Institute of Neural Information Processing | Ulm University

# LEARNING IN GRAPHICAL MODELS

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# RECAP: PROBABILITY CALCULUS

# PROBABILITY DISTRIBUTIONS IN ONE DIMENSION

For a finite set $\Omega = \{\omega_1, \dots, \omega_N\}$, we call any function $p : \Omega \to [0, 1]$ with the property

$$\sum_{i=1}^{N} p(\omega_i) = 1$$

a **probability distribution** on $\Omega$, and $p(\omega)$ is the *probability of* $\omega \in \Omega$.

Similarly, any non-negative function $f : \mathbb{R} \to \mathbb{R}_+$ with $\int_{\mathbb{R}} f(x)\, dx = 1$ is called a **probability density** on $\mathbb{R}$, where for any subset $A \subset \mathbb{R}$, the integral $p(A) := \int_A f(x)\, dx$ is the probability of $A$.

Examples:

- $p(\omega) = \frac{1}{N}$ for all $\omega \in \{\omega_1, \dots, \omega_N\}$ (*uniform* distribution)
- $p(\omega) = \delta_{\omega,\omega_0}$ for some fixed $\omega_0 \in \{\omega_1, \dots, \omega_N\}$ (*Dirac* distribution)
- $f(x) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-(x-\mu)^2/(2\sigma^2)}$ (*Gaussian* density)
- $f(x) = \lambda e^{-\lambda x}$ for all $x \geq 0, \lambda > 0$ (*Exponential* density)

**Note:** For distributions on countable sets $\Omega = \{\omega_1, \omega_2, \dots\}$, one also writes $p_i := p(\omega_i)$ for all $i$.

# PROBABILITY DISTRIBUTIONS IN MULTIPLE DIMENSIONS

Probability distributions on cartesian products $\Omega^n = \Omega \times \cdots \times \Omega$ of a finite set $\Omega$ are functions $p : \Omega^n \to [0, 1]$ such that $\sum_{i,\ldots,j} p(\omega_i, \ldots, \omega_j) = 1$ (and analogously for products of differing sets), also known as **multivariate distributions**.

Similarly, **multivariate probability densities** $f$ are probability densities on $\mathbb{R}^d$, i.e. $f : \mathbb{R}^d \to \mathbb{R}_+$ such that $\int_{\mathbb{R}^d} f(x_1, \ldots, x_d)\, dx^d = 1$.

Examples:

- $p(\omega, \omega') = \frac{1}{N^2}$ where $N = |\Omega|$ (*uniform distribution on* $\Omega \times \Omega$)
- $p(\omega, \omega') = p_1(\omega)p_2(\omega')$ (*products* of one-dimensional distributions $p_1, p_2$)
- $p(\mathbf{n}) = \frac{(\sum_{i=1}^k n_i)!}{n_1! \cdots n_k!} p_1^{n_1} \cdots p_k^{n_k}$ for $\mathbf{n} = (n_1, \ldots, n_k) \in \mathbb{N}^k$ (*Multinomial distribution*)
- $f(\mathbf{x}) = \frac{1}{\sqrt{(2\pi)^d \det(\Sigma)}} e^{-(\mathbf{x}-\mu)\Sigma^{-1}(\mathbf{x}-\mu)/2}$ for $\mathbf{x} = (x_1, \ldots, x_d) \in \mathbb{R}^d$ (*Multivariate Gaussian*)

# GENERALIZATION: PROBABILITY MEASURE

Consider the example of rolling a die with uniform probability $p(\omega) = \frac{1}{6}$ for all $\omega \in \Omega = \{1, \ldots, 6\}$. What is the probability of rolling an even number?

Since there are only two possibilities, even and odd, with equal counts, it is intuitively obvious that $\text{Prob}(\text{even}) = \frac{1}{2}$. But how would we calculate it in situations where we do not have an intuition?

Any probability distribution is an instance of a **probability measure** $\mathbb{P}$, which, by definition, maps sets $A$ to numbers $\mathbb{P}(A)$ between $0$ and $1$, with the extra property that

$$\mathbb{P}\Big(\bigcup_i A_i\Big) = \sum_i \mathbb{P}(A_i)$$

for any family of disjoint sets $A_i$.

Therefore, since $\text{even} = \{2, 4, 6\} = \{2\} \cup \{4\} \cup \{6\}$, we have

$$p(\text{even}) = p(2) + p(4) + p(6) = \frac{3}{6} = \frac{1}{2}$$

## RANDOM EXPERIMENTS

A **random experiment** is a trial with unknown outcome. The collection of all possible outcomes of such an experiment is called a **sample space**, often denoted by the letter $\Omega$.

For example:

- *Tossing a coin:* $\Omega = \{\text{heads}, \text{tails}\}$
- *Rolling a die:* $\Omega = \{1, 2, 3, 4, 5, 6\}$
- *Pick a card from a deck of* $52$ *cards:* $\Omega = \{\text{ace of clubs}, \ldots, \text{king of spades}\}$.
- *Observe the number of electric cars sold in a day:* $\Omega = \mathbb{N}$

## EVENTS

An event is a **subset $A \subset \Omega$ of a sample space $\Omega$**, i.e. a set of possible outcomes of a random experiment.

For example:

- $A =$ "the coin toss yields heads" $= \{\text{heads}\}$
- $A =$ "the die shows an even number" $= \{2, 4, 6\}$
- $A =$ "the card is red" $= \{\text{ace of diamonds}, \ldots, \text{king of hearts}\}$ (26 cards)
- $A =$ "the number of electric cars sold in a day is between 50 and 100" $= \{50, \ldots, 100\}$

The set of all allowed events (a so-called *sigma algebra*) is usually denoted by $\Sigma$. A common example is the **power set** $2^{\Omega}$, i.e. the set of all subsets of $\Omega$.

# PROBABILITY SPACE

A probability space is a triple $(\Omega, \Sigma, \mathbb{P})$, consisting of a **sample space** $\Omega$, a **set of events** $\Sigma$, and a **probability measure** $\mathbb{P}$, assigning probabilities $\mathbb{P}(A)$ to all events $A \in \Sigma$.

For example:

- *Rolling a die:* $(\Omega, \Sigma, \mathbb{P}) = (\{1, \dots, 6\}, 2^{\{1,\dots,6\}}, \mathbb{P})$, where $\mathbb{P}(\omega) = \frac{1}{6}\ \forall \omega = 1, \dots, 6$.
- *Tossing a biased coin twice:* $(\Omega, \Sigma, \mathbb{P})$ with $\Omega = \{HH, HT, TH, TT\}$,

  $$\Sigma = \{\emptyset, \{HH\}, \dots, \{TT\}, \{HH, HT\}, \dots, \{TH, TT\}, \{HH, HT, TH\}, \dots, \Omega\}$$

  and for $\omega = (\omega_0, \omega_1)$ with $\omega_i \in \{H, T\}$, we have $\mathbb{P}(\omega) = p(\omega_0) \cdot p(\omega_1)$, where $p$ is the probability distribution over $\{H, T\}$, given by $p(H) = b$ and $p(T) = 1 - b$ for some bias $b \in [0, 1]$.

**Note:** For the rest of the lecture, we always assume that a sample space $\Omega$ is part of a given probability space with probability measure $\mathbb{P}$ even if we do not explicitly mention it.

# RANDOM VARIABLES

A random variable is a **function from a sample space $\Omega$ to** (usually, real) **numbers**.

Examples:

- *Rolling a die:* $X : \Omega \to \Omega, X(\omega) = \omega$, i.e. $X$ is the number of dots on the die.
- *Tossing a coin:* $Y : \Omega \to \{0, 1\}, Y(\text{heads}) = 1, Y(\text{tails}) = 0$
- *Number of heads:* $Z(\omega) :=$ the number of heads in a sequence $\omega = (\omega_1, \dots \omega_n)$ of $n$ coin tosses, for example $Z(HHT) = 2$. Notice, with $Z_i : \Omega \to \{0, 1\}, Z_i(\omega) := Y(\omega_i)$ with $Y$ from above, we have

$$Z(\omega) = \sum_{i=1}^{n} Z_i(\omega)$$

**Note:** Random variables with a finite or countable number of values are known as **discrete random variables**, which will be our focus in this lecture. Most of the statements, however, directly generalize to **continuous random variables**, which is usually done by simply replacing summation by integration over the appropriate space.

## PROBABILITY MASS FUNCTIONS

Since any random variable $X$ is defined on a probability space $(\Omega, \Sigma, \mathbb{P})$, there is a straightforward way to assign a **probability measure** $P_X$ to (sets in) the target space of $X$:

$$P_X(A) := \mathbb{P}(X^{-1}(A)) = \mathbb{P}(X \in A)$$

where $X^{-1}(A) = \{\omega | X(\omega) \in A\}$ denotes the preimage of a set $A$ in the target space of $X$, also denoted as $\{X \in A\}$, in which case we drop the curly braces when evaluating $\mathbb{P}$.

For discrete random variables, we define the **probability distribution** $p_X$ **of** $X$, or its **probability mass function**, through

$$p_X(x) := P_X(\{x\}) = \mathbb{P}(\{\omega | X(\omega) = x\})$$

We also use the notation $p(X)$ for $p_X$ and $p(x)$ or $p(X{=}x)$ for $p_X(x)$.

**Note:** For *continuous random variables*, there exists a *probability density* $f_X$ such that $P_X(A) = \int_A f_X(x)dx$

EXAMPLE

# NUMBER OF HEADS

Consider sequences $\omega = (\omega_1, \ldots, \omega_n)$ of $n$ coin tosses with the same biased coin with probability $b$ of getting $\mathrm{heads}$. Let $Z(\omega)$ denote the number of heads in such a sequence. What is the probability distribution $p_Z$ of $Z$?

- Probability of a sequence $(\omega_1, \ldots, \omega_n)$ with $k$ heads: $b^k(1-b)^{n-k}$
- Number of permutations of $n$ elements: $n!$
- Number of sequences with $k$ heads: $\frac{n!}{k!(n-k)!}$ (divide $n!$ by the permutations of $1$s and $0$s)

$$\implies \qquad p_Z(k) = \frac{n!}{k!(n-k)!} b^k (1-b)^{n-k}$$

This is known as the **binomial distribution** (Note: $\sum_k p_Z(k) = 1$ is a special case of the *binomial formula*)

# INDICATOR AND SIMPLE RANDOM VARIABLES

Let $\Omega$ be a sample space and let $\mathbb{1}_A$ denote the indicator function of a set $A \subset \Omega$, i.e. $\mathbb{1}_A(\omega) = 1$ if $\omega \in A$ and $\mathbb{1}_A(\omega) = 0$ otherwise.

- **Indicator random variable:** $\mathbb{1}_A : \Omega \to \mathbb{R}, \omega \mapsto \mathbb{1}_A(\omega)$
- **Simple random variable:** $\sum_{i=1}^{N} a_i \mathbb{1}_{A_i} : \Omega \to \mathbb{R}, \omega \mapsto \sum_{i=1}^{N} a_i \mathbb{1}_{A_i}(\omega)$ (a *step function*)

Note that, if the sets $A_i$ are disjoint, then the corresponding simple random variable is a discrete random variable with values $a_i$.

**Theorem:** *Any random variable $X : \Omega \to \mathbb{R}$ can be approximated pointwise by a sequence of simple random variables $X_n$,* i.e. $X(\omega) = \lim_{n\to\infty} X_n(\omega)$ *for all $\omega \in \Omega$ (up to sets of probability zero).*

# EXPECTATION

One can define the expectation operator $\mathbb{E}$ for random variables $X$ inductively as follows:

- for indicator random variables $X = \mathbb{1}_A$, we define $\mathbb{E}[X] := \mathbb{P}(A)$
- for simple random variables $X = \sum_{i=1}^{N} a_i \mathbb{1}_{A_i}$, we define $\mathbb{E}[X] := \sum_i a_i \, \mathbb{E}[\mathbb{1}_{A_i}]$
- for arbitrary random variables $X$, we define $\mathbb{E}[X] := \lim_{n\to\infty} \mathbb{E}[X_n]$ where $(X_n)_n$ is a sequence of simple random variables that approximates $X$ pointwise.

One usually writes this as an integral with respect to the probability measure $\mathbb{P}$:

$$\mathbb{E}[X] = \int_\Omega X(\omega) \, d\mathbb{P}(\omega)$$

Note that, for discrete random variables $X$ with values $x_i$, by construction:

$$\mathbb{E}[X] = \sum_i x_i \, \mathbb{P}(X = x_i) = \sum_x x \, p_X(x)$$

**Remark:** Analogously, for continuous random variables with density $f_X$, we have $\mathbb{E}[X] = \int x \, f_X(x) dx$.

EXPECTATION

## SOME PROPERTIES

- **Linearity:** $\mathbb{E}[aX + bY] = a\mathbb{E}[X] + b\mathbb{E}[Y]$ for $a, b \in \mathbb{R}$ and random variables $X$, $Y$.
- **Functions of random variables:** For a (measurable) function $f$ defined on the range of a discrete random variable $X$ with probability mass function $p$,

$$\mathbb{E}[f(X)] = \sum_x f(x)\, p(x) \;=: \mathbb{E}_p[f]$$

- **Jensen's inequality:** If $g$ is a convex function on the range of a random variable $X$ (and all expectations are finite), then

$$g(\mathbb{E}[X]) \leq \mathbb{E}[g(X)]$$

with equality if and only if $g$ is linear or $X$ is constant.

EXAMPLE

## APPLICATION OF JENSEN'S INEQUALITY

Using Jensen's inequality and the fact that $g = -\log$ is a convex function, we find that the **Kullback-Leibler divergence** $D_{KL}(p\|q) := \sum_i p_i \log \frac{p_i}{q_i}$ **from** $q$ **to** $p$ satisfies

$$D_{KL}(p\|q) \;=\; \mathbb{E}_p\left[g\left(\frac{q}{p}\right)\right] \;\geq\; g\left(\mathbb{E}_p\left[\frac{q}{p}\right]\right) = g(1) = 0$$

and moreover, $D_{KL}(p\|q) = 0$ if and only if $\frac{q}{p}$ is constant, i.e.

$$\frac{q_1}{p_1} = \frac{q_2}{p_2} = \cdots = c \in \mathbb{R}$$

and thus $c = c\sum_i p_i = \sum_i q_i = 1$, which means that $p = q$.

## JOINT DISTRIBUTIONS

Usually one considers a random variable with values $\mathbf{X}$ in higher dimensional space as a tuple of multiple one-dimensional random variables, i.e. $\mathbf{X} = (X_1, \dots, X_d)$. The corresponding multivariate probability distribution $p_{\mathbf{X}}$ is called the **joint (distribution)** of the random variables $X_1, \dots, X_d$ with values

$$p(x_1, \dots, x_d) := p_{\mathbf{X}}(x_1, \dots, x_d)$$

Similarly, a multivariate probability density $f : \mathbb{R}^d \to [0, \infty)$ can be considered a **joint density** corresponding to continuous random variables $X_1, \dots, X_d$.

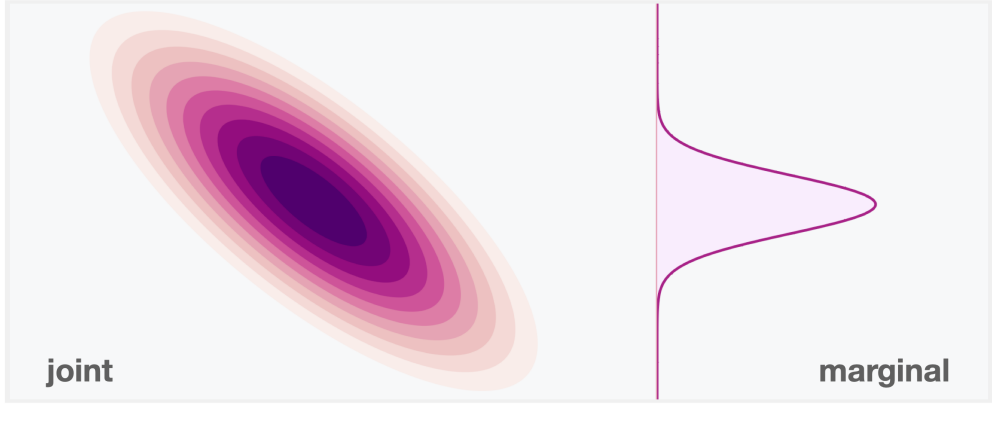
# MARGINALIZATION

For a joint probability distribution $p$ of two discrete random variables $X$ and $Y$,

$$p(y) := \sum_x p(x, y)$$

defines a probability distribution of $Y$, known as the **marginal** of $Y$ (with respect to $p$). Similarly, for continuous random variables $X$, $Y$, the **marginal density** of $Y$ (with respect to their joint density $f$) is given by $f(y) := \int f(x, y)\, dx$.

**Interpretation:** Marginals contain no information about the variables that have been summed out, i.e. the marginal distribution $p(Y) = \sum_x p(x, Y)$ represents the *knowledge about $Y$ given that $X$ is unknown*.



# CONDITIONING ON RANDOM VARIABLES: BAYES RULE

- Consider a joint $p(X, Y)$ of two random variables $X$, $Y$ and assume that the value of $X$ is known to be $x$ ("**the event $X = x$ is observed**").
- In general, this observation makes us more knowledgable about $Y$ than is represented by the marginal $p(Y)$: We can define **a new probability distribution for $Y$** by simply renormalizing $p(x, y)$ with respect to $y$, i.e.

$$\tilde{p}(y) := \frac{p(x, y)}{\sum_y p(x, y)} = \frac{p(x, y)}{p(x)} \qquad (*)$$

- The distribution $\tilde{p}$ thus depends on the value $x$, which is why $\tilde{p}(y)$ is denoted by $p(y|X=x)$, or simply $p(y|x)$. The expression $p(Y|X)$ is then interpreted as the distribution-valued function of $x$ with values $\tilde{p} = p(Y|X=x)$, known as the **conditional** of $Y$ given $X$.

**Note:** For continuous random variables, the same construction applied to densities can result in inconsistencies (Jaynes 1995, Ch. 15, The Borel-Kolmogorov paradox), which is why one has to rely on other methods (e.g. *conditional expectations*, see Gyenis et al. 2017) to properly define conditional distributions in this case.

## MARGINALIZATION AND CONDITIONING FOR ARBITRARILY MANY RVS

For random variables $X_1, \dots, X_d$, the marginal with respect to $X_k, \dots, X_l$ is obtained by summing $p$ over all variables besides of $X_k, \dots, X_l$, i.e.

$$p(x_k, \dots, x_l) = \sum_{\substack{x_1,\dots,x_i,\dots,x_d \\ \text{where } i \neq k,\dots,l}} p(x_1, \dots, x_d)$$

Similarly, conditioning on $X_k, \dots, X_l$ is analogous to the two-dimensional case,

$$p(x_i, \dots, x_j | X_k = x_k, \dots, X_l = x_l) := \frac{p(x_1, \dots, x_d)}{\sum_{x_i,\dots,x_j} p(x_1, \dots, x_d)} = \frac{p(x_1, \dots, x_d)}{p(x_k, \dots, x_l)}$$

## CANONICAL FACTORIZATION OF THE JOINT

The definition $(*)$ of conditional probabilities allows to rewrite the joint $p(X, Y)$ of two random variables $X$ and $Y$ as

$$p(X, Y) = p(X)\, p(Y|X)$$

Similarly, by induction, a joint $p(X_1, \ldots, X_d)$ can be factorized as

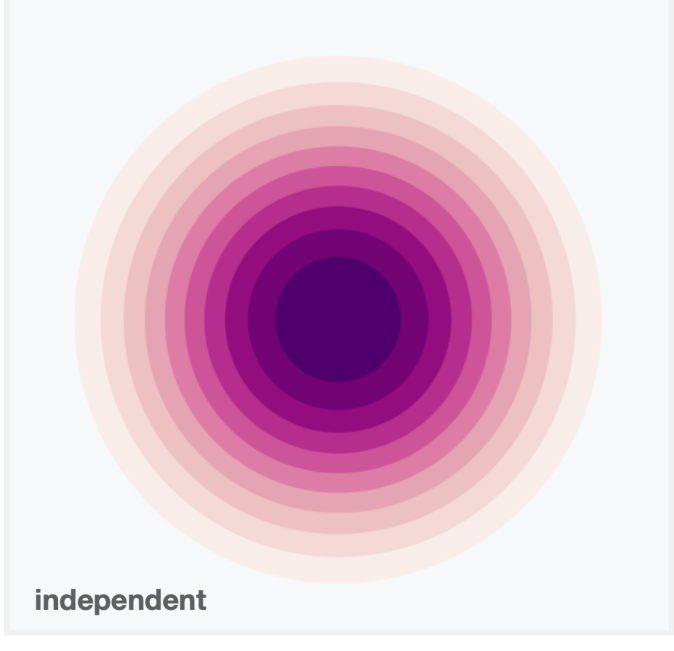
$$p(X_1, \ldots, X_d) = p(X_1)\, p(X_2|X_1) \cdots p(X_{d-1}|X_1, \ldots, X_{d-2})\, p(X_d|X_1, \ldots, X_{d-1})$$

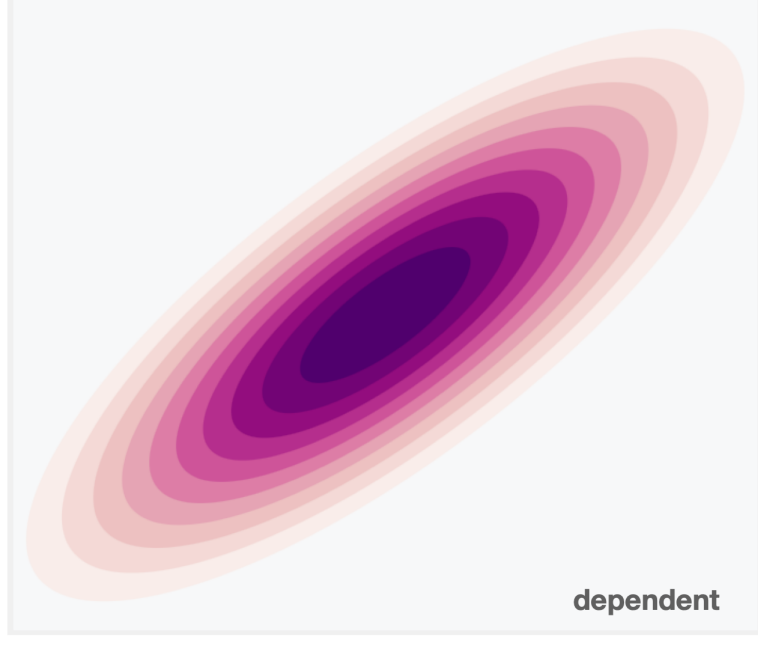
This is sometimes referred to as the **product rule**.

# STATISTICAL INDEPENDENCE OF RANDOM VARIABLES

If observing $X$ does not result in more information about $Y$ than considering $X$ to be unknown, i.e. if the conditional $p(Y|X)$ is the same as the marginal $p(Y)$, then $X$ and $Y$ are said to be *statistically* (or *stochastically*) *independent* (with respect to $p$). This is equivalent to

$$p(X, Y) = p(X)p(Y)$$

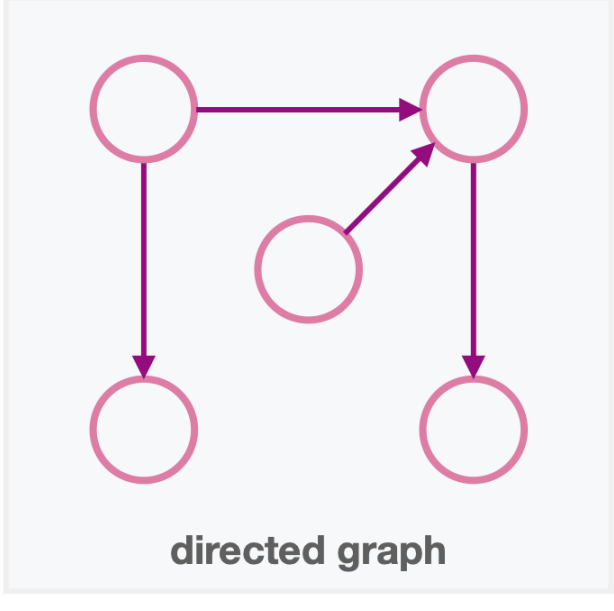


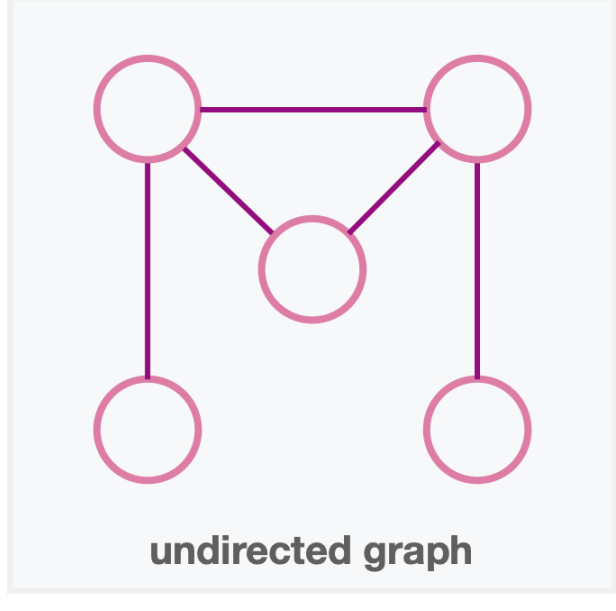
# DIRECTED GRAPHS

# GRAPHS

A **graph** is a tuple $(V, E)$, where $V$ is a set whose elements are called *vertices* or *nodes*, and $E$ consists of pairs of nodes called *edges*. In a **directed graph** the edges have orientation, representing a directed relationship between the nodes (graphically denoted by arrows). In an **undirected graph** the position of the nodes inside the edges is irrelevant, corresponding to a symmetric relationship (graphically represented by lines).



directed graph



undirected graph

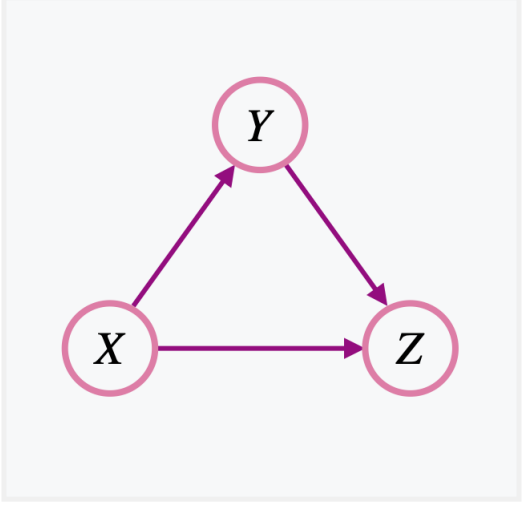
# REPRESENTING JOINTS GRAPHICALLY

*Example:* Can we represent $p(X, Y, Z) = p(X)\, p(Y|X)\, p(Z|X, Y)$ by a directed graph?

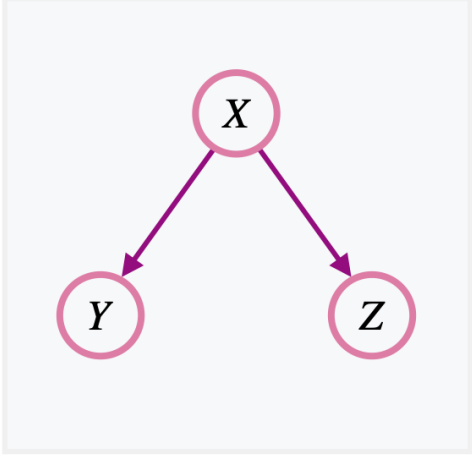
**Nodes** are the random variables.

**Edges** connect RVs that appear in a single conditional as a factor in the joint.

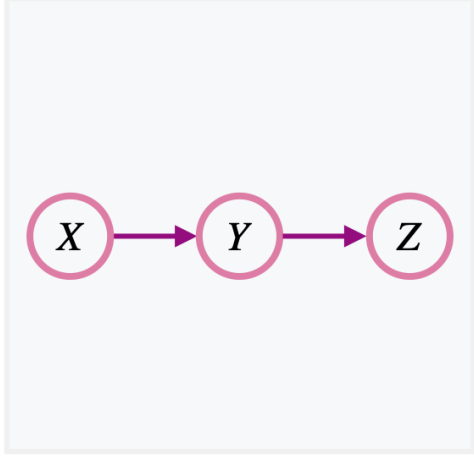
**Arrows** point from the variables in the condition to the variable over which the distribution is defined.



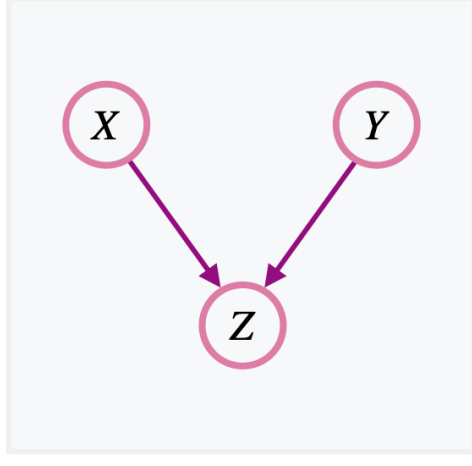
# MORE 3-VARIABLE EXAMPLES




$$p(X)\,p(Y|X)\,p(Z|X)$$




$$p(X)\,p(Y|X)\,p(Z|Y)$$




$$p(X)\,p(Y)\,p(Z|X,Y)$$

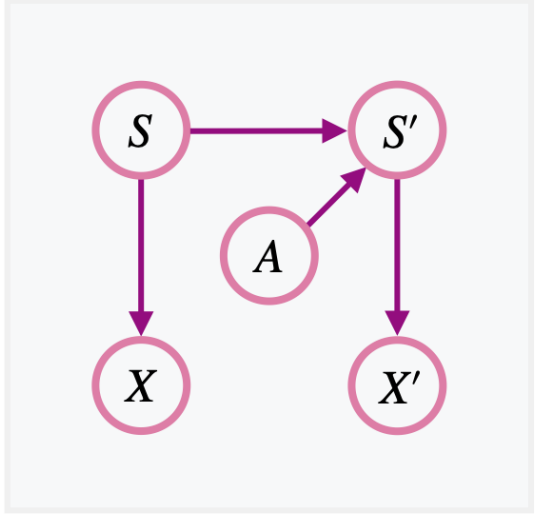
## GENERAL CASE

A directed graph is called **acyclic** if there is no path to visit a node twice by following the arrows.

Given a directed acyclic graph with nodes $X_1, \ldots, X_d$ (also called a *Bayesian network*), we can read off the joint

$$p(X_1, \ldots, X_d) = \prod_{k=1}^{d} p(X_k | \text{Parents}_k)$$

where $\text{Parents}_k$ are all parent nodes of node $X_k$.



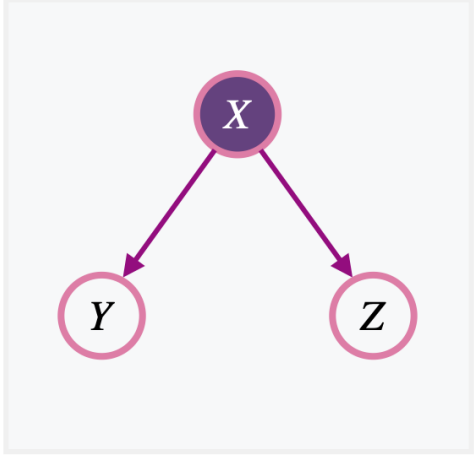

$$p(S)\,p(A)\,p(S' \mid S, A)\,p(X \mid S)\,p(X' \mid S')$$

An important use of graphical representations of joints is to **read off statistical independence** relations: In the above graph, when observing $S$, then $X$ and $S'$ are independent.

## CONDITIONAL INDEPENDENCE

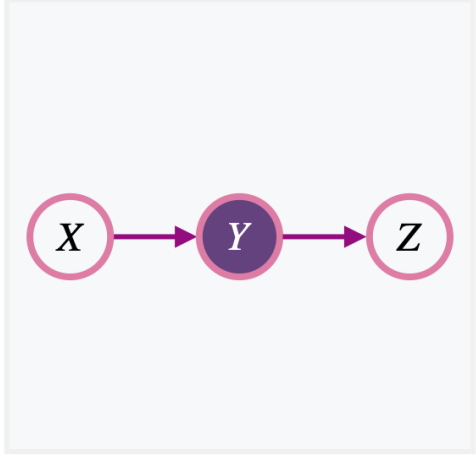
# 3-VARIABLE CASE REVISITED

*Tail-to-tail*



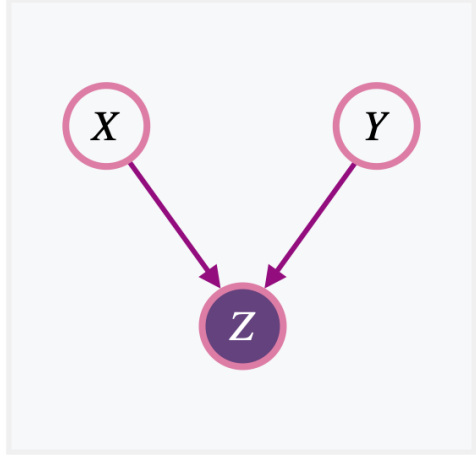

$$p(Y, Z \mid X) = p(Y \mid X)\, p(Z \mid X)$$

*Head-to-tail*




$$p(X, Z \mid Y) = p(X \mid Y)\, p(Z \mid Y)$$

*Head-to-head*




$$p(X, Y) = p(X)\, p(Y)$$
$$p(X, Y \mid Z) \neq p(X \mid Z)\, p(Y \mid Z)$$

**Note:** When making a negative statement about conditional independence, we mean that this does not follow *in general*. A specific model that satisfies a given graph can always have more independence properties than is specified by the graph.

CONDITIONAL INDEPENDENCE

# D-SEPARATION

The three cases on the previous slide contain the essentials for deriving conditional independence relations for general directed acyclic graphs, known as **d-separation**.

Consider three sets of nodes $A$, $B$, and $C$. A **path** (along edges, ignoring direction of arrows) from a node in $A$ to a node in $B$ is called **blocked** by $C$ if

$(i)$ *it contains a node in* $C$ *that is tail-to-tail or head-to-tail*, or

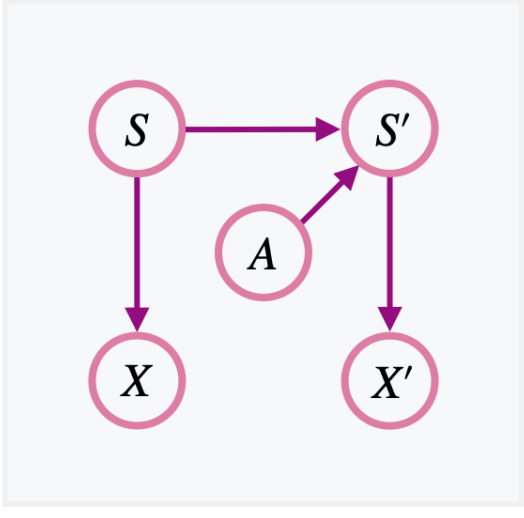
$(ii)$ *it contains a head-to-head node that is* ***not*** *in* $C$*, nor any of its descendants is in* $C$

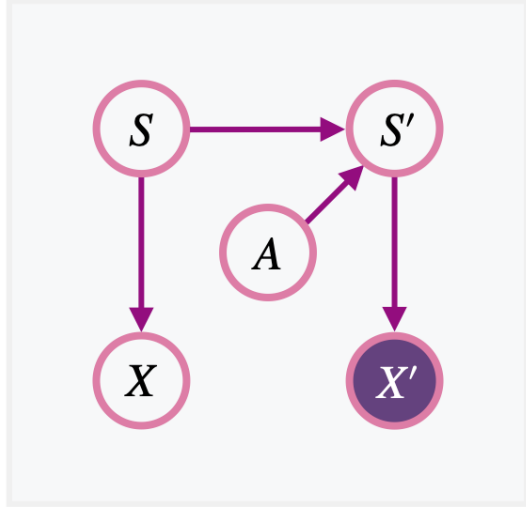
Here, a *descendant* of a (oparent) node is any node that can be reached from its parent by following arrows.

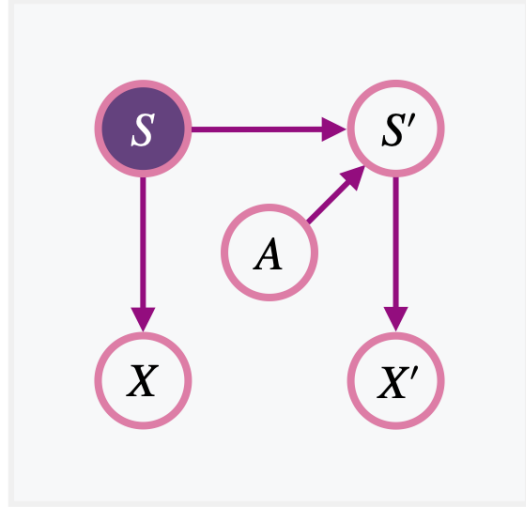
**Theorem** (Pearl 1988): *If all possible paths from* $A$ *to* $B$ *are blocked by* $C$ *then the random variables in* $A$ *are independent from the ones in* $B$ *given the random variables in* $C$*.*

CONDITIONAL INDEPENDENCE

# ILLUSTRATION OF D-SEPARATION




$p(X, A) = p(X)p(A)$

$S'$ **blocks** because it is head-to-head and it is not in $C = \{\}$ (nor its descendants)

$p(X, A|X') \neq p(X|X')p(A|X')$

$S'$ is **unblocked** because it is head-to-head and its descendant $X'$ is in $C$

$p(X, A|S) = p(X|S)p(A|S)$

$S$ **blocks** because it is tail-to-tail and in $C$ (also, $S'$ blocks for the same reason as before)

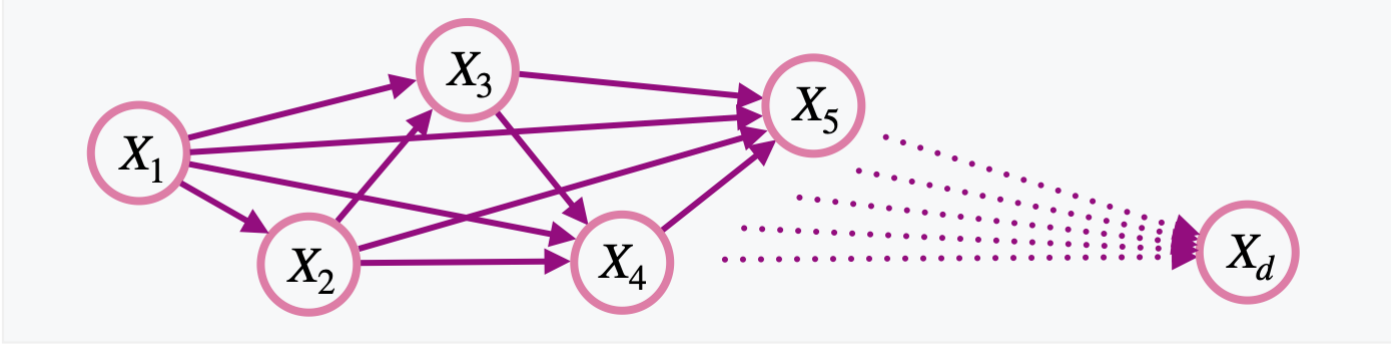
# FULLY CONNECTED MODEL

Two nodes with a direct connection cannot have any conditional independence property (since there are no nodes that could satisfy $(i)$ or $(ii)$ of d-separation).

In particular, the **most general model** for $d$ random variables $X_1, \ldots, X_d$ has a canonical factorization

$$p(X_1, \ldots, X_d) = p(X_1)\, p(X_2|X_1)\, p(X_3|X_1, X_2) \cdots p(X_d|X_1, \ldots, X_{d-1})$$

that cannot be simplified (there is a connection between all nodes), and thus does not have any conditional independence properties.

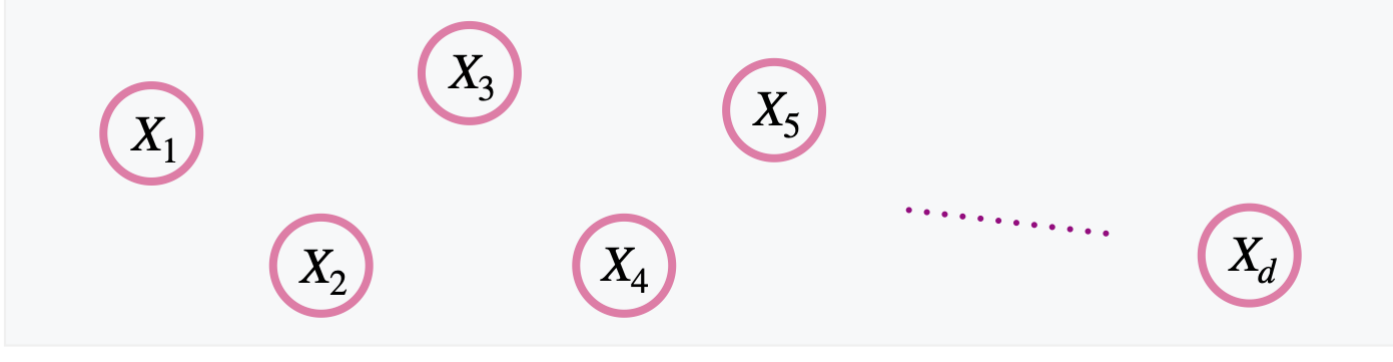


## THE MEAN-FIELD ASSUMPTION

In contrast, the **most simple model** would have no connections at all and therefore fully factorizes, i.e.

$$p(X_1, \ldots, X_d) = p(X_1) \cdots p(X_d)$$

This is sometimes called a *mean-field* assumption.



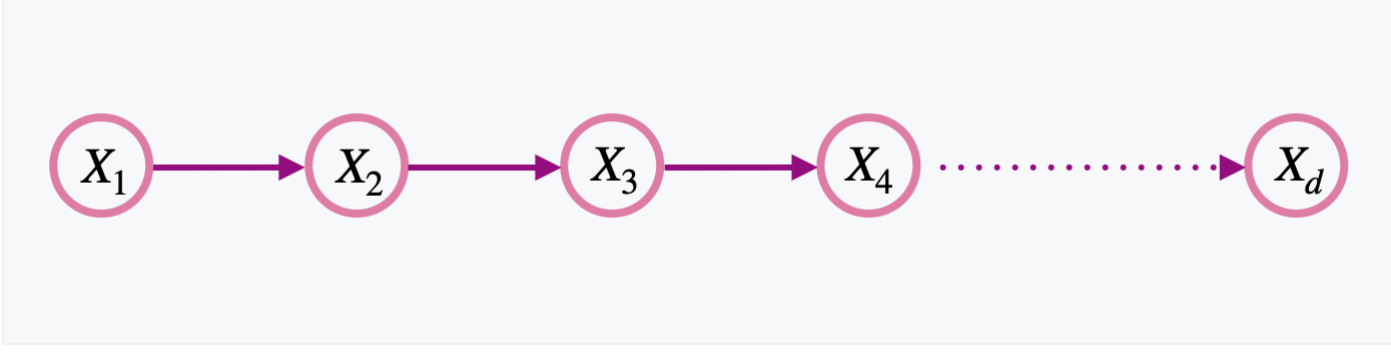
## THE MARKOV PROPERTY

# MARKOV CHAINS

If we want to allow just slightly more dependence among the variables than in the mean-field assumption, we arrive at what is known to be a **Markov chain**

$$p(X_1, \ldots, X_d) = p(X_1)\, p(X_2|X_1)\, p(X_3|X_2) \cdots p(X_d|X_{d-1})$$

which got its name from the **Markov property** $p(X_k|X_1, \ldots, X_{k-1}) = p(X_k|X_{k-1})$.



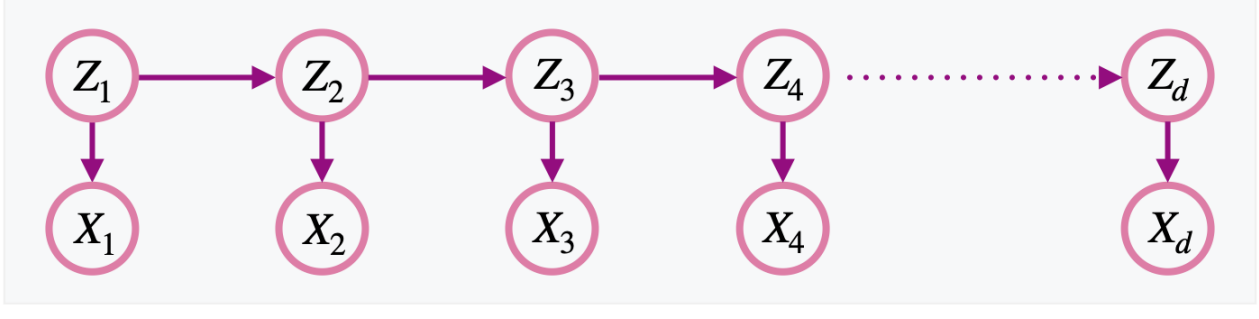

**Note:** In many applications, the additional assumption is made that the **transition probability** $p(X_k|X_{k-1})$ is independent of $k$ (*homogeneity*), i.e. the conditional distributions in the factorization above are all identical (share parameters), just evaluated at different "time steps" (naming from modeling temporal data).

# HIDDEN MARKOV MODELS

Most sequential data has the property that $X_k$ does not only depend on the predecessor (Markov chains) but on many or all previous time steps. However, simply allowing more and more dependencies of $p(X_k|X_m, \ldots, X_{k-1})$ results in *higher-order Markov models* potentially with many parameters to determine.

In contrast, *Hidden Markov Models (HMMs)* achieve dependence on all previous time steps, while keeping the model complexity low:

- introduce **latent variables** $Z_1, \ldots, Z_d$ that **satisfy the Markov property**
- $Z_k$ **generates** $X_k$ through a distribution $p(X_k|Z_k)$ (*emission probability*) $\forall k = 1, \ldots, d$.

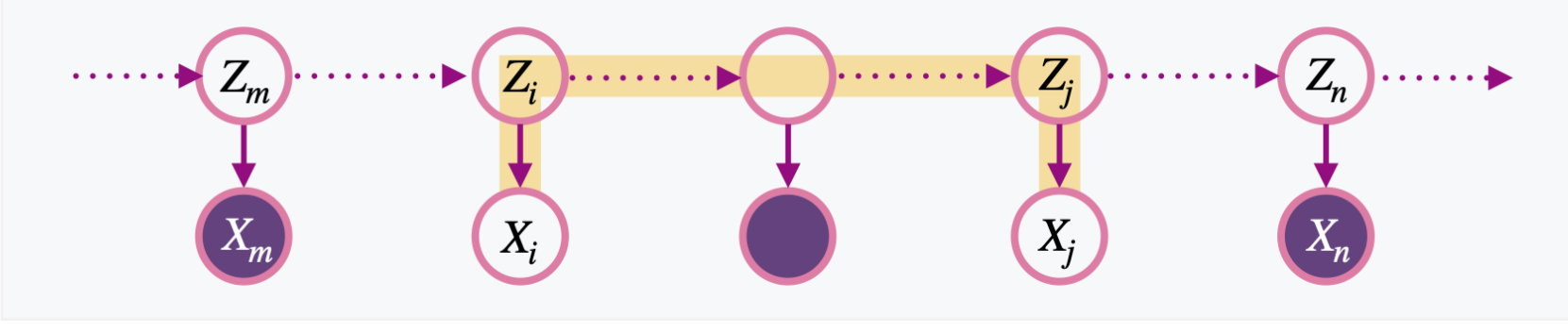


# D-SEPARATION IN HIDDEN MARKOV MODELS

For any $i, j = 1, \dots d$, conditioned on observations $X_m, \dots, X_n$, there is an unblocked path between $X_i$ and $X_j$ along the latent variables with no head-to-head nodes, and thus

$$p(X_i, X_j | X_m, \dots, X_n) \neq p(X_i | X_m, \dots, X_n)\, p(X_j | X_m, \dots, X_n)$$

for any $X_m, \dots, X_n$.




In particular, conditionals of the form $p(X_i | X_1, \dots, X_{i-1})$ generally do depend on all previous random variables.

# MARKOV BLANKETS

For a joint $p$ of a set of discrete random variables $X_1, \ldots, X_d$, we have

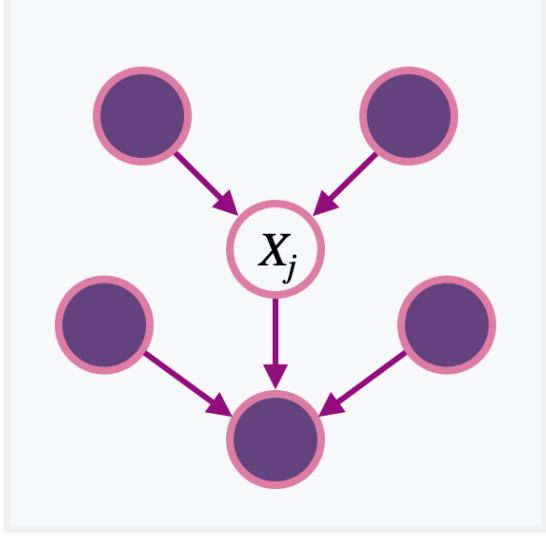
$$p(x_j|x_1, \ldots, x_{i\neq j}, \ldots, x_d) = \frac{p(x_1, \ldots, x_d)}{\sum_{x_j} p(x_1, \ldots, x_d)} = \frac{\prod_{k=1}^{d} p(x_k|\text{parents}_k)}{\sum_{x_j} \prod_{l=1}^{d} p(x_l|\text{parents}_l)}$$

Consider the two properties of a factor in the denominator:

- $l = j$, i.e. the factor is $p(x_j|\text{parents}_j)$, or
- $x_j \in \text{parents}_l$, i.e. the $X_l$ is a child of $X_j$

In any other case, the factor can be pulled out of the sum and cancels with the numerator.

$\Longrightarrow p(X_j|X_1, \ldots, X_{i\neq j}, \ldots, X_d)$ only depends on the **parents** of $X_j$, the **children** of $X_j$, and the **other parents of the children** of $X_j$, forming the so-called *Markov Blanket*.



# INFERENCE

There are mainly three types of inference:

- parameter estimation through **maximum (log-)likelihood**

$$\theta^*(x_1, \ldots, x_d) = \text{argmax}_\theta \ \log p_\theta(x_1, \ldots, x_d)$$

- inferring distributions over unknown variables, known as **Bayesian inference**

$$p(Z|x_1, \ldots, x_d) = \frac{p(x_1, \ldots, x_d|Z)\ p(Z)}{\sum_z p(x_1, \ldots, x_d|z)p(z)}$$

- approximating Bayes' posteriors, known as **variational inference**

$$q^*(Z) = \text{argmin}_{q \in \Gamma}\ \text{error}(\text{q(Z)}, \text{p(Z}|\text{x}_1, \ldots, \text{x}_\text{d}))$$

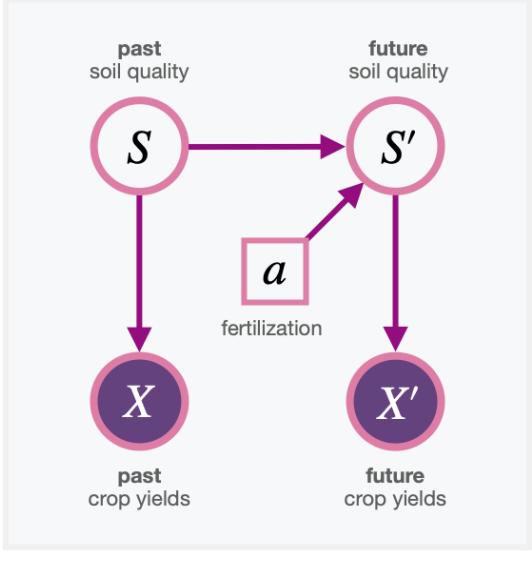
**Note:** Variational inference can be considered a generalization of both, maximum likelihood and Bayesian inference, which are recovered as limiting cases by the choice of trial distributions.

# MAXIMUM LIKELIHOOD

Consider the example of a model

$$p_a(S, S', X, X') = p(S)\, p(X|S)\, p_a(S'|S)\, p(X'|S')$$

consisting of the (for simplicity, discrete) variables *past* and *future soil quality* $S, S'$, *past* and *future crop yields* $X, X'$, where the future soil quality $S'$ depends on $S$ and an action $a$, e.g. representing the amount of fertilization.




**Note:** For fixed $a$, this is a one-step hidden markov model.

As a farmer, we might only be able to **observe the past crop yields** $X = x$. In order to determine an action $a$ leading to **desired future crop yields** $X' = x'$, the farmer could employ maximum log-likelihood as follows:

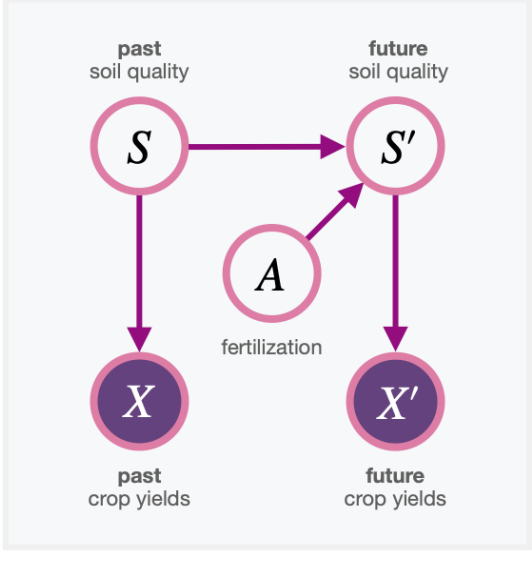
$$a^*(x, x') = \operatorname{argmax}_a \log p_a(x, x') = \operatorname{argmax}_a \log \sum_{s,s'} p_a(s, s', x, x')$$

# BAYESIAN INFERENCE

Instead of greedily looking for the best action $a$, the farmer could also **treat the action as a random variable** $A$ following some prior distribution $p(A)$, resulting in the joint

$$p(S, S', X, X', A) = p(S)\, p(X|S)\, p(A)\, p(S'|S, A)\, p(X'|S')$$

The farmer can then infer the distribution $p(A|X{=}x, X'{=}x')$ using Bayes' rule:




$$p(A|x, x') = \frac{p(x, x', A)}{p(x, x')} = \frac{\sum_{s,s'} p(s, s', x, x', A)}{\sum_{s,s',a} p(s, s', x, x', a)}$$

**Note:** Depending on the sharpness of the prior $p(A)$, the Bayes' posterior $p(A|x, x')$ will be more or less sharp and can only be non-zero where $p(A)$ is non-zero. If $p(A)$ is uniform, then Bayes' rule is the *softmax* version of maximum log-likelihood.

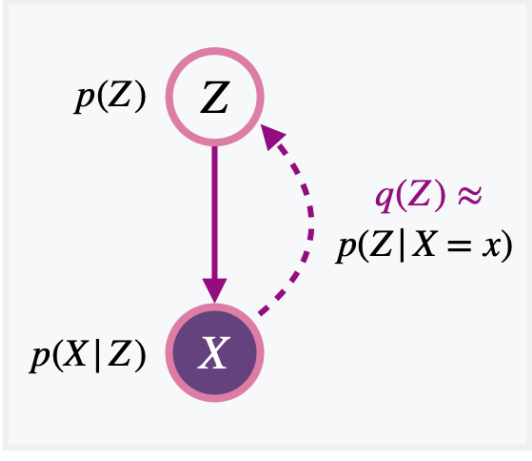
VARIATIONAL INFERENCE

# MOTIVATION

Before considering the model from the previous slide, assume a simple model $p(X, Z) = p(Z)\, p(X|Z)$ of two variables. When observing $X{=}x$, we can determine

$$p(Z|X{=}x) = \frac{p(Z)\, p(x|Z)}{\sum_z p(z)\, p(x|z)}$$

over hidden causes $Z$ using Bayes' rule.




*Problem:* The calculation of the normalization $\sum_z p(z)\, p(x|z)$ is often intractable.

*Idea:* Approximate $p(Z|x)$ by a family of **trial distributions** $q(Z)$ by **minimizing some error** measuring the difference between $q(Z)$ and $p(Z|x)$.

*But:* We cannot use ANY discrimination measure between distributions because we would have to know $p(Z|x)$ in advance!

## VARIATIONAL INFERENCE

# FREE ENERGY

We have

$$D_{KL}(q(Z)\|p(Z|x)) = \sum_z q(z)\log\frac{q(z)}{p(z|x)} = \underbrace{\sum_z q(z)\log\frac{q(z)}{p(x,z)}}_{=:F(q(Z)\|p(x,Z))} + C(x)$$

where $C(x) := \sum_z q(z)\log p(x) = \log p(x)$ is independent of $q$.

Hence, minimizing the Kullback-Leibler divergence between $q(Z)$ and $q(Z|x)$ is equivalent to minimizing the so-called **(variational) free energy** $F(q(Z)\|p(x,Z))$ with respect to $q(Z)$, for which we **do NOT have to know** $p(Z|x)$ in advance.

In particular,

$$\operatorname*{argmin}_{q(Z)} F(q(Z)\|p(x,Z)) = p(Z|x), \qquad \min_{q(Z)} F(q(Z)\|p(x,Z)) = -C(x) = -\log\sum_z p(x,z)$$

VARIATIONAL INFERENCE

# GENERAL FREE ENERGY MINIMIZATION

Let $\phi \geq 0$ be an arbitrary non-negative function of one variable. In the exercises, using Jensen's inequality we show that

$$F(q\|\phi) := \sum_z q(z) \log \frac{q(z)}{\phi(z)}$$

is minimized at $q^*$ given by

$$q^*(Z) = \frac{\phi(Z)}{\sum_z \phi(z)}$$

with the minimum $F(q^*\|\phi) = -\log \sum_z \phi(z)$.

In variational inference, the reference function $\phi$ is usually given by a **joint distribution evaluated at the observed variables** (as shown on the previous slide).

VARIATIONAL INFERENCE

# NORMALIZATION THROUGH OPTIMIZATION

Hence, minimizing the free energy $F(q\|\phi)$ simply normalizes the reference function $\phi$, in order to obtain a probability distribution with the same shape as $\phi$. This is relevant in particular when this normalization is hard or intractable to do directly.

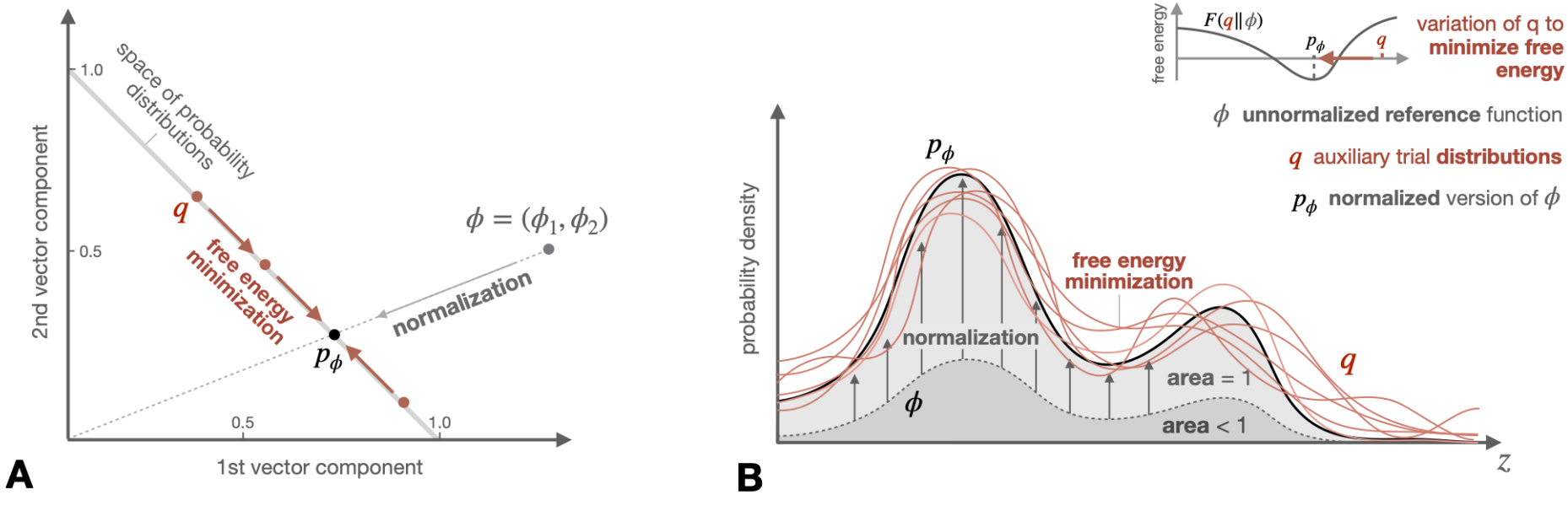



Image source: Gottwald, Braun 2020.

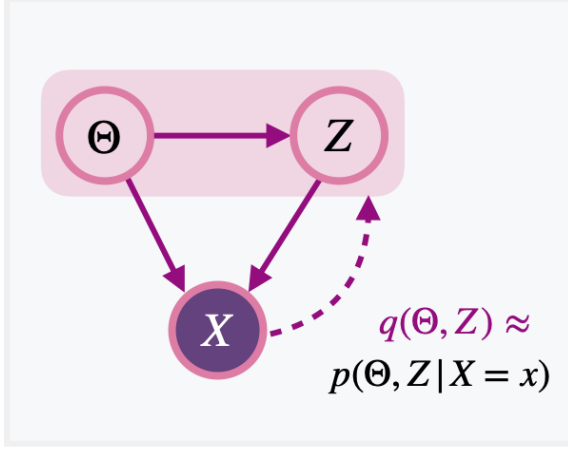
## VARIATIONAL INFERENCE

# 2 HIDDEN DIMENSIONS

Consider the previous model parametrized by a parameter $\theta$, i.e. $p_\theta(Z, X) = p_\theta(Z)p_\theta(X|Z)$, and treat $\theta$ also as a random variable, so that we have a model of the form

$$p(\Theta, Z, X) = p(\Theta)\, p(Z|\Theta)\, p(X|Z, \Theta).$$

As previously, instead of calculating the Bayes' posterior $p(\Theta, Z|X{=}x)$ directly, we can minimize the free energy




$$F(q(\Theta, Z)|p(\Theta, Z, x)) = \sum_{\theta,z} q(\theta, z) \log \frac{q(\theta, z)}{p(\theta)\, p(z|\theta)\, p(x|z, \theta)}$$

with respect to $q(\Theta, Z)$.

# MEAN-FIELD SOLUTIONS

Assume that $\Theta$ and $Z$ are **statistically independent under** $q$, i.e. $q(\Theta, Z) = q(\Theta)q(Z)$. Then the free energy can be written as

$$F(q\|p) = \sum_{\theta} q(\theta) \log \frac{q(\theta)}{p(\theta)\, e^{\sum_z q(z) \log p(x|z,\theta)p(z|\theta)}} + C_1 = F(q(\Theta)\|\phi_1(\Theta)) + C_1$$

where $\phi_1(\theta) := p(\theta)\, e^{\sum_z q(z) \log p(x|z,\theta)p(z|\theta)}$ and $C_1 := \sum_z q(z) \log q(z)$, or, equivalently, as

$$F(q\|p) = \sum_{z} q(z) \log \frac{q(z)}{e^{\sum_\theta q(\theta) \log p(x|z,\theta)p(z|\theta)p(\theta)}} + C_2 = F(q(Z)\|\phi_2(Z)) + C_2$$

where $\phi_2(z) := e^{\sum_\theta q(\theta) \log p(x|z,\theta)p(z|\theta)p(\theta)}$ and $C_2 := \sum_\theta q(\theta) \log q(\theta)$.

This motivates to **alternatingly minimize** with respect to $q(\Theta)$ and $q(Z)$ (while keeping the other one fixed), with the solutions

$$q^*(\theta) = \frac{\phi_1(\theta)}{\sum_\theta \phi_1(\theta)}, \quad q^*(z) = \frac{\phi_2(z)}{\sum_z \phi_2(z)}$$

VARIATIONAL INFERENCE

# APPROXIMATIONS AND ITERATIONS

In summary, representing Bayes' rule as an optimization principle has **two main applications**:

- **Approximate inference:** Approximating Bayes' posteriors by parametrized trial distributions $q_\theta$ (e.g. Gaussians):

$$\theta^*(x) = \operatorname{argmin}_\theta F(q_\theta(Z) \| p(x, Z))$$

- **Iterative inference algorithms:** Minimize the free energy with respect to factors of $q$ alternatingly, for example the mean-field algorithm on the previous slide (an example of the *variational Bayesian EM algorithm*, see e.g. Beal 2003, and the exercises).

# VARIATIONAL INFERENCE
# OVERVIEW

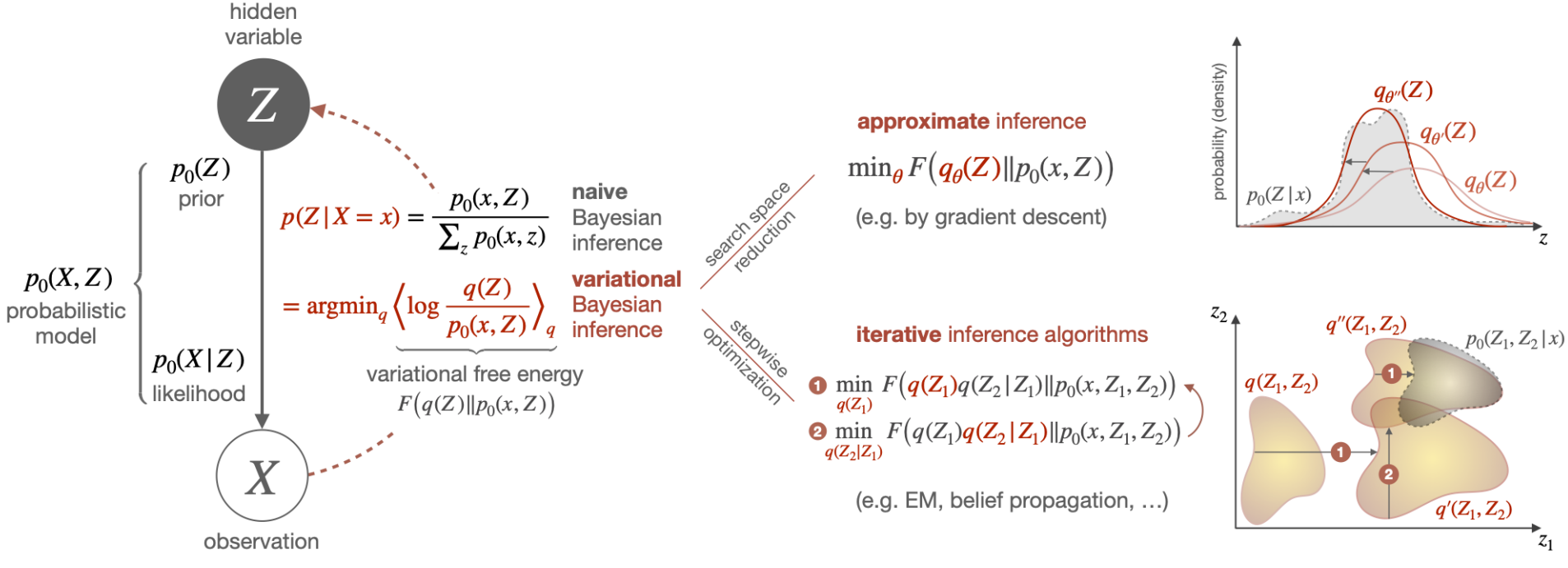



Image source: Gottwald, Braun 2020.

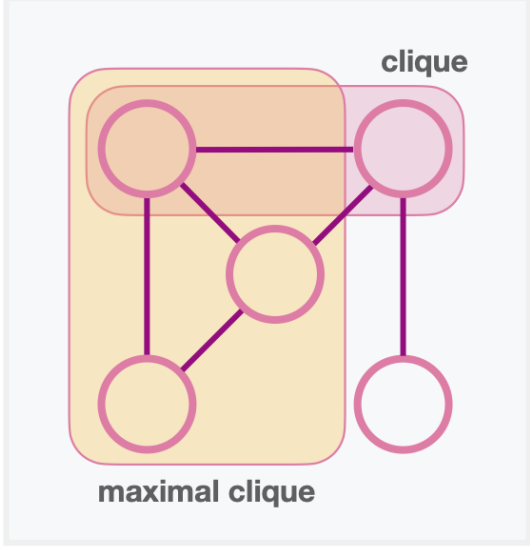
# UNDIRECTED GRAPHS

# CLIQUES

Undirected graphs are useful to model mutual and cyclic dependencies. They rely on the concept of a *clique*:

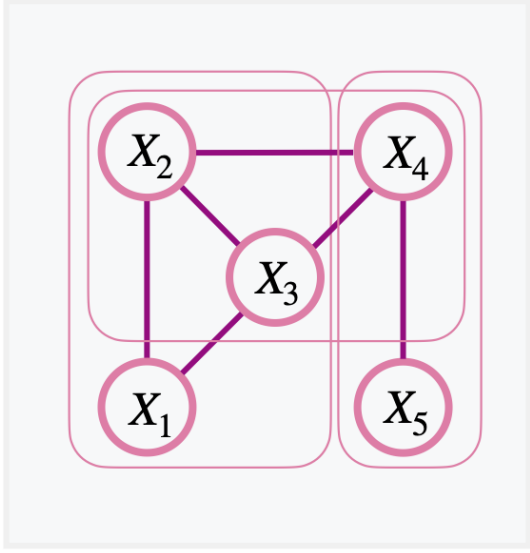
A **clique** is a fully connected set of nodes in an undirected graph, i.e. there is an edge connecting any two nodes of a clique.

A **maximal clique** is a clique that cannot be extended by including one more node, i.e. a maximal clique is not allowed to be part of a larger clique.



# JOINT PROBABILITY REPRESENTED BY AN UNDIRECTED GRAPH

Let $X_1, \ldots, X_d$ be the random variables corresponding to the nodes of a undirected graph, also called a *(Markov) Random Field*, and let $\mathbf{X}_c$ denote the subset of random variables belonging to a clique $c$. The corresponding joint distribution takes the form



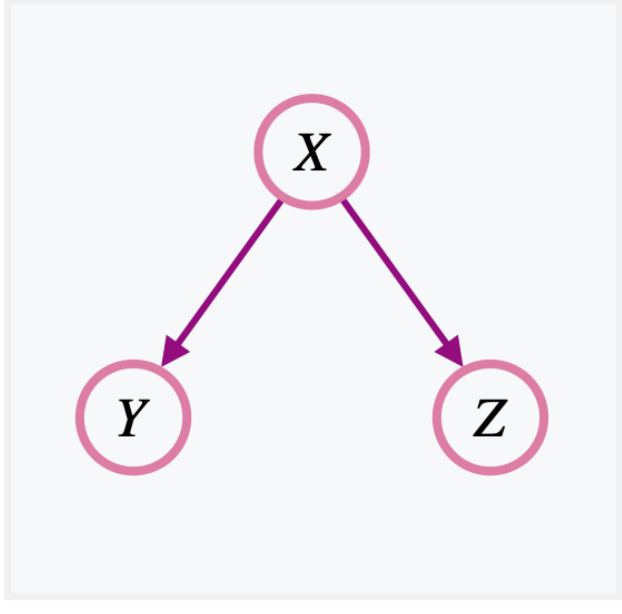

$$p(X_1, \ldots, X_d) = \frac{1}{Z} \prod_c \psi_c(\mathbf{X}_c)$$

where the product is over all cliques (can be restricted to maximal cliques). Here, $Z := \sum_{x_1,\ldots,x_d} \prod_c \psi_c(\mathbf{x}_c)$ denotes the normalization constant and $\psi_c \geq 0$ is the so-called **potential function** belonging to clique $c$.

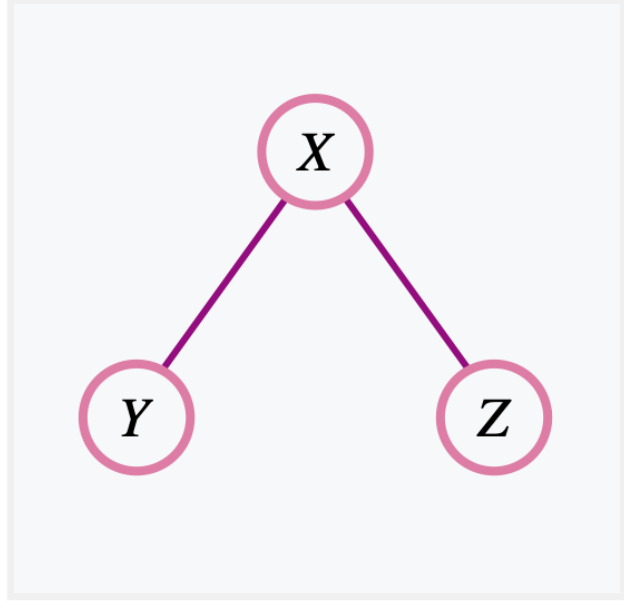
**Example:** The graphical model shown above takes the form

$$p(x_1, \ldots, x_5) = \frac{1}{Z} \psi_1(x_1, x_2, x_3)\, \psi_2(x_2, x_3, x_4)\, \psi_3(x_4, x_5)$$

# DIRECTED TO UNDIRECTED GRAPHS

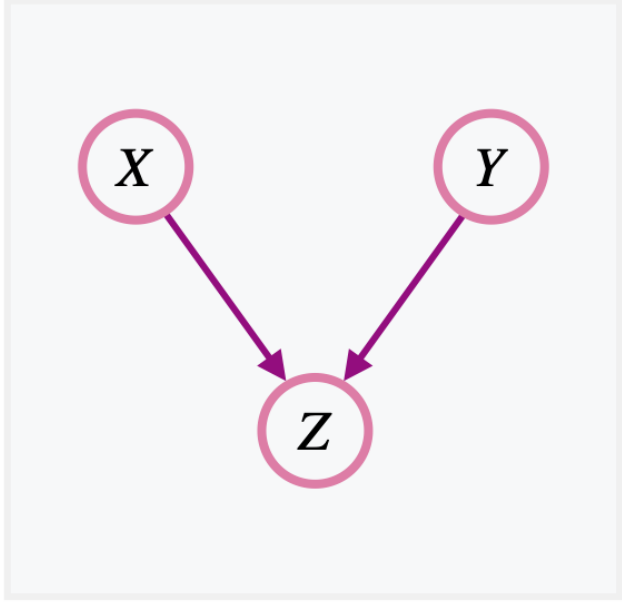



$$p(X)\,p(Y\,|\,X)\,p(Z\,|\,X)$$

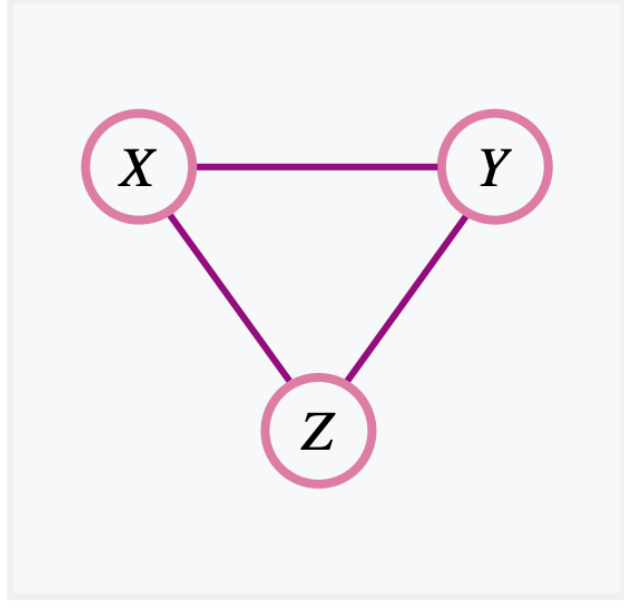



$$\frac{1}{Z}\,\psi_1(X,Y)\,\psi_2(X,Z)$$

# DIRECTED TO UNDIRECTED GRAPHS: "MORALIZATION"

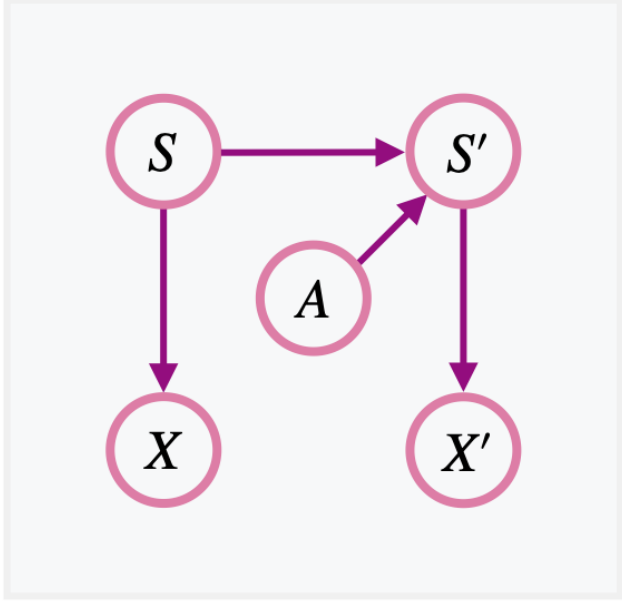



$$p(X)\,p(Y)\,p(Z|X,Y)$$

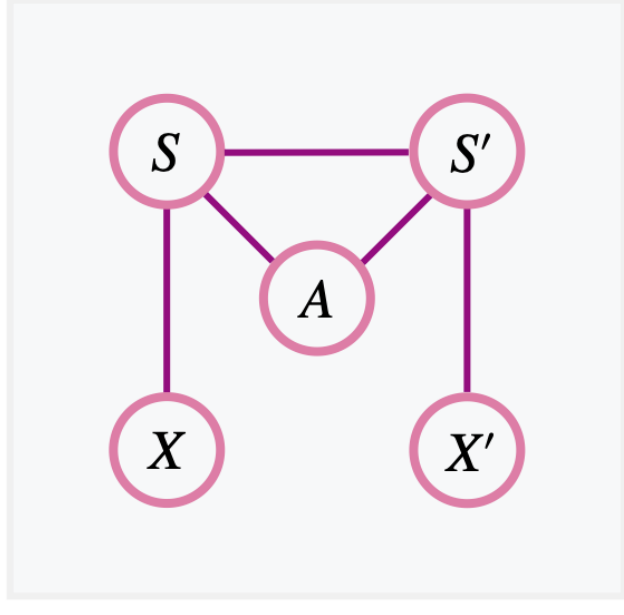



$$\frac{1}{Z}\psi(X,Y,Z)$$

# DIRECTED TO UNDIRECTED GRAPHS: "MORALIZATION"

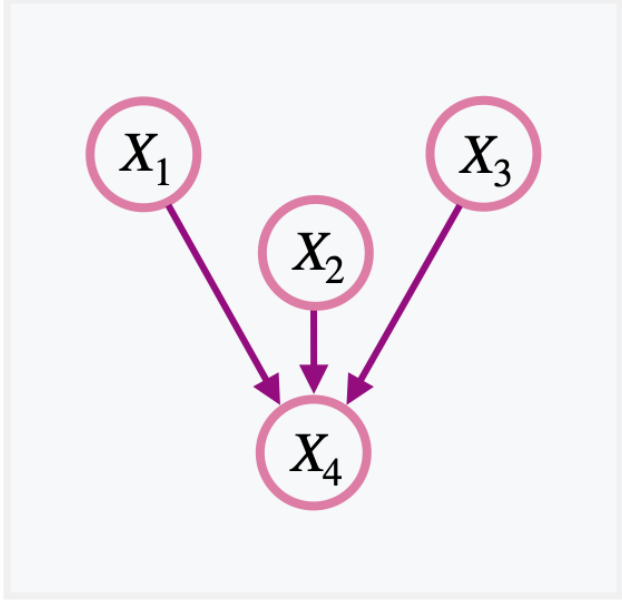


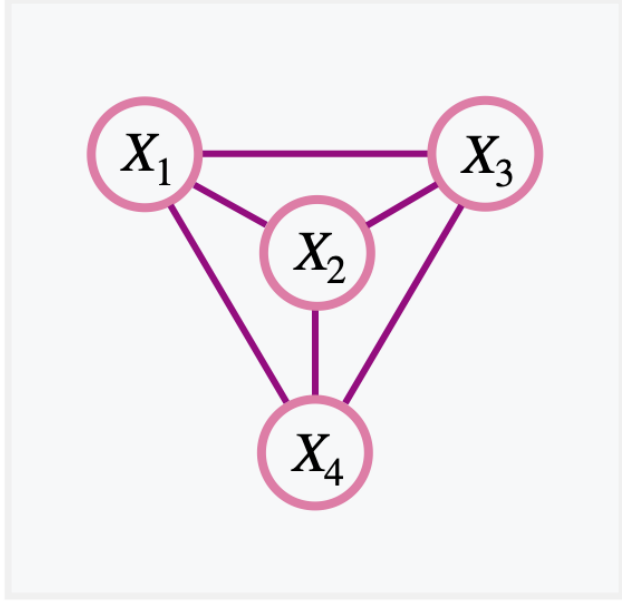

$$p(S)\,p(A)\,p(S' \mid S, A)\,p(X \mid S)\,p(X' \mid S')$$




$$\frac{1}{Z}\,\psi_1(S, X)\,\psi_2(S, S', A)\,\psi_3(S', X')$$

# DIRECTED TO UNDIRECTED GRAPHS: "MORALIZATION"



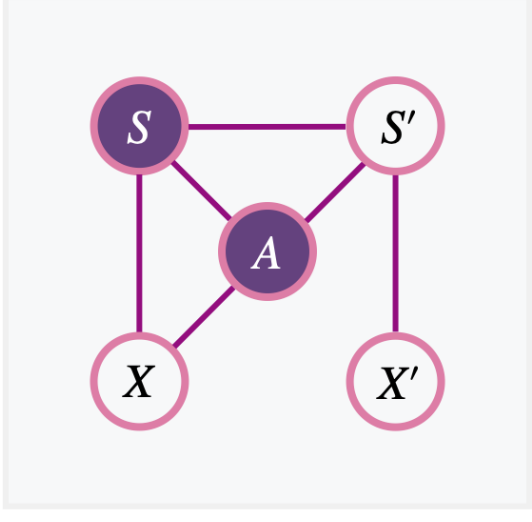

$$p(X_1)\,p(X_2)\,p(X_3)\,p(X_4 \mid X_1, X_2, X_3)$$

$$\frac{1}{Z}\,\psi(X_1, X_2, X_3, X_4)$$

# CONDITIONAL INDEPENDENCE FOR UNDIRECTED GRAPHS

Much simpler than d-separation:

Consider three sets of nodes $A$, $B$, and $C$ of an undirected graph. A path from a node in $A$ to a node in $B$ is called **blocked** by $C$ if it passes through a node belonging to $C$.



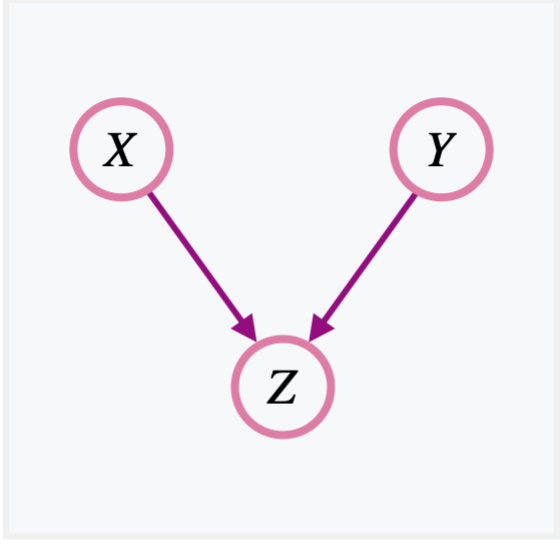

**Theorem** (Clifford 1990): *If all paths from $A$ to $B$ are blocked by $C$, then the set of random variables in $A$ is independent from the set of random variables in $B$, given the set of random variables in $C$.*

**Example:** In the graph to the right, the paths between $X$ and $S'$ (and $X'$) is blocked by $\{S, A\}$, i.e.

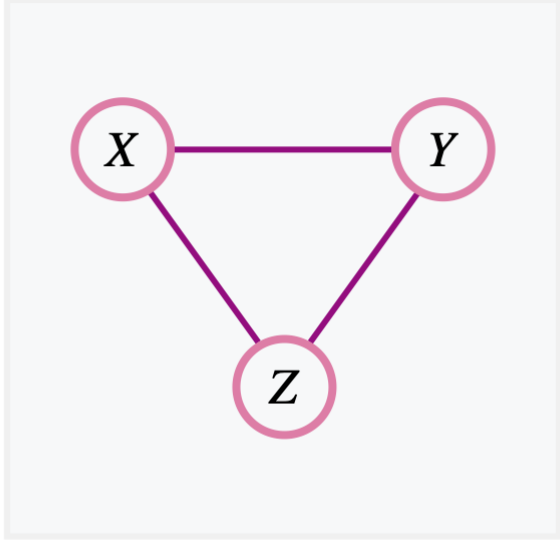
$$p(X, S' | S, A) = p(X|S, A)\, p(S' | S, A)$$

CONDITIONAL INDEPENDENCE

# COMPARISON TO DIRECTED GRAPHS



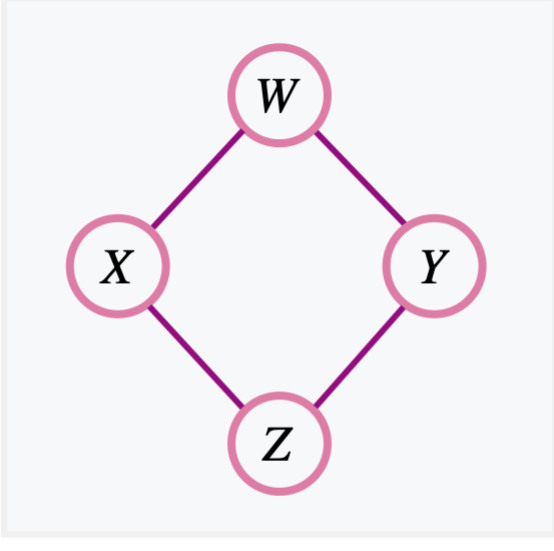

$$p(X, Y) = p(X)\,p(Y)$$
$$p(X, Y \mid Z) \neq p(X \mid Z)\,p(Y \mid Z)$$



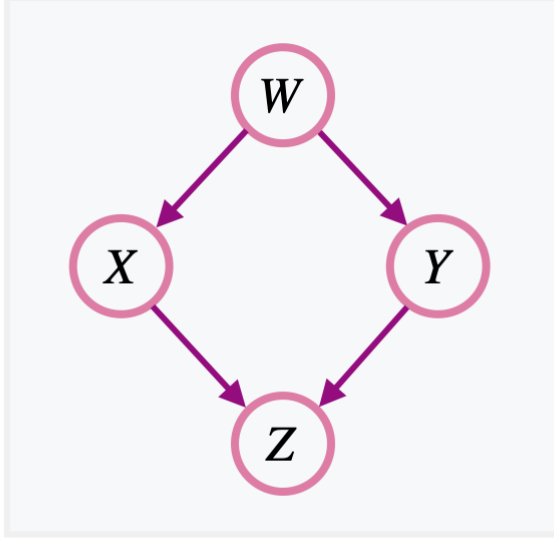

$$p(X, Y) \neq p(X)\,p(Y)$$
$$p(X, Y \mid Z) \neq p(X \mid Z)\,p(Y \mid Z)$$

CONDITIONAL INDEPENDENCE

# COMPARISON TO DIRECTED GRAPHS




$$p(X, Y \mid W, Z) = p(X \mid W, Z)\, p(Y \mid W, Z)$$
$$p(W, Z \mid X, Y) = p(W \mid X, Y)\, p(Z \mid X, Y)$$



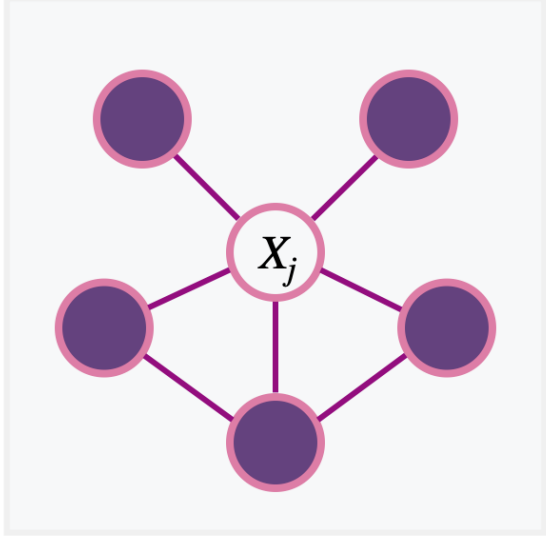

$$p(X, Y \mid W, Z) \neq p(X \mid W, Z)\, p(Y \mid W, Z)$$
$$p(W, Z \mid X, Y) = p(W \mid X, Y)\, p(Z \mid X, Y)$$

# MARKOV BLANKETS IN UNDIRECTED GRAPHS

Due to the simple conditional independence properties of undirected models, their Markov Blankets take also a particularly simple form:

The Markov Blanket of a node $X_j$ consists of **all neighbouring nodes** (directly connected through a single edge).

In particular, given all neighbouring nodes, $X_j$ is independent from all other nodes in the undirected graph.



## EXPONENTIAL REPRESENTATION

Since the potential functions $\psi_c$ have to be non-negative, sometimes they are represented using so-called **energy functions** $E_c$ through

$$\psi_c(\mathbf{x}_c) = e^{-E_c(\mathbf{x}_c)}$$

so that the joint distribution corresponding to an undirected graph takes the form of a **Boltzmann distribution**

$$p(x_1, \ldots, x_d) = \frac{1}{Z} e^{-\sum_c E_c(\mathbf{x}_c)}$$

where the summation is over the maximal cliques of the undirected graph. Notice, *low energy means high probability* and *high energy means low probability*.

## BOLTZMANN MACHINES

Boltzmann machines are fully connected undirected graphs with **binary nodes** defined through **1-clique** and **2-clique energies** of the form

$$E_{\{X_i\}}(x_i) = b_i x_i \qquad E_{\{X_i,X_j\}}(x_i, x_j) = -w_{ij} x_i x_j$$

where the so-called *biases* $b_i \in \mathbb{R}$ and *weights* $w_{i,j} \in \mathbb{R}$ are the parameters of the machine. The weight matrix $w$ is taken to be **symmetric** and with **0s on the diagonal**. The total energy can therefore be written as

$$E_{\mathbf{X}}(x_1, \dots, x_N) = -\sum_{i=1}^{N} \sum_{j=1}^{i-1} w_{ij} x_i x_j + \sum_{i=1}^{N} b_i x_i = -\frac{1}{2} \sum_{i,j=1}^{N} w_{ij} x_i x_j + \sum_{i=1}^{N} b_i x_i$$

where $\mathbf{X} := \{X_1, \dots, X_N\}$.

# INTERPRETATION AS NETWORKS OF THRESHOLD UNITS

Consider a Boltzmann machine with $N$ units and assume that unit $k$ is in state $x_k = 0$. The change in total energy when unit $k$ changes from $0$ to $1$ is

$$\Delta E_k := E_{\mathbf{X}}(x_1, \dots, x_k = 1, \dots, x_N) - E_{\mathbf{X}}(x_1, \dots, x_k = 0, \dots, x_N) = -\sum_{i=1}^{N} w_{ki} x_i + b_k$$

Thus, in order to minimize the total energy, i.e. $\Delta E_k < 0$, unit $k$ should change its state from $0$ to $1$ if $\sum_i w_{ki} x_i > b_k$.

$\Longrightarrow b_k$ can be interpreted as a **threshold**, whereas $\sum_i w_{ki} x_i$ is the **input to unit** $k$, which activates the unit if it exceeds its threshold.

**Note:** This is exact for the deterministic versions of Boltzmann machines, so-called **Hopfield networks**. Boltzmann machines are their "soft-max" version (see next slide).

# SAMPLING MINIMUM ENERGY CONFIGURATIONS

Given a Boltzmann machine with fixed weights $w_{ij}$ and biases $b_i$, samples from the joint can be generated by successively sampling from the conditionals

$$p(X_k | X_1, \ldots, X_{i \neq k}, \ldots, X_N) \; .$$

That is, we start with a random configuration $\mathbf{x} = (x_1, \ldots, x_N)$ of the network and update it with new samples from the corresponding conditionals (this is also known as **Gibbs sampling**). We have

$$p(x_k | x_1, \ldots, x_{i \neq k}, \ldots, x_N) = \frac{1}{Z} \, e^{-E_{\mathbf{X}}(\mathbf{x})} = \frac{1}{Z} \, e^{\text{terms dep. on } k \, + \, \text{const wrt. } k} = \frac{1}{\tilde{Z}} \, e^{-\Delta E_k x_k}$$

where $\tilde{Z}$ depends on $x_1, \ldots, x_N$ except $x_k$.

Thus, in order to decide whether $X_k$ takes the value $0$ or $1$, we simply calculate the difference between the bias/threshold $b_k$ and the input to unit $k$, resulting in $\Delta E_k$, which determines the probability of $X_k = 1$ given all other samples by $p_k := \frac{1}{1+e^{\Delta E_k}}$.

# INVERSE TEMPERATURE

It is convenient, to introduce a scaling parameter $\beta > 0$, known as the **inverse temperature** due to its analogy with the Boltzmann distribution from thermodynamics, which is multiplied to the total energy, so that

$$p(x_1, \dots, x_N) = \frac{1}{Z} e^{-\beta E_{\mathbf{X}}(x_1, \dots, x_N)}, \qquad p_k = \frac{1}{1 + e^{\beta \Delta E_k}}$$

This allows to scale between deterministic Boltzmann machines (Hopfield networks) and very "soft" Boltzmann machines:

- $\beta \to \infty$: In this case, the sign of $\Delta E_k$ decides deterministically between $X_k = 1$ and $X_k = 0$ (i.e. $b_k$ is a hard threshold), since $\frac{1}{1+e^{\beta|\Delta E|}} \to 0$ and $\frac{1}{1+e^{-\beta|\Delta E|}} \to 1$ as $\beta \to \infty$.
- $\beta \to 0$: We have $p_k = \frac{1}{2}$, in particular the state of $X_k$ is independent of the energy.

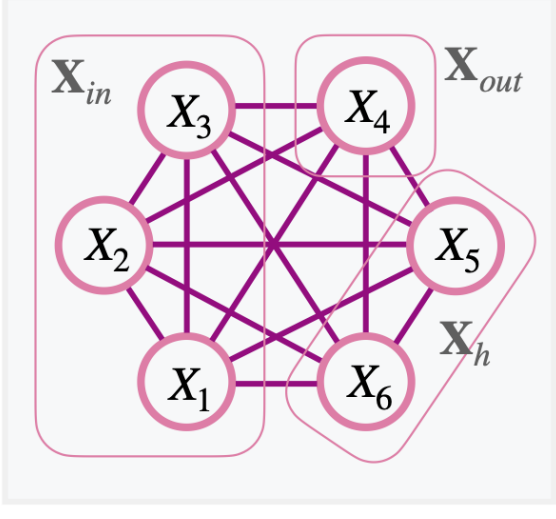
**Note:** This can be used for a **cooling** scheme, known as *simulated annealing*: start with small $\beta$, i.e. "high temperature" (to avoid getting stuck in local minima) and increase $\beta$ over time.

# LEARNING: VISIBLE AND HIDDEN UNITS

Using **maximum log-likelihood** the weights and biases of a Boltzmann machine can be adjusted such that its minimum energy configurations resemble a given set of binary example vectors as closely as possible.

To this end, the set $\mathbf{X} = \{X_1, \ldots, X_N\}$ of all nodes is split into two parts: $\mathbf{X} = \mathbf{X}_v \cup \mathbf{X}_h$:

- **Visible units** $\mathbf{X}_v = \mathbf{X}_{in} \cup \mathbf{X}_{out}$: These consist of all inputs and possibly (in case of supervised learning) outputs
- **Hidden units** $\mathbf{X}_h$: These are latent variables that are only used internally (marginalized out in the likelihood)



# LEARNING: OPTIMIZATION PROBLEM

Thus, learning in Boltzmann machines consists in solving the optimization problem

$$\max_{w,b} \mathbb{E}_{p_{\text{data}}(\mathbf{X}_v)} \Big[ \log p(\mathbf{X}_v) \Big] = \max_{w,b} \frac{1}{|\mathcal{D}|} \sum_{\mathbf{x}_v \in \mathcal{D}} \log \sum_{\mathbf{x}_h} p(\mathbf{x}_v, \mathbf{x}_h)$$

where $\mathcal{D}$ denotes a given dataset of $|\mathcal{D}|$ binary vectors corresponding to the visible units.

We have

$$\frac{\partial}{\partial w_{ij}} \log p(\mathbf{x}_v) = \cdots = \sum_{\mathbf{x}_h} \underbrace{\frac{e^{-\beta E(\mathbf{x}_v, \mathbf{x}_h)}}{\sum_{\mathbf{x}_h} e^{-\beta E(\mathbf{x}_v, \mathbf{x}_h)}}}_{p(\mathbf{x}_h | \mathbf{x}_v)} x_i x_j - \sum_{\mathbf{x}_v, \mathbf{x}_h} p(\mathbf{x}_v, \mathbf{x}_h) x_i x_j$$

and the derivative wrt. $b_i$ is the same, except of the sign and that $x_j$ is not present.

# LEARNING: GRADIENT ASCENT

In particular, using gradient ascent, we obtain the update equations ($\lambda$ is the learning rate)

$$w_{ij}^{t+1} \leftarrow w_{ij}^{t} + \lambda\left(\mathbb{E}_{p_{\text{data}}(\mathbf{X_v})p(\mathbf{X}_h|\mathbf{X}_v)}[X_iX_j] - \mathbb{E}_{p(\mathbf{X}_v,\mathbf{X}_h)}[X_iX_j]\right)$$

$$b_{i}^{t+1} \leftarrow b_{i}^{t} - \lambda\left(\mathbb{E}_{p_{\text{data}}(\mathbf{X_v})p(\mathbf{X}_h|\mathbf{X}_v)}[X_i] - \mathbb{E}_{p(\mathbf{X}_v,\mathbf{X}_h)}[X_i]\right)$$

In practice, these expected values are approximated using Gibbs sampling, in particular, every gradient ascent update step requires to simulate the boltzmann machine in two different ways (if hidden states are present):

- $\mathbb{E}_{p(\mathbf{X}_v,\mathbf{X}_h)}[\cdot]$ requires **samples from the equilibrium** (as before)
- $\mathbb{E}_{p_{\text{data}}(\mathbf{X_v})p(\mathbf{X}_h|\mathbf{X}_v)}[\cdot]$ requires to **fix the visible units** at the current datapoint $\mathbf{x}_v$ and to let the **hidden units equilibrate** using the same sampling scheme as for the second term.

**Note:** The update increment of $w_{ij}$ is sometimes written as $\lambda(\langle X_iX_j\rangle_{\text{data}} - \langle X_iX_j\rangle_{\text{model}})$ (analogous for $b_i$) because in the case of no hidden units, the first term is simply the expectation of $X_iX_j$ under the data distribution.

# DEGREES OF FREEDOM

A Boltzmannn machine with nodes $X_1, \ldots, X_N$ is not able to represent all possible distributions over these variables, because of the **restricting form of its energy,** which only considers $1$- and $2$-cliques.

This can be seen immediately when counting the degrees of freedom in the case of $N > 2$, e.g. for $N = 3$:

- a joint of 3 binary variables $X_1, X_2, X_3$ has $2^3 - 1 =$ **7 independent values**, whereas
- Boltzmann machines with three nodes have **6 parameters**: $b_1, b_2, b_3, w_{12}, w_{13}, w_{23}$.

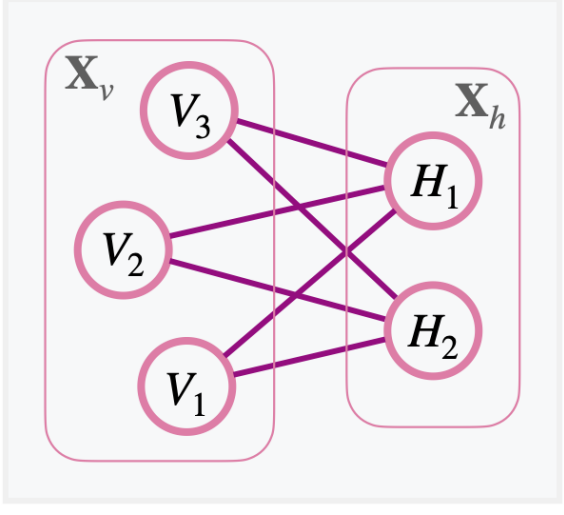
In general, Boltzmann machines have $N + N(N-1)/2 = N(N+1)/2$ parameters, which is smaller than the $2^N - 1$ parameters of a joint of $N$ binary variables if $N > 2$.

**Note:** Using hidden nodes the expressive power of a Boltzmann machine is increased, but the number of hidden units must grow exponentially in the number of variables to achieve full expressibility (see e.g. Le Roux, Bengio).

# RESTRICTED BOLTZMANN MACHINES

As can be seen in the exercises, even very simple tasks such as representing the XOR function can be challenging for a simple Boltzmann machine.

A more efficent model is obtained by removing all connections between visible nodes and between hidden nodes and **only keep the connections between hidden and visible nodes** in tact, resulting in *restricted Boltzmann machines* (RBMs).




Denoting the visible variables by $V_1, \ldots, V_n$ and the hidden variables by $H_1, \ldots, H_m$, and the biases of visible nodes by $a$ and the biases of hidden nodes by $b$, we obtain

$$E_{\mathbf{X}}(v_1, \ldots, v_n, h_1, \ldots, h_m) = -\sum_{i=1}^{n}\sum_{j=1}^{m} w_{ij} v_i h_j + \sum_{i=1}^{n} a_i v_i + \sum_{j=1}^{m} b_j h_j$$

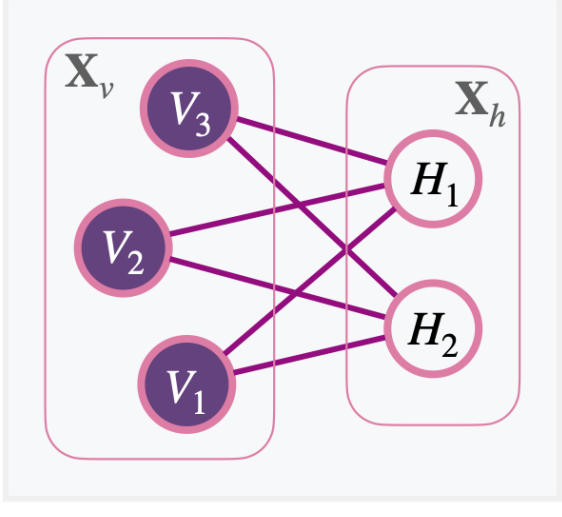
# CONDITIONAL INDEPENDENCE

In restricted Boltzmann machines, all hidden nodes are statistically independent given the set of visible nodes, and all visible nodes are statistically independent given the set of hidden nodes, because every path connecting any two nodes in one group of nodes has to go through a node of the other group.

We therefore have

$$p(\mathbf{H}|\mathbf{V}=\mathbf{v}) = \prod_{i=1}^{m} p(H_i|\mathbf{V}=\mathbf{v})$$

$$p(\mathbf{V}|\mathbf{H}=\mathbf{h}) = \prod_{i=1}^{n} p(V_i|\mathbf{H}=\mathbf{h})$$



# SAMPLING MINIMUM ENERGY CONFIGURATIONS

Due to the conditional independence properties, Gibbs sampling now consists of only two steps that are alternated:

- Given a random sample $\mathbf{V} = \mathbf{v}$, update all hidden states in parallel by sampling from $p(H_j|\mathbf{v})$, where

$$p(H_j = 1|\mathbf{v}) = \frac{1}{1 + e^{\beta \Delta E_j^h}}, \quad \Delta E_j^h = -\sum_i w_{ij} v_i + b_j$$

- Update all visible states in parallel by sampling from $p(V_i|\mathbf{h})$, where

$$p(V_i = 1|\mathbf{h}) = \frac{1}{1 + e^{\beta \Delta E_i^v}}, \quad \Delta E_i^v = -\sum_j w_{ij} h_j + a_i$$

# LEARNING: STANDARD LEARNING RULE

Maximum log-likelihood estimation using Gradient ascent results in the same learning rule as in regular Boltzmann machines, where $p(\mathbf{H}|\mathbf{V})$ in the first term is replaced by $p(H_j|\mathbf{V})$:

$$w_{ij}^{t+1} \leftarrow w_{ij}^{t} + \lambda\left(\mathbb{E}_{p_{\text{data}}(\mathbf{V})p(H_j|\mathbf{V})}[V_i H_j] - \mathbb{E}_{p(\mathbf{V},\mathbf{H})}[V_i H_j]\right)$$

with an analogous simplified rule for the biases, as previously.

- The first term is determined by selecting random training samples $\mathbf{v}$ and **sampling hidden states in parallel** using $p(H_j|\mathbf{v})$ (see previous slide).
- The second term requires samples of minimum energy configurations using **Gibbs sampling**.

Even though learning in RBMs is more stable than in regular Boltzmann machines, Gibbs sampling can still take a long time. In Hinton 2002, a **faster learning rule** was proposed, approximately minimizing the so-called **contrastive divergence**.

# LEARNING: CONTRASTIVE DIVERGENCE

Let $q^0, q^1, \ldots, q^\infty$ denote the distributions over visible states $\mathbf{v}$ that result from Gibbs sampling steps $0, 1, \ldots, \infty$, starting at the data distribution, i.e. $q^0 = p_{\text{data}}$, and eventually ending at the equilibrium distribution, i.e. $q^\infty = p$. For example,

$$q^1(\mathbf{v}) = \sum_{\mathbf{h}} p(\mathbf{v}|\mathbf{h}) \sum_{\mathbf{v}'} p(\mathbf{h}|\mathbf{v}')q^0(\mathbf{v}') = \sum_{\mathbf{v}'} p(\mathbf{v}|\mathbf{v}')q^0(\mathbf{v}'), \quad q^2(\mathbf{v}) = \sum_{\mathbf{v}'} p(\mathbf{v}|\mathbf{v}')q^1(\mathbf{v}'), \ldots$$

Maximizing the average log-likelihood $\mathbb{E}_{q^0(\mathbf{V})}[\log q^\infty(\mathbf{V})]$ is equivalent to minimizing $D_{\text{KL}}(q^0 \| q^\infty) = \mathbb{E}_{q^0}[\log q^0] - \mathbb{E}_{q^0}[\log q^\infty]$. Note the following facts:

- By Jensen's inequality, $D_{\text{KL}}(q^1 \| q^\infty) \leq D_{\text{KL}}(q^0 \| q^\infty)$ with equality only if $q^1 = q^0$, expressing the fact that $q^1$ is one step closer to $q^\infty$ than $q^0$.
- If $q^1 = q^0$ then $q^\infty = q^0$ ($\Pi q^0 = q^0 \Rightarrow \Pi^n q^0 = q^0$, where $\Pi q(\mathbf{v}) := \sum_{\mathbf{v}'} p(\mathbf{v}|\mathbf{v}')q(\mathbf{v}')$)

**Contrastive Divergence Learning:** Minimize the difference $D_{\text{KL}}(q^0 \| q^\infty) - D_{\text{KL}}(q^1 \| q^\infty)$ which is non-negative and takes its minimum at $q^\infty = q^0$.

# LEARNING: APPROXIMATE CONTRASTIVE DIVERGENCE

Contrastive divergence is usually applied to cancel untractable expectations with respect to $q^\infty$ that appear in both divergences. This is also true in RBMs, even though the following learning rule only approximately minimizes contrastive divergence:

$$w_{ij}^{t+1} \leftarrow w_{ij}^t + \lambda\Big(\mathbb{E}_{q^0(\mathbf{V})p(H_j|\mathbf{V})}[V_i H_j] - \mathbb{E}_{q^1(\mathbf{V})p(H_j|\mathbf{V})}[V_i H_j]\Big)$$

It is motivated by

$$\frac{\partial}{\partial w_{ij}} D_{\mathrm{KL}}(q^0 \| q^\infty) = -\mathbb{E}_{q^0}\left[\frac{\partial}{\partial w_{ij}} \log q^\infty\right] = -\Big(\mathbb{E}_{q^0(\mathbf{V})p(H_j|\mathbf{V})}[V_i H_j] - \mathbb{E}_{q^\infty}[V_i H_j]\Big)$$

$$\frac{\partial}{\partial w_{ij}} D_{\mathrm{KL}}(q^1 \| q^\infty) \approx -\mathbb{E}_{q^1}\left[\frac{\partial}{\partial w_{ij}} \log q^\infty\right] = -\Big(\mathbb{E}_{q^1(\mathbf{V})p(H_j|\mathbf{V})}[V_i H_j] - \mathbb{E}_{q^\infty}[V_i H_j]\Big)$$

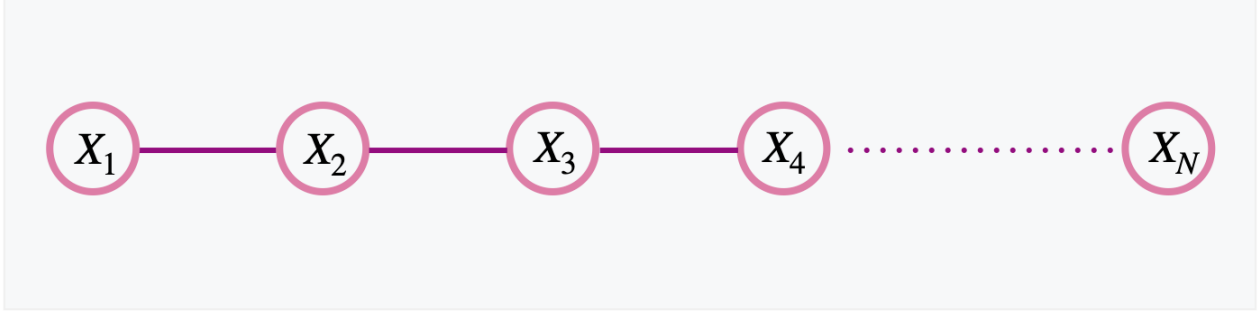
where the approximation consists in ignoring the $w$-dependency of $q^1$. The simplified update rules for the biases are analogous as before.

# MESSAGE PASSING

# INFERENCE ON A CHAIN

Consider a graphical model with nodes $X_1, \ldots, X_N$ only consisting of $2$-cliques with every node being part of exactly two cliques, except of $X_1$ and $X_N$ that are only part of one, i.e. the variables can be ordered as a chain with joint

$$p(\mathbf{X}) = \frac{1}{Z}\psi_{1,2}(X_1, X_2)\,\psi_{2,3}(X_2, X_3)\cdots\psi_{N-2,N-1}(X_{N-2}, X_{N-1})\,\psi_{N-1,N}(X_{N-1}, X_N)$$




**Note:** Examples of such graphical models are Markov chains, where each clique potential takes the form of a conditional probability of one node given another node, turning the undirected into a directed graph.

# MARGINALS

Assume that we want to dermine the distribution of node $k$ given that no other variables are observed, i.e. we want to calculate the marginal $p(X_k)$.

The naive approach is to calculate the full joint $p(X_1, \dots, X_N)$ and then to take sum over all other variables $\mathbf{x}_{\setminus k} = (x_1, \dots, x_{i \neq k}, \dots, x_N)$, i.e. $p(X_k) = \sum_{\mathbf{x}_{\setminus k}} p(x_1, \dots, x_{k-1}, X_k, x_{k+1}, \dots, x_N)$. Assuming that all variables $X_i$ have $K$ possible values, the joint $p(\mathbf{X})$ consists of $K^N$ numbers, i.e. the amount of terms that have to be added in the naive calculation of $p(X_k)$ grows exponentially with $N$.

Another approach is to use the factorization of $p$ in order to reduce the number of calculations: $\psi_{1,2}$ is the only factor that depends on $x_1$, and similarly $\psi_{N-1,N}$ is the only factor that depends on $x_N$, so that the sum over $x_1$ and $x_N$ can be taken immediately, and so on:

$$p(X_k) = \frac{1}{Z} \sum_{x_{k-1}} \psi_{k-1,k}(x_{k-1}, X_k) \cdots \sum_{x_2} \psi_{2,3}(x_2, x_3) \sum_{x_1} \psi_{1,2}(x_1, x_2)$$

$$\times \sum_{x_{k+1}} \psi_{k,k+1}(X_k, x_{k+1}) \cdots \sum_{x_{N-1}} \psi_{N-2,N-1}(x_{N-2}, x_{N-1}) \sum_{x_N} \psi_{N-1,N}(x_{N-1}, x_N)$$

INFERENCE ON A CHAIN

# MARGINALS: MESSAGES

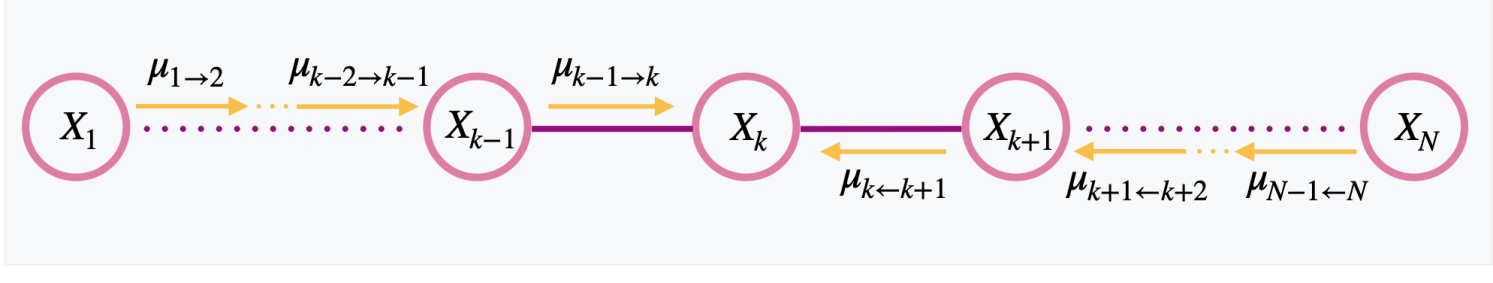
If we define the **forward message from** $1$ **to** $2$ and **backward message from** $N$ **to** $N-1$

$$\mu_{1\to 2}(x_2) := \sum_{x_1} \psi_{1,2}(x_1, x_2), \qquad \mu_{(N-1)\leftarrow N}(x_{N-1}) := \sum_{x_N} \psi_{N-1,N}(x_{N-1}, x_N)$$

and for $1 < i < N$, the **forward** and **backward messages from** $i$ **to** $i+1$ **and** $i-1$,

$$\mu_{i\to i+1}(x_{i+1}) := \sum_{x_i} \psi_{i,i+1}(x_i, x_{i+1})\, \mu_{i-1\to i}(x_i),$$
$$\mu_{i-1\leftarrow i}(x_{i-1}) := \sum_{x_i} \psi_{i-1,i}(x_{i-1}, x_i)\, \mu_{i\leftarrow i+1}(x_i),$$

then $p(X_k) = \frac{1}{Z}\, \mu_{k-1\to k}(X_k)\, \mu_{k\leftarrow k+1}(X_k)$ is the **product of messages sent from the preceding node** $X_{k-1}$ **and the succeeding node** $X_{k+1}$ **to node** $X_k$.



INFERENCE ON A CHAIN

# MARGINALS: COMPUTATIONAL COMPLEXITY

Assuming that all variables have $K$ possible values, then each of the $K - 1$ independent values of $p(X_k)$ requires to calculate $N - 1$ messages

$$\underbrace{\mu_{1\to 2}, \dots, \mu_{k-1\to k}}_{k-1 \text{ messages}}, \underbrace{\mu_{k\leftarrow k+1}, \dots, \mu_{N-1\leftarrow N}}_{N-k \text{ messages}},$$

where each message is determined by a sum of at most $K$ terms. In particular, the number of terms that have to be summed **grows linearly in** $N$, whereas in the naive calculation that number grows **exponentially in** $N$ (more precisely, $\mathcal{O}(K^2 N)$ vs. $\mathcal{O}(K^N)$).

Additionally, if we want to determine all $N$ marginals $p(X_1), \dots, p(X_N)$, then each message only has to be calculated once and can be used in multiple places, i.e. we only need twice the amount of messages than for a single marginal.

## CONDITIONALS

If a variable is observed, then **the summation over that variable is simply replaced by evaluating the corresponding clique potentials at the observed value**. Otherwise, the messages are calculated by the same iteration as before, in particular

$$p(X_k|\mathbf{X}_o = \mathbf{x}_o) = \frac{1}{Z}\,\mu_{k-1\to k}(X_k, \mathbf{x}_o)\,\mu_{k\leftarrow k+1}(X_k, \mathbf{x}_o)$$

where $\mathbf{X}_o \subset \{X_1, \ldots, X_N\}$ denotes the set of observed variables, and the extra dependency on $\mathbf{x}_o$ in the backward and forward messages indicates that those variables are not summed out in the iteration.

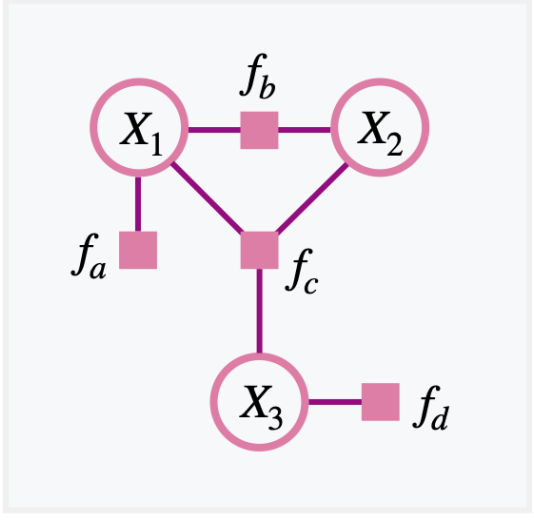
The inference algorithm discussed so far can be considered a special case of the **sum-product algorithm** for tree-structured graphs, for which we need to introduce **factor graphs**.

# FACTOR GRAPHS

Factor graphs are similar to undirected graphs in that they do not contain arrows, but they can contain **more specific information about the decomposition of the joint**, e.g.,

$$p(X_1, X_2, X_3) = f_a(X_1)\, f_b(X_1, X_2)\, f_c(X_1, X_2, X_3)\, f_d(X_3),$$

because **each factor** $f_a, f_b, \ldots,$ **obtains its own node** in the graph, indicated by a filled square, and is connected to the variables of that factor.




In an undirected graph, the joint above would simply contain the three variables and links between them (see e.g. this slide)

# INFERENCE IN FACTOR GRAPHS

Factor graphs allow a very simple message passing algorithm, generalizing what we derived for chains to the so-called **sum-product algorithm**.

- To this end, messages are always considered to be sent **from factors to nodes** and **from nodes to factors** (thereby getting rid of "backward" messages, since direction is artificial in undirected graphs anyways), denoted by $\mu$ and $\nu$, respectively.
- It is traditional to denote **variable indices** by $i, j, k, \ldots \in \{1, 2, 3, \ldots\}$ and **factor indices** by $s, t, u, \ldots \in \{a, b, c, \ldots\}$, i.e. the two types of messages may generally be denoted by $\mu_{s \to i}$ (factor to variable) and $\nu_{i \to s}$ (variable to factor).
- *Goal*: The marginal of a variable is calculated by the (normalized) **product of all incoming messages** from the neighbouring factors.

Based on this goal, in the following, we construct messages for various cases in order to **motivate the sum-product algorithm** for general graphs (for a more detailed derivation see e.g. Bishop, Chapter 8.4).

# EXAMPLE: CHAINS

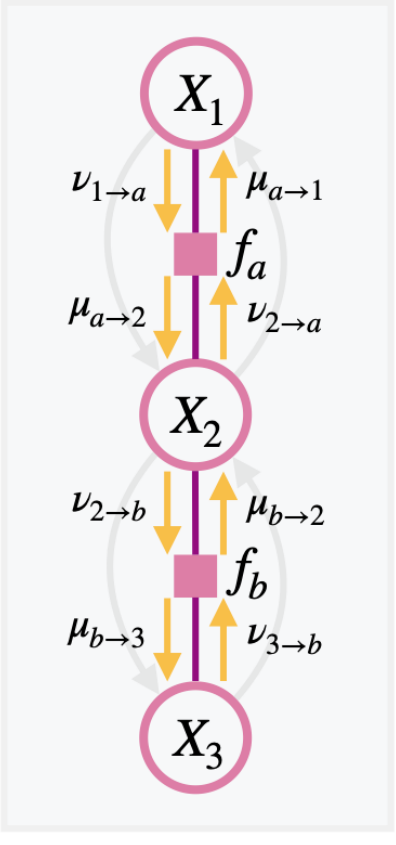
Consider a chain of three variables $X_1, X_2, X_3$. Writing $f_a := \psi_{1,2}$ and $f_b := \psi_{2,3}$ then the message equations are given by

$$\mu_{1\to 2}(x_2) = \sum_{x_1} f_a(x_1, x_2)\, \nu_{1\to a}(x_1) \quad =: \mu_{a\to 2}(x_2)$$

$$\mu_{2\to 3}(x_3) = \sum_{x_2} f_b(x_2, x_3)\, \nu_{2\to b}(x_2) \quad =: \mu_{b\to 3}(x_3)$$

$$\mu_{2\leftarrow 3}(x_2) = \sum_{x_3} f_b(x_2, x_3)\, \nu_{3\to b}(x_3) \quad =: \mu_{b\to 2}(x_2)$$

$$\mu_{1\leftarrow 2}(x_1) = \sum_{x_2} f_a(x_1, x_2)\, \nu_{2\to a}(x_2) \quad =: \mu_{a\to 1}(x_1)$$




$\Longrightarrow$ For **boundary variables** $X_i$ (only connected to a single factor $f_s$): $\nu_{i\to s}(x_i) = 1$.

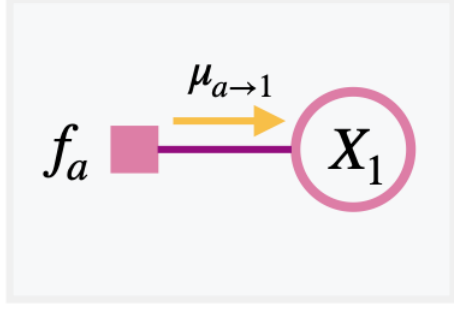
$\Longrightarrow$ In a chain, **interior variables** pass through the incoming message from the factor

# EXAMPLE: BOUNDARY FACTOR

Consider a factor graph consisting of only one variable $X_1$ and one factor node $f_a$. Since the distribution $p(X_1)$ must be the (normalized) product of all incoming messages, we have

$$p(x_1) = \frac{1}{Z} f_a(x_1) = \frac{1}{Z} \mu_{a \to 1}(x_1)$$

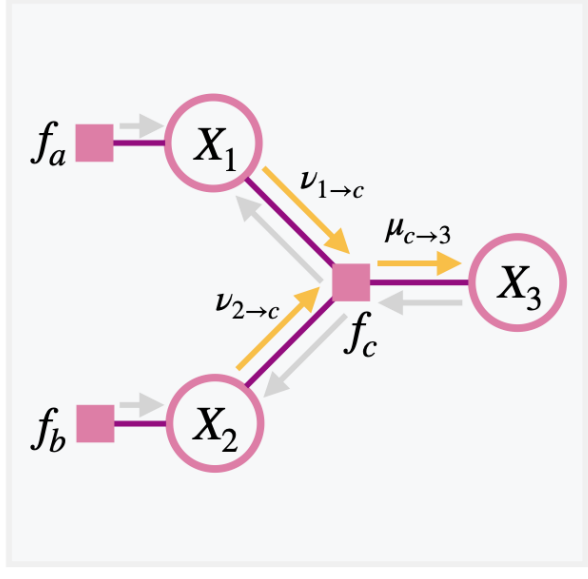
and thus $\mu_{a \to 1}(x_1) = f_a(x_1)$.




$\Longrightarrow$ The message from a **boundary factor** $f_s$ to its only node $X_i$ is simply $\mu_{s \to i}(x_i) = f_s(x_i)$.

# EXAMPLE: MESSAGE FROM FACTOR TO NODE

For **interior factor nodes** in chains, we know that the message to the next variable is created by multiplying the incoming message from the previous variable with the factor and summing out the previous variable. Here, we have




$$p(x_3) \propto \sum_{x_1,x_2} f_c(x_1,x_2,x_3)\, f_a(x_1)\, f_b(x_2) \;\propto\; \mu_{c\to 3}(x_3)$$

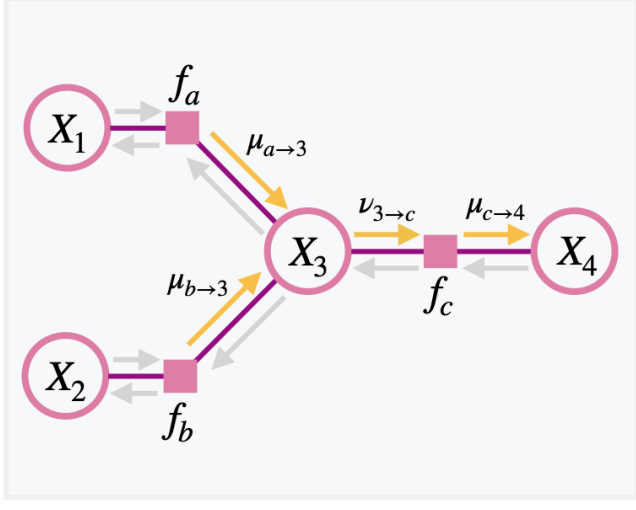
and we know already $f_a(x_1) = \mu_{a\to 1}(x_1) = \nu_{1\to c}(x_1)$ and similarly $f_b(x_2) = \nu_{2\to c}(x_2)$. Hence,

$$\mu_{c\to 3}(x_3) = \sum_{x_1,x_2} f_c(x_1,x_2,x_3)\, \nu_{1\to c}(x_1)\, \nu_{2\to c}(x_2)$$

$\Longrightarrow$ For the message of an **interior factor node** $s$ to one of its variables $X_i$, we **multiply** $f_s$ **with the incoming messages** from the other variables $X_j \neq X_i$ and **sum out** those variables.

# EXAMPLE: MESSAGE FROM NODE TO FACTOR

For **interior variable nodes** in chains, we alredy know that the incoming message from the previous factor is simply passed through to the next factor. Here, we have




$$p(x_4) \propto \sum_{x_1,x_2,x_3} f_a(x_1,x_3)\, f_b(x_2,x_3)\, f_c(x_3,x_4) \propto \mu_{c\to 4}(x_4)$$

and since $f_c$ is an interior node like in a chain, we know that $\mu_{c\to 4}(x_4) = \sum_{x_3} f_c(x_3,x_4)\, \nu_{3\to c}(x_3)$, so that

$$\nu_{3\to c}(x_3) = \Big(\sum_{x_1} f_a(x_1,x_3)\Big)\Big(\sum_{x_2} f_b(x_2,x_3)\Big) = \mu_{a\to 3}(x_3)\, \mu_{b\to 3}(x_3)$$

$\Longrightarrow$ For the message of an **interior variable node** $X_i$ to one of the connected factors $f_s$, we **multiply the incoming messages** from the other factors connected to $X_i$.

# FINAL FORM OF MESSAGES

Consider a factor graph of random variables $X_1, X_2, \ldots$ and factors $f_a, f_b, \ldots$. Let $N(i)$ denote the index set of neighbours of $X_i$, i.e. the **indices $a, b, \ldots$ of factors that depend on $X_i$**, and $N(s)$ the index set of neighbours of $f_s$, i.e. the **indices $i, j, \ldots$ of the variables of $f_s$**.

Let messages $\mu_{s \to i}$ and $\nu_{i \to s}$ be calculated as follows:

$$\nu_{i \to s}(x_i) := \prod_{t \in N(i) \setminus \{s\}} \mu_{t \to i}(x_i)$$

$$\mu_{s \to i}(x_i) := \sum_{\mathbf{x}_s \setminus \{x_i\}} f_s(\mathbf{x}_s) \prod_{j \in N(s) \setminus \{i\}} \nu_{j \to s}(x_j)$$

where $\mathbf{x}_s$ denotes the set of variables of factor $f_s$.

Moreover, for the cases of no incoming messages: the message $\nu_{i \to s}$ from a variable that only appears in a single factor ($f_s$) is set to $1$, whereas the message $\mu_{s \to i}(x_i)$ of a factor that only depends on a single variable ($x_i$) is set to $f_a(x_i)$.

THE SUM-PRODUCT ALGORITHM

# MARGINALS

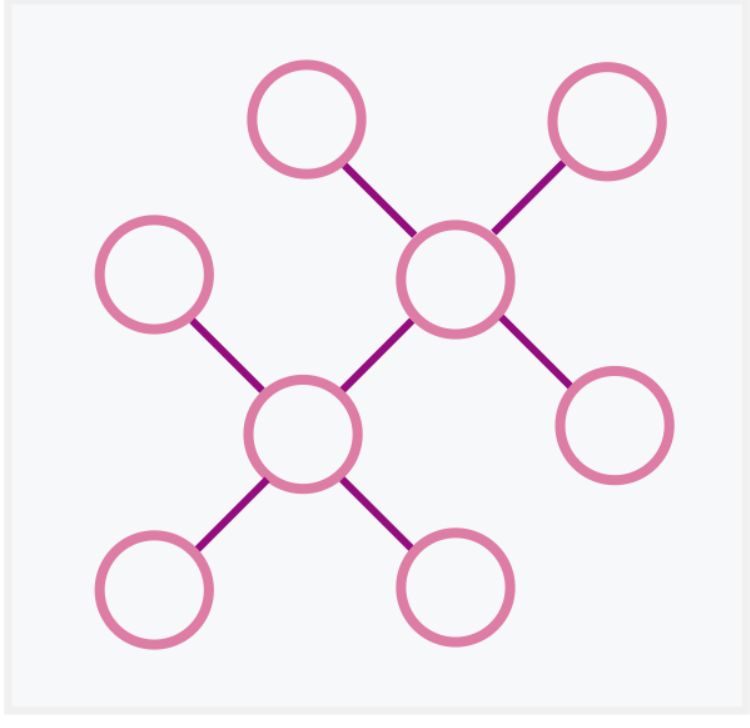
**Theorem**: *For tree-structured graphs, the marginal $p(X_k)$ is given by the (normalized) product of all incoming messages:*

$$p(X_k) = \frac{1}{Z} \prod_{s \in N(k)} \mu_{s \to k}(X_k)$$

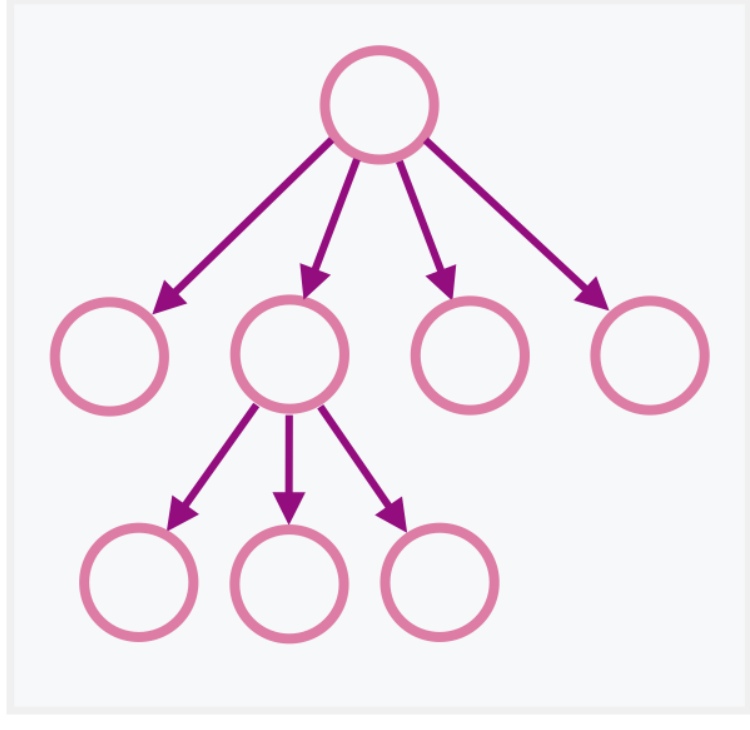
where **tree-structured graphs** are

- **trees**: undirected graphs with only one path between any two nodes, and directed graphs whose moral graph is a tree (i.e. each node has at most one parent), and
- **polytrees**: directed graphs where each node can have more than one parent but there is still only one path between any two nodes in the directed graph (their moral graphs can have cycles, i.e. are not trees)

# TREES

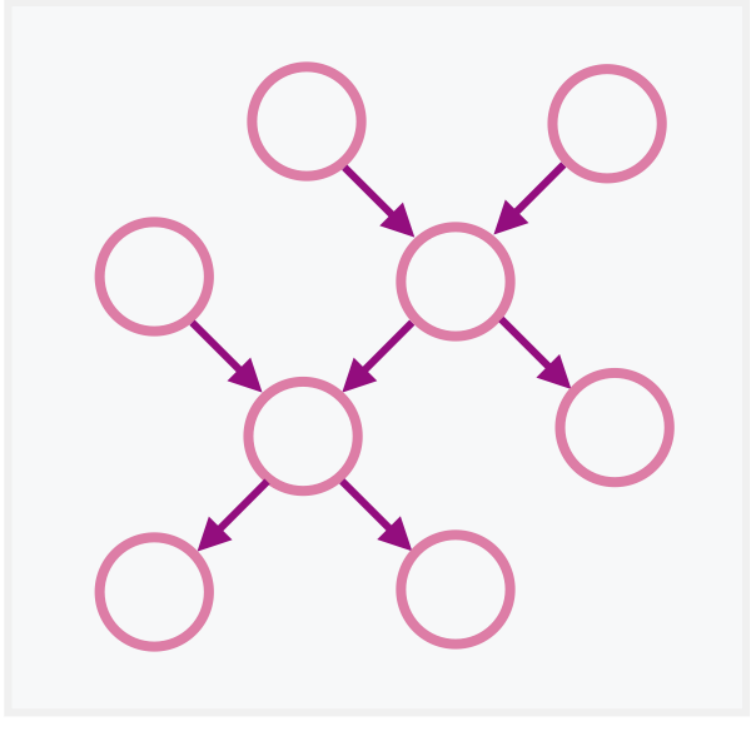


a **tree**

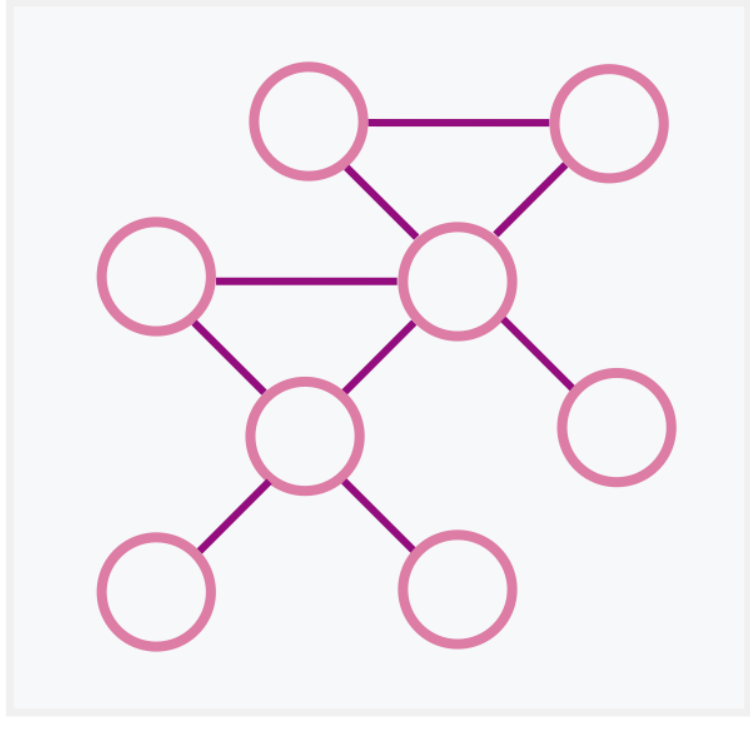


a **directed tree** with a single root node

# POLYTREES



a **polytree**



corresponding moral graph
(**not** necessarily coming from a polytree)

# CONDITIONALS

**So far**: calculate marginals $p(X_k)$ given that all other variables are unknown.

**Conditioning on observed variables $\mathbf{X}_o$** is analogous to marginalization except that sums over $\mathbf{X}_o$ are replaced by evaluations at the observed values $\mathbf{x}_o$.

In particular, **messages from factors to nodes** are determined by the same procedure as before, just that now the **summation is only over unobserved variables**, whereas any variable $X_j \in \mathbf{X}_o$ is simply evaluated at its observed value $x_j \in \mathbf{x}_o$,

$$\mu_{s \to i}(x_i) := \sum_{\mathbf{x}_s \setminus \{x_i, \mathbf{x}_o\}} f_s(\mathbf{x}_s) \prod_{j \in N(s) \setminus \{i\}} \nu_{j \to s}(x_j)$$

where $\mathbf{x}_s$ contains both, unobserved variables of $f_s$ over which is summed and observed variables of $f_s$ which are simply clamped at their values.

All the other messages are the same.

# FACTOR MARGINALS AND CONDITIONALS

In analogy to marginals of single variable nodes, we can also use the messages to determine the marginal of a factor, i.e. the joint distribution of the variables $\mathbf{X}_s$ connected to a given factor $f_s$, by the normalized product of all incoming messages and the corresponding factor,

$$p(\mathbf{x}_s) \;=\; \tfrac{1}{Z}\, f_s(\mathbf{x}_s) \prod_{i \in N(s)} \nu_{i \to s}(x_i)$$

and similarly for the conditionals $p(\mathbf{X}_s | \mathbf{X}_o = \mathbf{x}_o)$ with the corresponding messages as for single-variable conditionals.

Having an efficient way to calculate single-variable conditionals *and* factor conditionals is particularly useful in the **EM algorithm for Hidden Markov Models**, as we shall see later.

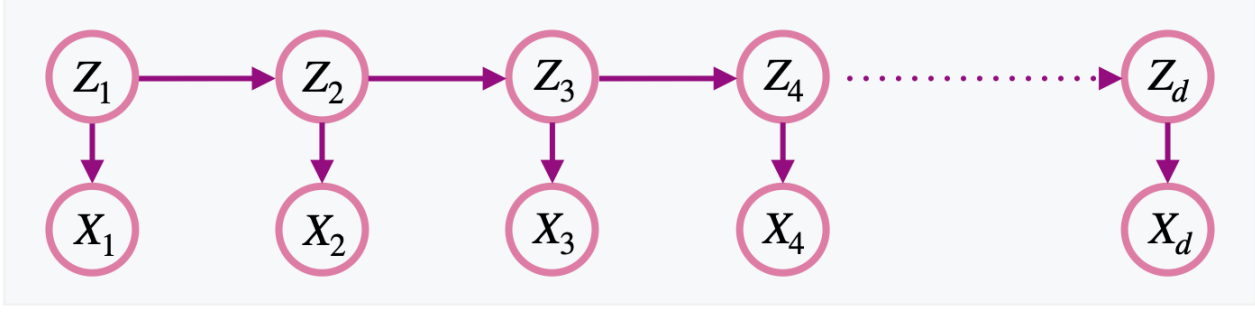
## OTHER MESSAGE PASSING ALGORITHMS

- *Max-sum algorithm*: Very similar to the sum-product algorithm, but for **MAP estimation** (the sum-product algorithm performs exact Bayesian inference on trees).
- *Junction tree algorithm*: message-passing for **more general graphical models** by first creating a new tree (the *junction tree*) that represents the relations between cliques of a processed version of the original graph and then performing message passing on that tree.
- *Loopy belief propagation*: **approximate inference** through message-passing in graphical models with loops. For some models, this converges, for others it does not.

# LEARNING IN HMMS

As we have seen in Section 2, a Hidden Markov Model (HMM) consists of observable variables $X_1, \ldots, X_d$ and hidden states $Z_1, \ldots, Z_d$, related by a joint of the form

$$p(\mathbf{X}, \mathbf{Z}) = p(Z_1) \prod_{k=2}^{d} p(Z_k|Z_{k-1}) \prod_{n=1}^{d} p(X_n|Z_n)$$




In the following, we will use **message-passing** to perform Bayesian inference over the hidden states, which is required for **maximum likelihood estimation** through the **EM algorithm**.

LEARNING IN HMMS

# EM ALGORITHM

Assuming that the emission and transition probabilities $p_\theta(X_i|Z_i)$ and $p_\theta(Z_{i+1}|Z_i)$, as well as $p_\theta(Z_1)$, are parametrized by a set of parameters $\theta$, we can perform **maximum likelihood estimation** in order to learn from given sequential data $\mathbf{x} = (x_1, \dots, x_d)$:

$$\theta^* = \operatorname{argmax}_\theta \log p_\theta(\mathbf{x}) = \operatorname{argmax}_\theta \log \sum\nolimits_{\mathbf{z}} p_\theta(\mathbf{x}, \mathbf{z})$$

where, if we assume that each hidden variable has $K$ states, the marginalization over $\mathbf{Z}$ consists of $K^d$ terms and thus is intractible for practical values of $d$.

This is the use-case of the standard EM algorithm (which can be considered a **special case of the variational EM algorithm**, see the exercises): Initialize $\theta$ and iterate the two steps

- **E-step**: Given $\theta$, determine the Bayes' posterior $q(\mathbf{Z}) := p_\theta(\mathbf{Z}|\mathbf{x})$
- **M-step**: Update $\theta$ by maximizing $\mathbb{E}_{q(\mathbf{Z})}[\log p_\theta(\mathbf{x}, \mathbf{Z})]$

# M-STEP

The M-step consists in maximizing

$$\mathbb{E}_{q(\mathbf{Z})}[\log p_\theta(\mathbf{x}, \mathbf{Z})] = \mathbb{E}_{q(\mathbf{Z})}\Big[\sum_{k=1}^{d}\Big(\log p_\theta(x_k|Z_k) + \log p_\theta(Z_k|Z_{k-1})\Big)\Big]$$

where, for simplicity, we write $p_\theta(Z_1|Z_0) := p_\theta(Z_1)$. Using the linearity of expectation,

$$\mathbb{E}_{q(\mathbf{Z})}[\log p_\theta(\mathbf{x}, \mathbf{Z})] = \sum_{k=1}^{d}\Big(\mathbb{E}_{q(Z_k)}\Big[\log p_\theta(x_k|Z_k)\Big] + \mathbb{E}_{q(Z_{k-1},Z_k)}\Big[\log p_\theta(Z_k|Z_{k-1})\Big]\Big)$$

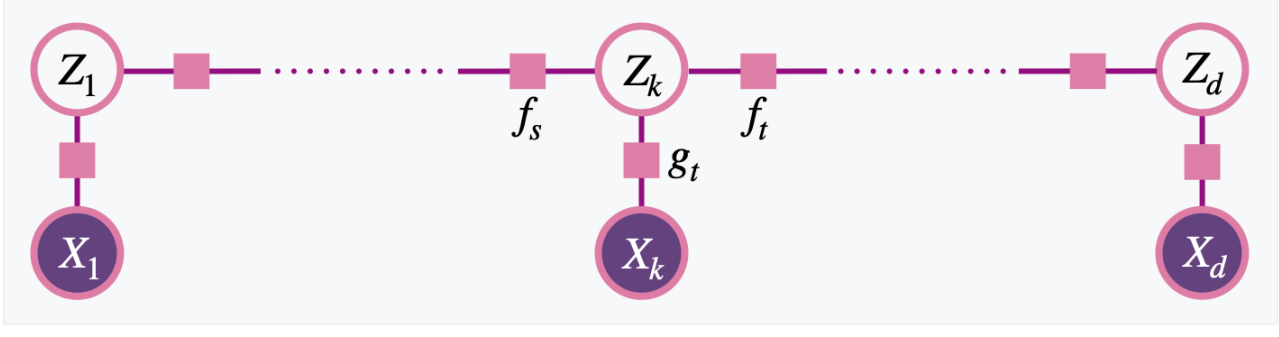
from which it follows that we **only need the single-variable marginals** $q(Z_k)$ and **two-variable marginals** $q(Z_{k-1}, Z_k)$.

LEARNING IN HMMS

# E-STEP: FACTOR GRAPH FOR THE SUM-PRODUCT-ALGORITHM

Canonical choice for a **factor graph of an HMM**: Variables $\mathbf{X}, \mathbf{Z}$ and factors

$$f_s(z_{k-1}, z_k) := p_\theta(z_k | z_{k-1}), \qquad g_t(x_k, z_k) := p_\theta(x_k | z_k)$$




**Note:** Another choice would be to absorb the emission probabilities in the transition probabilities, since $x_1, \ldots, x_d$ are assumed to be constant throughout.

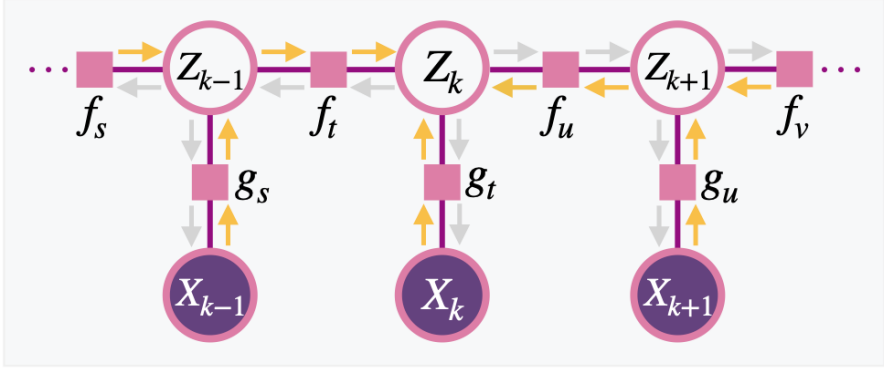
**Notation:** Here, we need to include the variable and factor names in the messages, e.g., $\mu_{f_s \to Z_k}$, $\mu_{g_t \to Z_k}$, etc...

LEARNING IN HMMS

# E-STEP: SINGLE-VARIABLE MARGINALS

For each hidden state $Z_k$ there are three incoming messages (except at the boundary),

$$q(z_k) = \frac{1}{Z}\, \mu_{g_t \to Z_k}(z_k)\, \mu_{f_t \to Z_k}(z_k)\, \mu_{f_u \to Z_k}(z_k)$$



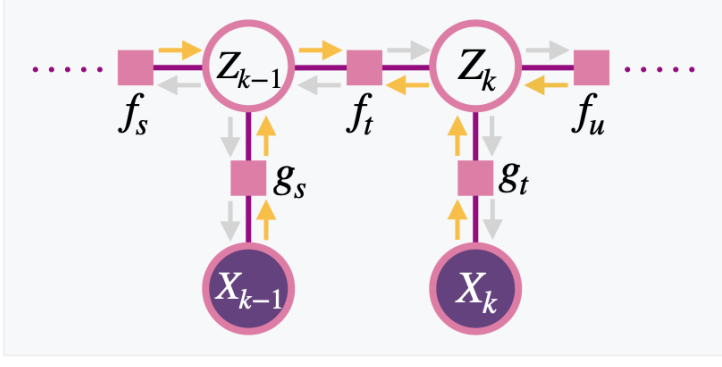

where the message from $g_t$ is simply the emission probability, and the messages from $f_t$ and $f_u$ are calculated iteratively:

- $\mu_{g_t \to Z_k}(z_k) = g_t(z_k, x_k) = p_\theta(x_k | z_k)$
- $\mu_{f_t \to Z_k}(z_k) = \sum_{z_{k-1}} f_t(z_{k-1}, z_k)\, g_s(z_{k-1}, x_{k-1})\, \mu_{f_s \to Z_{k-1}}(z_{k-1})$
- $\mu_{f_u \to Z_k}(z_k) = \sum_{z_{k+1}} f_u(z_k, z_{k+1})\, g_u(z_{k+1}, x_{k+1})\, \mu_{f_v \to Z_{k+1}}(z_{k+1})$

# E-STEP: FACTOR MARGINALS

The two-variable factor marginals are determined by the product of the factor itself and the two incoming messages from the nodes $Z_{k-1}$ and $Z_k$,

$$q(Z_{k-1}, Z_k) = \frac{1}{Z} f_t(z_{k-1}, z_k)\, \nu_{Z_{k-1}\to f_t}(z_{k-1})\, \nu_{Z_k\to f_t}(z_k)$$




which can be determined from the factor-to-node messages that we already have to calculate for the single-variable marginals:

- $\nu_{Z_{k-1}\to f_t}(z_{k-1}) = g_s(z_{k-1}, x_{k-1})\, \mu_{f_s\to Z_{k-1}}(z_{k-1})$
- $\nu_{Z_k\to f_t}(z_k) = g_t(z_k, x_k)\, \mu_{f_u\to Z_k}(z_k)$