, \ldots, x_d|x_1, x_2, x_3) \\
&\vdots \\
&= p(x_1)p(x_2|x_1)p(x_3|x_1, x_2) \ldots p(x_d|x_1, \ldots x_{d-1}) \\
&= p(x_1)\prod_{i=2}^{d} p(x_i|x_1, \ldots, x_{i-1}) \\
&= \prod_{i=1}^{d} p(x_i|\mathrm{pre}_i)
\end{aligned}$$

with $\mathrm{pre}_i = \mathrm{pre}(x_i) = \{x_1, \ldots, x_{i-1}\}$, $\mathrm{pre}_1 = \varnothing$ and $p(x_1|\varnothing) = p(x_1)$

The chain rule can be applied to any ordering $x_{k_1}, \ldots x_{k_d}$. Different orderings give different factorisations.

From (conditional) independence to factorisation

$p(\mathbf{x}) = \prod_{i=1}^{d} p(x_i|\mathrm{pre}_i)$ for the ordering $x_1, \ldots, x_d$

- For each x_i, we condition on all previous variables in the ordering.
- Assume that, for each i, there is a minimal subset of variables $\pi_i \subseteq \mathrm{pre}_i$ such that $p(\mathbf{x})$ satisfies

$$x_i \perp\!\!\!\perp (\mathrm{pre}_i \setminus \pi_i) \mid \pi_i$$

  for all i.
- $p(\mathbf{x})$ is then said to satisfy the ordered Markov property .
- By definition of conditional independence: $p(x_i|x_1, \ldots, x_{i-1}) = p(x_i|\mathrm{pre}_i) = p(x_i|\pi_i)$
- With the convention $\pi_1 = \varnothing$, we obtain the factorisation

$$p(x_1, \ldots, x_d) = \prod_{i=1}^{d} p(x_i|\pi_i)$$

- See later: the π_i correspond to the parents of x_i in graphs.

From (conditional) independence to factorisation

- Assume the variables are ordered as $x_1, \ldots, x_d$, let $\mathrm{pre}_i = \{x_1, \ldots x_{i-1}\}$ and $\pi_i \subseteq \mathrm{pre}_i$.
- We have seen that

$$\begin{aligned} \text{if} \qquad & x_i \perp\!\!\!\perp (\mathrm{pre}_i \setminus \pi_i) \mid \pi_i \text{ for all } i \\ \text{then} \qquad & p(x_1, \ldots, x_d) = \prod_{i=1}^{d} p(x_i|\pi_i) \end{aligned}$$

- The chain rule corresponds to the case where $\pi_i = \mathrm{pre}_i$.
- Do we also have the reverse?

$$\begin{aligned} \text{if} \qquad & p(x_1, \ldots, x_d) = \prod_{i=1}^{d} p(x_i|\pi_i) \quad \text{with } \pi_i \subseteq \mathrm{pre}_i \\ \text{then} \qquad & x_i \perp\!\!\!\perp (\mathrm{pre}_i \setminus \pi_i) \mid \pi_i \text{ for all } i\,? \end{aligned}$$

From factorisation to (conditional) independence

- Let us first check whether $x_d \perp\!\!\!\perp (\mathrm{pre}_d \setminus \pi_d) \mid \pi_d$ holds.
- We do that by checking whether

$$p(x_d | \overbrace{x_1, \ldots, x_{d-1}}^{\mathrm{pre}_d}) = p(x_d | \pi_d)$$

  holds.
- Since

$$p(x_d | x_1, \ldots, x_{d-1}) = \frac{p(x_1, \ldots, x_d)}{p(x_1, \ldots, x_{d-1})}$$

  we start with computing $p(x_1, \ldots, x_{d-1})$.

From factorisation to (conditional) independence

Assume that the x_i are ordered as $x_1, \ldots, x_d$ and that $p(x_1, \ldots, x_d) = \prod_{i=1}^{d} p(x_i|\pi_i)$ with $\pi_i \subseteq \mathrm{pre}_i$.

We compute $p(x_1, \ldots, x_{d-1})$ using the sum rule:

$$
\begin{aligned}
p(x_1, \ldots, x_{d-1}) &= \int p(x_1, \ldots, x_d) \mathrm{d}x_d \\
&= \int \prod_{i=1}^{d} p(x_i|\pi_i) \mathrm{d}x_d \\
&= \int \prod_{i=1}^{d-1} p(x_i|\pi_i) p(x_d|\pi_d) \mathrm{d}x_d \quad (x_d \notin \pi_i, i < d) \\
&= \prod_{i=1}^{d-1} p(x_i|\pi_i) \int p(x_d|\pi_d) \mathrm{d}x_d \\
&= \prod_{i=1}^{d-1} p(x_i|\pi_i)
\end{aligned}
$$

From factorisation to (conditional) independence

Hence:

$$
\begin{aligned}
p(x_d|x_1, \ldots, x_{d-1}) &= \frac{p(x_1, \ldots, x_d)}{p(x_1, \ldots, x_{d-1})} \\
&= \frac{\prod_{i=1}^{d} p(x_i|\pi_i)}{\prod_{i=1}^{d-1} p(x_i|\pi_i)} \\
&= p(x_d|\pi_d)
\end{aligned}
$$

And $p(x_d|x_1, \ldots, x_{d-1}) = p(x_d|\mathrm{pre}_d) = p(x_d|\pi_d)$ means that $x_d \perp\!\!\!\perp (\mathrm{pre}_d \setminus \pi_d) \mid \pi_d$ as desired.

$p(x_1, \ldots, x_{d-1})$ has the same form as $p(x_1, \ldots, x_d)$: apply same procedure to all $p(x_1, \ldots, x_k)$, for smaller and smaller $k \leq d-1$

Proves that

(1) $p(x_1, \ldots, x_k) = \prod_{i=1}^{k} p(x_i|\pi_i)$ and that

(2) factorisation implies $x_i \perp\!\!\!\perp (\mathrm{pre}_i \setminus \pi_i) \mid \pi_i$ for all i

Brief summary

- Let $\mathbf{x} = (x_1, \ldots, x_d)$ be a d-dimensional random vector with pdf/pmf $p(\mathbf{x})$.
- Denote the predecessors of x_i in the ordering by $\mathrm{pre}(x_i) = \mathrm{pre}_i = \{x_1, \ldots, x_{i-1}\}$, and let $\pi_i \subseteq \mathrm{pre}_i$.

$$p(\mathbf{x}) = \prod_{i=1}^{d} p(x_i|\pi_i) \Longleftrightarrow x_i \perp\!\!\!\perp (\mathrm{pre}_i \setminus \pi_i) \mid \pi_i \text{ for all } i$$

- Equivalence of factorisation and ordered Markov property of the pdf/pmf

Why does it matter?

- Denote the predecessors of x_i in the ordering by $\mathrm{pre}_i = \{x_1, \ldots, x_{i-1}\}$, and let $\pi_i \subseteq \mathrm{pre}_i$.

$$p(\mathbf{x}) = \prod_{i=1}^{d} p(x_i|\pi_i) \iff x_i \perp\!\!\!\perp (\mathrm{pre}_i \setminus \pi_i) \mid \pi_i \text{ for all } i$$

- Why does it matter?
  - Relatively strong result: It holds for sets of pdfs/pmfs and not only single instances
  - For all members of the set: Fewer numbers are needed for their representation (computational advantage)
  - Given the independencies, we know what form $p(\mathbf{x})$ must have (helpful for specifying models)
  - Increased understanding of the properties of the model (independencies and data generation mechanism)
  - Visualisation as a graph

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Program

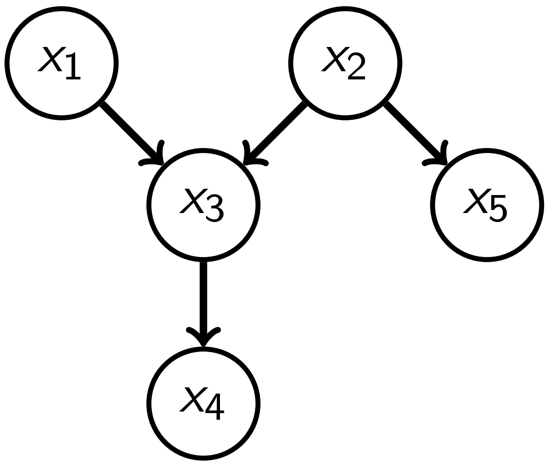
1. Equivalence of factorisation and ordered Markov property
2. Understanding models from their factorisation
   - Visualisation as a directed graph
   - Description of directed graphs and topological orderings

Visualisation as a directed graph

If $p(\mathbf{x}) = \prod_{i=1}^{d} p(x_i|\pi_i)$ with $\pi_i \subseteq \mathrm{pre}_i$ we can visualise the model as a graph with the random variables x_i as nodes, and directed edges that point from the $x_j \in \pi_i$ to the x_i. This results in a directed acyclic graph (DAG).

Example:

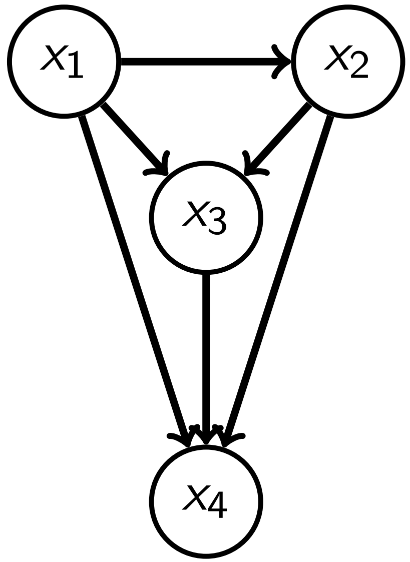
$$p(x_1, x_2, x_3, x_4, x_5) = p(x_1)p(x_2)p(x_3|x_1, x_2)p(x_4|x_3)p(x_5|x_2)$$



Visualisation as a directed graph

Example:

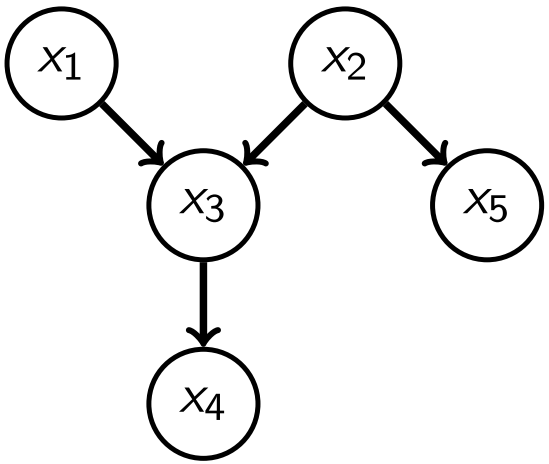
$$p(x_1, x_2, x_3, x_4) = p(x_1)p(x_2|x_1)p(x_3|x_1, x_2)p(x_4|x_1, x_2, x_3)$$



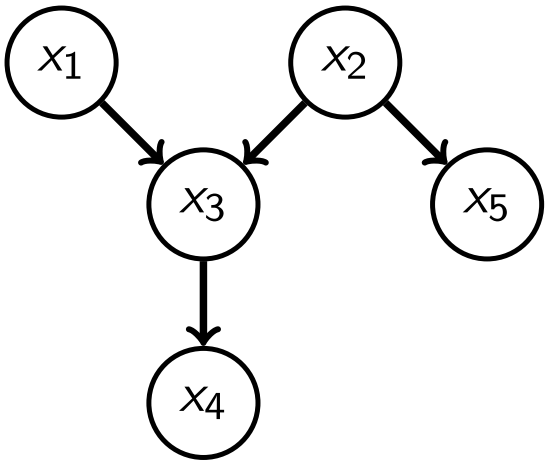
Factorisation obtained by chain rule $\equiv$ fully connected directed acyclic graph.

Graph concepts

- Directed graph: graph where all edges are directed
- Directed acyclic graph (DAG): by following the direction of the arrows you will never visit a node more than once
- x_i is a parent of x_j if there is a (directed) edge from x_i to x_j. The set of parents of x_i in the graph is denoted by $\mathrm{pa}(x_i) = \mathrm{pa}_i$, e.g. $\mathrm{pa}(x_3) = \mathrm{pa}_3 = \{x_1, x_2\}$.
- x_j is a child of x_i if $x_i \in \mathrm{pa}(x_j)$, e.g. x_3 and x_5 are children of x_2.

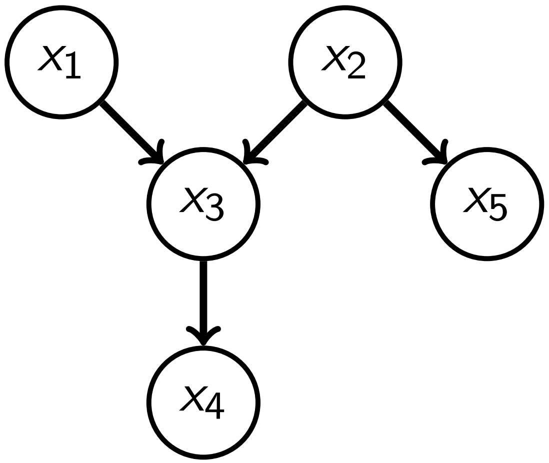


- A path or trail from x_i to x_j is a sequence of distinct connected nodes starting at x_i and ending at x_j. The direction of the arrows does *not* matter. For example: x_5, x_2, x_3, x_1 is a trail.
- A directed path is a sequence of connected nodes where we follow the direction of the arrows. For example: x_1, x_3, x_4 is a directed path. But x_5, x_2, x_3, x_1 is not a directed path.



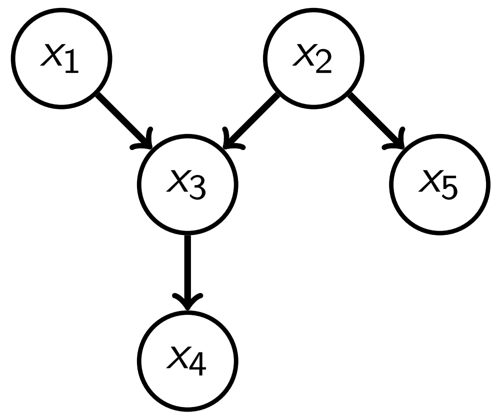
Graph concepts

- The ancestors $\mathrm{anc}(x_i)$ of x_i are all the nodes where a directed path leads to x_i. For example, $\mathrm{anc}(x_4) = \{x_1, x_3, x_2\}$.
- The descendants $\mathrm{desc}(x_i)$ of x_i are all the nodes that can be reached on a directed path from x_i. For example, $\mathrm{desc}(x_1) = \{x_3, x_4\}$.
  (Note: sometimes, x_i is included in the set of ancestors and descendants)
- The non-descendents of x_i are all the nodes in a graph without x_i and without the descendants of x_i. For example, $\mathrm{nondesc}(x_3) = \{x_1, x_2, x_5\}$



Graph concepts

- Topological ordering: an ordering $(x_1, \ldots, x_d)$ of some variables x_i is topological relative to a graph if parents come before their children in the ordering.
  (whenever there is a directed edge from x_i to x_j, x_i occurs prior to x_j in the ordering.)
- There is always at least one such ordering for DAGs.
- For a pdf $p(\mathbf{x})$, assume you order the random variables x_i in some manner and compute the corresponding factorisation, e.g. $p(\mathbf{x}) = p(x_1)p(x_2)p(x_3|x_1, x_2)p(x_4|x_3)p(x_5|x_2)$
- When you visualise the factorised pdf as a graph, the graph is always such that the ordering used for the factorisation is topological to it.
- The π_i in the factorisation are equal to the parents pa_i in the graph. We may call both sets the "parents" of x_i.



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