Undirected Graphical Models I

Definition and Basic Properties

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Recap

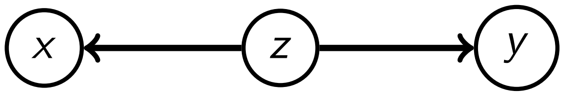
- The number of free parameters in probabilistic models increases with the number of random variables involved.
- Making statistical independence assumptions reduces the number of free parameters that need to be specified.
- Starting with the chain rule and an ordering of the random variables, we used statistical independencies to simplify the representation.
- We thus obtained a factorisation in terms of a product of conditional pdfs that we visualised as a DAG.
- In turn, we used DAGs to define sets of distributions ("directed graphical models").
- We discussed independence properties satisfied by the distributions, d-separation, and the equivalence to the factorisation.

The directionality in directed graphical models

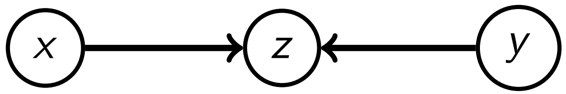
- So far we mainly exploited the property

$$\mathbf{x} \perp\!\!\!\perp \mathbf{y} \mid \mathbf{z} \Longleftrightarrow p(\mathbf{x}, \mathbf{y}|\mathbf{z}) = p(\mathbf{x}|\mathbf{z})p(\mathbf{y}|\mathbf{z})$$

- But when working with $p(\mathbf{x}, \mathbf{y}|\mathbf{z})$ we impose an ordering or directionality from $\mathbf{z}$ to $\mathbf{x}$ and $\mathbf{y}$.
- Directionality matters in directed graphical models



versus



- In some cases, directionality is natural but in others we do not want to choose one direction over another.
- We now discuss how to visualise and represent probability distributions and independencies in a symmetric manner without assuming a directionality or ordering of the variables.

Program

1. Visualising factorisations with undirected graphs
2. Undirected graphical models

Program

1. Visualising factorisations with undirected graphs
   - Undirected characterisation of statistical independence
   - Gibbs distributions
   - Visualising Gibbs distributions with undirected graphs

2. Undirected graphical models

Further characterisation of statistical independence

- For non-negative functions $a(\mathbf{x}, \mathbf{z}), b(\mathbf{y}, \mathbf{z})$:

$$\mathbf{x} \perp\!\!\!\perp \mathbf{y} \mid \mathbf{z} \Longleftrightarrow p(\mathbf{x}, \mathbf{y}, \mathbf{z}) = a(\mathbf{x}, \mathbf{z}) b(\mathbf{y}, \mathbf{z})$$

  (see below for proof)
- Equivalent to $p(\mathbf{x}, \mathbf{y}, \mathbf{z}) = p(\mathbf{x}|\mathbf{z}) p(\mathbf{y}|\mathbf{z}) p(\mathbf{z})$ but does not assume that the factors are (conditional) pdfs/pmfs.
- No directionality or ordering of the variables is imposed.
- Unconditional version: For non-negative functions $a(\mathbf{x}), b(\mathbf{y})$:

$$\mathbf{x} \perp\!\!\!\perp \mathbf{y} \Longleftrightarrow p(\mathbf{x}, \mathbf{y}) = a(\mathbf{x}) b(\mathbf{y})$$

- The important point is the factorisation of $p(\mathbf{x}, \mathbf{y}, \mathbf{z})$ into two non-negative factors:
  - if the factors share a variable $\mathbf{z}$, then we have conditional independence,
  - if not, we have unconditional independence.

Proof for $p(\mathbf{x}, \mathbf{y}, \mathbf{z}) = a(\mathbf{x}, \mathbf{z})b(\mathbf{y}, \mathbf{z}) \iff \mathbf{x} \perp\!\!\!\perp \mathbf{y} \mid \mathbf{z}$

We prove the equivalence for pmfs. For pdfs, the arguments stay the same, we just replace the sums with integrals.

The proof uses the sum rule (SR) and the product rule (PR).

$\Rightarrow$ Assume $p(\mathbf{x}, \mathbf{y}, \mathbf{z}) = a(\mathbf{x}, \mathbf{z})b(\mathbf{y}, \mathbf{z})$ $(*)$

$$
\begin{aligned}
p(\mathbf{x}, \mathbf{z}) &\overset{(SR)}{=} \sum_{\mathbf{y}} p(\mathbf{x}, \mathbf{y}, \mathbf{z}) \overset{(*)}{=} \sum_{\mathbf{y}} a(\mathbf{x}, \mathbf{z})b(\mathbf{y}, \mathbf{z}) \\
&= a(\mathbf{x}, \mathbf{z}) \sum_{\mathbf{y}} b(\mathbf{y}, \mathbf{z}) = a(\mathbf{x}, \mathbf{z})\tilde{b}(\mathbf{z}) \\
p(\mathbf{y}, \mathbf{z}) &\overset{(SR)}{=} \sum_{\mathbf{x}} p(\mathbf{x}, \mathbf{y}, \mathbf{z}) \overset{(*)}{=} \sum_{\mathbf{x}} a(\mathbf{x}, \mathbf{z})b(\mathbf{y}, \mathbf{z}) \\
&= b(\mathbf{y}, \mathbf{z}) \sum_{\mathbf{x}} a(\mathbf{x}, \mathbf{z}) = b(\mathbf{y}, \mathbf{z})\tilde{a}(\mathbf{z}) \\
p(\mathbf{z}) &\overset{(SR)}{=} \sum_{\mathbf{y}} p(\mathbf{y}, \mathbf{z}) = \tilde{a}(\mathbf{z}) \sum_{\mathbf{y}} b(\mathbf{y}, \mathbf{z}) = \tilde{a}(\mathbf{z})\tilde{b}(\mathbf{z})
\end{aligned}
$$

Assume $p(\mathbf{z}) > 0$, then $\tilde{a}(\mathbf{z}) > 0, \tilde{b}(\mathbf{z}) > 0$ and

$$a(\mathbf{x}, \mathbf{z}) = \frac{p(\mathbf{x}, \mathbf{z})}{\tilde{b}(\mathbf{z})}, \qquad b(\mathbf{y}, \mathbf{z}) = \frac{p(\mathbf{y}, \mathbf{z})}{\tilde{a}(\mathbf{z})}$$

Hence

$$\begin{aligned}
p(\mathbf{x}, \mathbf{y}, \mathbf{z}) &\overset{(*)}{=} a(\mathbf{x}, \mathbf{z}) b(\mathbf{y}, \mathbf{z}) && (1)\\
&= \frac{p(\mathbf{x}, \mathbf{z})}{\tilde{b}(\mathbf{z})} \frac{p(\mathbf{y}, \mathbf{z})}{\tilde{a}(\mathbf{z})} && (2)\\
&= \frac{p(\mathbf{x}, \mathbf{z}) p(\mathbf{y}, \mathbf{z})}{p(\mathbf{z})} && (3)\\
&\overset{(PR)}{=} \frac{p(\mathbf{x}|\mathbf{z}) p(\mathbf{z}) p(\mathbf{y}|\mathbf{z}) p(\mathbf{z})}{p(\mathbf{z})} && (4)\\
&= p(\mathbf{x}|\mathbf{z}) p(\mathbf{y}|\mathbf{z}) p(\mathbf{z}) && (5)
\end{aligned}$$

and thus

$$p(\mathbf{x}, \mathbf{y}|\mathbf{z}) = p(\mathbf{x}|\mathbf{z}) p(\mathbf{y}|\mathbf{z}) \quad (\text{for } p(\mathbf{z}) > 0) \qquad (6)$$

which was one of our initial criteria for $\mathbf{x} \perp\!\!\!\perp \mathbf{y} \mid \mathbf{z}$.

$\Leftarrow$ Assume $\mathbf{x} \perp\!\!\!\perp \mathbf{y} \mid \mathbf{z}$.

We thus have $p(\mathbf{x}, \mathbf{y}, \mathbf{z}) = p(\mathbf{z})p(\mathbf{x}|\mathbf{z})p(\mathbf{y}|\mathbf{z})$

- Identify $a(\mathbf{x}, \mathbf{z}) = p(\mathbf{z})p(\mathbf{x}|\mathbf{z})$ and $b(\mathbf{y}, \mathbf{z}) = p(\mathbf{y}|\mathbf{z})$,
- Or, $a(\mathbf{x}, \mathbf{z}) = p(\mathbf{x}|\mathbf{z})$ and $b(\mathbf{y}, \mathbf{z}) = p(\mathbf{z})p(\mathbf{y}|\mathbf{z})$,
- Or, $a(\mathbf{x}, \mathbf{z}) = p^{1/2}(\mathbf{z})p(\mathbf{x}|\mathbf{z})$ and $b(\mathbf{y}, \mathbf{z}) = p^{1/2}(\mathbf{z})p(\mathbf{y}|\mathbf{z})$,
- etc.

Reformulation to ensure normalisation

- Since $p(\mathbf{x}, \mathbf{y}, \mathbf{z})$ must sum (integrate) to one, we must have

$$\sum_{\mathbf{x},\mathbf{y},\mathbf{z}} a(\mathbf{x}, \mathbf{z}) b(\mathbf{y}, \mathbf{z}) = 1$$

- Normalisation condition often ensured by re-defining $a(\mathbf{x}, \mathbf{z}) b(\mathbf{y}, \mathbf{z})$: we have $\mathbf{x} \perp\!\!\!\perp \mathbf{y} \mid \mathbf{z}$ iff

$$p(\mathbf{x}, \mathbf{y}, \mathbf{z}) = \frac{1}{Z} \phi_A(\mathbf{x}, \mathbf{z}) \phi_B(\mathbf{y}, \mathbf{z}) \qquad Z = \sum_{\mathbf{x},\mathbf{y},\mathbf{z}} \phi_A(\mathbf{x}, \mathbf{z}) \phi_B(\mathbf{y}, \mathbf{z})$$

- Z: normalisation constant (related to partition function, see later)
- ϕ_i: factors (also called potential functions).
  Do generally not correspond to (conditional) pdfs/pmfs.
- Key point remains the same: conditional independence if the factors share a variable $\mathbf{z}$.

What does it mean?

$$\mathbf{x} \perp\!\!\!\perp \mathbf{y} \mid \mathbf{z} \iff p(\mathbf{x}, \mathbf{y}, \mathbf{z}) = \frac{1}{Z}\phi_A(\mathbf{x}, \mathbf{z})\phi_B(\mathbf{y}, \mathbf{z})$$

"$\Rightarrow$" If we want our model to satisfy $\mathbf{x} \perp\!\!\!\perp \mathbf{y} \mid \mathbf{z}$ we should write the pdf (pmf) as

$$p(\mathbf{x}, \mathbf{y}, \mathbf{z}) \propto \phi_A(\mathbf{x}, \mathbf{z})\phi_B(\mathbf{y}, \mathbf{z})$$

"$\Leftarrow$" If the pdf (pmf) can be written as

$$p(\mathbf{x}, \mathbf{y}, \mathbf{z}) \propto \phi_A(\mathbf{x}, \mathbf{z})\phi_B(\mathbf{y}, \mathbf{z})$$

then we have $\mathbf{x} \perp\!\!\!\perp \mathbf{y} \mid \mathbf{z}$

equivalent for unconditional version

Example

Consider $p(x_1, x_2, x_3, x_4) \propto \phi_1(x_1, x_2)\phi_2(x_2, x_3)\phi_3(x_4)$

What independencies does p satisfy?

- We can write

$$
\begin{aligned}
p(x_1, x_2, x_3, x_4) &\propto \underbrace{[\phi_1(x_1, x_2)\phi_2(x_2, x_3)]}_{\tilde{\phi}_1(x_1, x_2, x_3)}[\phi_3(x_4)] \\
&\propto \tilde{\phi}_1(x_1, x_2, x_3)\phi_3(x_4)
\end{aligned}
$$

  so that $x_4 \perp\!\!\!\perp x_1, x_2, x_3$.

- Integrating out x_4 gives

$$
p(x_1, x_2, x_3) = \int p(x_1, x_2, x_3, x_4)\mathrm{d}x_4 \propto \phi_1(x_1, x_2)\phi_2(x_2, x_3)
$$

  so that $x_1 \perp\!\!\!\perp x_3 \mid x_2$

Gibbs distributions

- Example is a special case of a class of pdfs/pmfs that factorise as
$$p(x_1, \ldots, x_d) = \frac{1}{Z} \prod_c \phi_c(\mathcal{X}_c)$$
  - $\mathcal{X}_c \subseteq \{x_1, \ldots, x_d\}$
  - ϕ_c are non-negative factors (potential functions)
    Do generally not correspond to (conditional) pdfs/pmfs.
    They measure "compatibility", "agreement", or "affinity"
  - Z is a normalising constant so that $p(x_1, \ldots, x_d)$ integrates (sums) to one.
- Known as Gibbs (or Boltzmann) distributions
- $\tilde{p}(x_1, \ldots, x_d) = \prod_c \phi_c(\mathcal{X}_c)$ is said to be an unnormalised model: $\tilde{p} \geq 0$ but does not necessarily integrate (sum) to one.

Energy-based model

- With $\phi_c(\mathcal{X}_c) = \exp\left(-E_c(\mathcal{X}_c)\right)$, we have equivalently

$$p(x_1, \ldots, x_d) = \frac{1}{Z} \exp\left[-\sum_c E_c(\mathcal{X}_c)\right]$$

- $\sum_c E_c(\mathcal{X}_c)$ is the energy of the configuration $(x_1, \ldots, x_d)$.
  low energy $\iff$ high probability

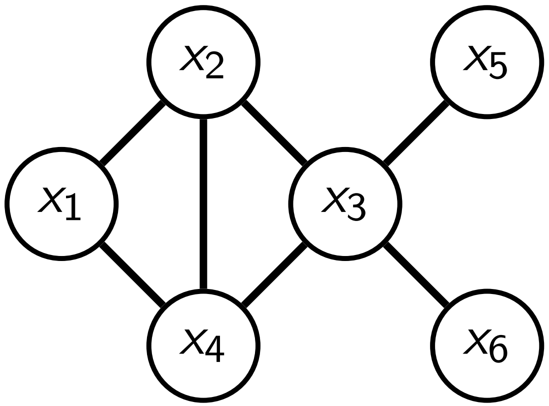
Visualising Gibbs distributions with undirected graphs

$p(x_1, \ldots, x_d) \propto \prod_c \phi_c(\mathcal{X}_c)$

- Node for each x_i
- For all factors ϕ_c: draw an undirected edge between all x_i and x_j that belong to $\mathcal{X}_c$
- Results in a fully-connected subgraph for all x_i that are part of the same factor (this subgraph is called a clique).

Example:

Graph for $p(x_1, \ldots, x_6) \propto \phi_1(x_1, x_2, x_4)\phi_2(x_2, x_3, x_4)\phi_3(x_3, x_5)\phi_4(x_3, x_6)$



Program

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   - Undirected characterisation of statistical independence
   - Gibbs distributions
   - Visualising Gibbs distributions with undirected graphs

2. Undirected graphical models

Program

1. Visualising factorisations with undirected graphs

2. Undirected graphical models
   - Definition
   - Examples
   - Conditionals, marginals, and change of measure (tilting)

Undirected graphical models (UGMs)

- We started with a factorised pdf/pmf and associated a undirected graph with it. We now go the other way around and start with an undirected graph.
- *Definition* An undirected graphical model based on an undirected graph H with d nodes and associated random variables x_i is the set of pdfs/pmfs that factorise as

$$p(x_1, \ldots, x_d) = \frac{1}{Z} \prod_c \phi_c(\mathcal{X}_c)$$

  where Z is the normalisation constant, $\phi_c(\mathcal{X}_c) \geq 0$, and the $\mathcal{X}_c$ correspond to the maximal cliques in the graph.
- Remark: a pdf/pmf $p(x_1, \ldots, x_d)$ that can be written as above is said to "factorise over the graph H". We say that it has property $F(H)$ ("F" for factorisation).

Remarks

- An undirected graph defines the pdfs/pmfs in terms of Gibbs distributions.
- The undirected graphical model corresponds to a set of probability distributions . This is because, like in DGMs, we did not specify any numerical values for the factors $\phi_c(\mathcal{X}_c)$. We only specified which variables the factors take as input.
- Individual pdfs/pmf in the set are typically also called a undirected graphical model.
- Other names for an undirected graphical model: Markov network (MN), Markov random field (MRF)
- The $\mathcal{X}_c$ form maximal cliques in the graph.

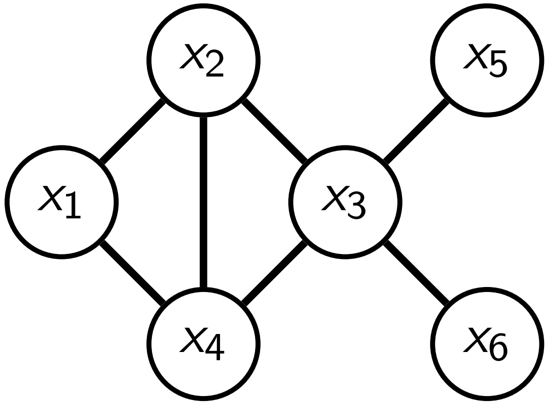
  Maximal clique: a set of fully connected nodes (clique) that is not contained in another clique.

Why maximal cliques?

- The mapping from Gibbs distribution to graph is many to one. We may obtain the same graph for different Gibbs distributions, e.g.

$$p(\mathbf{x}) \propto \phi_1(x_1, x_2, x_4)\phi_2(x_2, x_3, x_4)\phi_3(x_3, x_5)\phi_4(x_3, x_6)$$

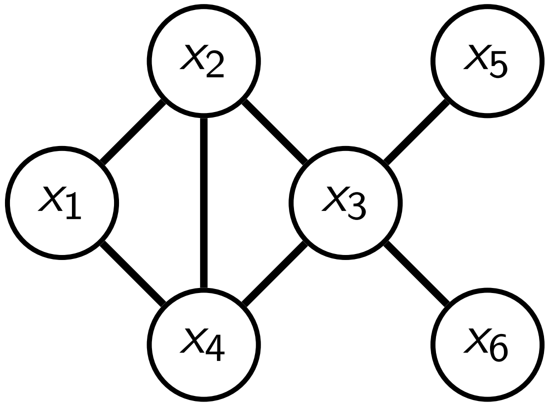
$$p(\mathbf{x}) \propto \tilde{\phi}_1(x_1, x_2)\tilde{\phi}_2(x_1, x_4)\tilde{\phi}_3(x_2, x_4)\tilde{\phi}_4(x_2, x_3)\tilde{\phi}_5(x_3, x_4)\tilde{\phi}_6(x_3, x_5)\tilde{\phi}_7(x_3, x_6)$$



- By using maximal cliques, we take a conservative approach and do not make additional assumptions on the factorisation.

Example

Undirected graph:



Random variables: $\mathbf{x} = (x_1, \ldots, x_6)$

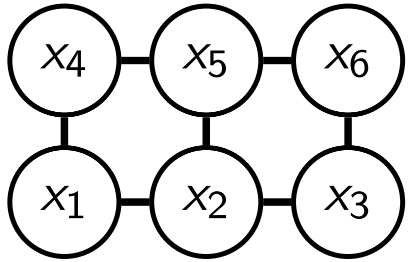
Maximal cliques: $\{x_1, x_2, x_4\}, \quad \{x_2, x_3, x_4\}, \quad \{x_3, x_5\}, \quad \{x_3, x_6\}$

Undirected graphical model: set of pdfs/pmfs $p(\mathbf{x})$ that factorise as:

$$
\begin{aligned}
p(\mathbf{x}) &= \frac{1}{Z}\phi_1(x_1, x_2, x_4)\phi_2(x_2, x_3, x_4)\phi_3(x_3, x_5)\phi_4(x_3, x_6) \\
&\propto \phi_1(x_1, x_2, x_4)\phi_2(x_2, x_3, x_4)\phi_3(x_3, x_5)\phi_4(x_3, x_6)
\end{aligned}
$$

Example (pairwise Markov network)

Graph:



Random variables: $\mathbf{x} = (x_1, \ldots, x_6)$

Maximal cliques: all neighbours

$\{x_1, x_2\}$ $\{x_2, x_3\}$ $\{x_4, x_5\}$ $\{x_5, x_6\}$ $\{x_1, x_4\}$ $\{x_2, x_5\}$ $\{x_3, x_6\}$

Undirected graphical model: set of pdfs/pmfs $p(\mathbf{x})$ that factorise as:

$$p(\mathbf{x}) \propto \phi_1(x_1, x_2)\phi_2(x_2, x_3)\phi_3(x_4, x_5)\phi_4(x_5, x_6)\phi_5(x_1, x_4)\phi_6(x_2, x_5)\phi_7(x_3, x_6)$$

This is an example of a pairwise Markov network.

Classical instances of pairwise Markov networks

- For pairwise Markov networks, the functional form of the factors is not constrained, and neither is the domain of $\mathbf{x}$.
- They can thus represent a large number of different distributions.
- Classical instances are the multivariate Gaussian distribution for continuous variables and the Boltzmann machine (Ising model) for binary variables.

Multivariate Gaussians are pairwise Markov networks

- The pdf of multivariate Gaussian is

$$p(\mathbf{x}) = \frac{1}{\sqrt{(2\pi)^n \det(\boldsymbol{\Sigma})}} \exp\left(-\frac{1}{2}(\mathbf{x}-\boldsymbol{\mu})^\top \boldsymbol{\Sigma}^{-1}(\mathbf{x}-\boldsymbol{\mu})\right) \tag{7}$$

- Re-writing the quadratic term in the exponential gives

$$\begin{aligned}
(\mathbf{x}-\boldsymbol{\mu})^\top \boldsymbol{\Sigma}^{-1}(\mathbf{x}-\boldsymbol{\mu}) &= (\mathbf{x}-\boldsymbol{\mu})^\top \boldsymbol{\Lambda}(\mathbf{x}-\boldsymbol{\mu}) && (8)\\
&= \mathbf{x}^\top\boldsymbol{\Lambda}\mathbf{x} - \mathbf{x}^\top\boldsymbol{\Lambda}\boldsymbol{\mu} - \boldsymbol{\mu}^\top\boldsymbol{\Lambda}\mathbf{x} + \boldsymbol{\mu}^\top\boldsymbol{\mu} && (9)\\
&= \mathbf{x}^\top\boldsymbol{\Lambda}\mathbf{x} - 2\mathbf{x}^\top\boldsymbol{\Lambda}\boldsymbol{\mu} + \boldsymbol{\mu}^\top\boldsymbol{\mu} && (10)\\
&= \mathbf{x}^\top\boldsymbol{\Lambda}\mathbf{x} - 2\mathbf{x}^\top\mathbf{b} + \boldsymbol{\mu}^\top\boldsymbol{\mu} && (11)
\end{aligned}$$

with $\mathbf{b} = \boldsymbol{\Lambda}\boldsymbol{\mu}$ and where we have used that $\boldsymbol{\Lambda} = \boldsymbol{\Sigma}^{-1}$ is symmetric.

Multivariate Gaussians are pairwise Markov networks

- Hence

$$p(\mathbf{x}) \propto \exp\left(-\frac{1}{2}\mathbf{x}^\top \boldsymbol{\Lambda}\mathbf{x} + \mathbf{x}^\top \mathbf{b} - \frac{1}{2}\boldsymbol{\mu}^\top \boldsymbol{\mu}\right) \tag{12}$$

$$\propto \exp\left(-\frac{1}{2}\mathbf{x}^\top \boldsymbol{\Lambda}\mathbf{x} + \mathbf{x}^\top \mathbf{b}\right) \tag{13}$$

$$\propto \exp\left(-\frac{1}{2}\sum_{ij} \lambda_{ij} x_i x_j + \sum_i x_i b_i\right) \tag{14}$$

$$\propto \prod_{ij} \exp\left(-\frac{1}{2}\lambda_{ij} x_i x_j\right) \prod_i \exp\left(x_i b_i\right) \tag{15}$$

- Visualising the distribution as an undirected graph shows that it is a pairwise Markov network.

Boltzmann machines are pairwise Markov networks

- The Boltzmann machine has exactly the same expression, but the variables are binary

$$p(\mathbf{x}) \propto \exp\left(-\frac{1}{2}\sum_{ij}\lambda_{ij}x_ix_j + \sum_i x_i b_i\right) \quad x_i \in \{0,1\} \quad (16)$$

  where (as for Gaussians) $\lambda_{ij} = \lambda_{ji}$
- Properties have been extensively studied in physics
- Have been used by Hopfield and Hinton to model associative memory and to find patterns in large data sets (Nobel Prize in Physics 2024).

  Talk by Hinton, April 2025: `https://informatics.ed.ac.uk/news-events/events/informatics-distinguished-lectures/professor-geoffrey-hinton-distinguished`

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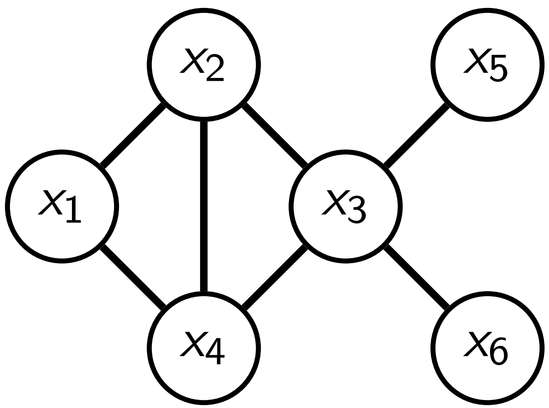
Conditionals

- For DGMs, the factors $k(x_i|\mathrm{pa}_i)$ defining $p(\mathbf{x})$ are the conditional pdfs/pmfs of x_i given pa_i under $p(\mathbf{x})$, i.e. $p(x_i|\mathrm{pa}_i)$. We do not have such a correspondence for UGMs.
- But conditioning on random variables corresponds to a simple graph operation: removing their nodes from the graph.
- Example: For $p(x_1, \ldots, x_6)$ specified by the graph below, what is $p(x_1, x_2, x_4, x_5, x_6|x_3 = \alpha)$?



Conditionals

- The graph specifies the factorisation

$$p(x_1, \ldots, x_6) \propto \phi_1(x_1, x_2, x_4)\phi_2(x_2, x_3, x_4)\phi_3(x_3, x_5)\phi_4(x_3, x_6)$$

- By definition: $p(x_1, x_2, x_4, x_5, x_6 | x_3 = \alpha)$

$$\begin{aligned}
&= \frac{p(x_1, x_2, x_3 = \alpha, x_4, x_5, x_6)}{\int p(x_1, x_2, x_3 = \alpha, x_4, x_5, x_6) \mathrm{d}x_1 \mathrm{d}x_2 \mathrm{d}x_4 \mathrm{d}x_5 \mathrm{d}x_6} \\
&= \frac{\phi_1(x_1, x_2, x_4)\phi_2(x_2, \alpha, x_4)\phi_3(\alpha, x_5)\phi_4(\alpha, x_6)}{\int \phi_1(x_1, x_2, x_4)\phi_2(x_2, \alpha, x_4)\phi_3(\alpha, x_5)\phi_4(\alpha, x_6) \mathrm{d}x_1 \mathrm{d}x_2 \mathrm{d}x_4 \mathrm{d}x_5 \mathrm{d}x_6} \\
&= \frac{1}{Z(\alpha)} \phi_1(x_1, x_2, x_4)\phi_2^\alpha(x_2, x_4)\phi_3^\alpha(x_5)\phi_4^\alpha(x_6)
\end{aligned}$$

- Gibbs distribution with derived factors ϕ_i^α of reduced domain and new normalisation "constant" $Z(\alpha)$
- Note that $Z(\alpha)$ depends on the conditioning value α.

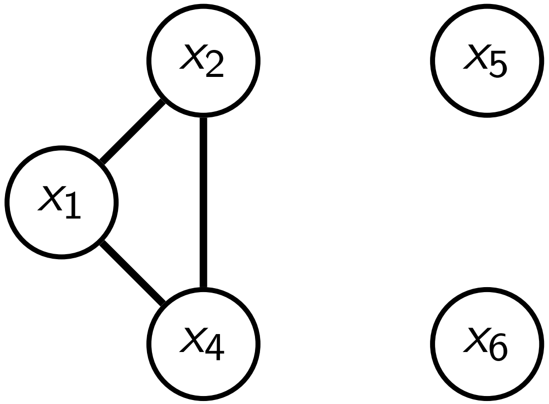
Conditionals

Let $p(x_1, \ldots, x_6) \propto \phi_1(x_1, x_2, x_4)\phi_2(x_2, x_3, x_4)\phi_3(x_3, x_5)\phi_4(x_3, x_6)$.

- Conditional $p(x_1, x_2, x_4, x_5, x_6 | x_3 = \alpha)$ is

$$\frac{1}{Z(\alpha)}\phi_1(x_1, x_2, x_4)\phi_2^\alpha(x_2, x_4)\phi_3^\alpha(x_5)\phi_4^\alpha(x_6)$$

- Conditioning on variables removes the corresponding nodes and connecting edges from the undirected graph



Marginals

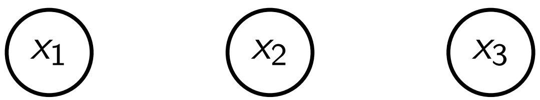
- For DGMs, the product of the first j terms in the factorisation, $\prod_{i=1}^{j} p(x_i|\mathrm{pa}_i)$, equaled the marginal $p(x_1, \ldots, x_j)$.
- UGMs do not have such a general property. But we can exploit the factorisation when computing the marginals.
- Will be the discussed in the "inference part" of the course.

Change of measure (tilting)

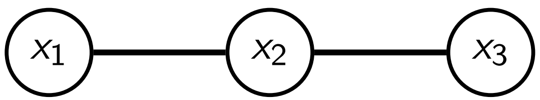
- A way to create new pdf/pmfs is to reweight existing ones, which is a special instance of a "change of measure" also called "tilting".
- For example, assume $q(x_1, x_2, x_3) = \prod_i q_i(x_i)$ to be a given pmf. We want to generate a new pmf that assigns higher probabilities to $(x_1, x_2) \in A$, and to $(x_2, x_3) \in B$, for some sets A and B.
- We can thus define the Gibbs distribution

$$p(\mathbf{x}) = \frac{1}{Z}\phi_A(x_1, x_2)\phi_B(x_2, x_3)\prod_{i=1}^{3} q_i(x_i)$$

where $\phi_A(x_1, x_2) = 1$ for $(x_1, x_2) \notin A$, $\phi_A(x_1, x_2) > 1$ for $(x_1, x_2) \in A$, and equivalently for ϕ_B.



graph for $q(\mathbf{x})$



graph for $p(\mathbf{x})$

Change of measure (tilting)

- Similarly, we can think that an undirected graph defines how a base distribution, e.g. $q(\mathbf{x}) = \prod_i q_i(x_i)$, should be reweighted by factors $\phi_c(\mathcal{X}_c)$, thus defining a change of measure.
- Two different ways of defining models: Reweighting for UGMs vs data generation for DGMs.
- Reweighting is clear when computing expectations, e.g.

$$\begin{aligned}
\mathbb{E}_p[h] &= \sum_{\mathbf{x}} h(\mathbf{x})p(\mathbf{x}) \\
&= \frac{1}{Z} \sum_{x_1,x_2,x_3} h(x_1,x_2,x_3)\phi_A(x_1,x_2)\phi_B(x_2,x_3) \prod_i q_i(x_i) \\
&= \frac{1}{Z} \mathbb{E}_q[h\phi_A\phi_B]
\end{aligned}$$

- Since $Z = \sum_{x_1,x_2,x_3} \phi_A(x_1,x_2)\phi_B(x_2,x_3) \prod_i q_i(x_i) = \mathbb{E}_q[\phi_A\phi_B]$

$$\mathbb{E}_p[h] = \frac{\mathbb{E}_q[h\phi_A\phi_B]}{\mathbb{E}_q[\phi_A\phi_B]}$$

Change of measure

Program recap

1. Visualising factorisations with undirected graphs
    - Undirected characterisation of statistical independence
    - Gibbs distributions
    - Visualising Gibbs distributions with undirected graphs

2. Undirected graphical models
    - Definition
    - Examples
    - Conditionals, marginals, and change of measure (tilting)