3. Probabilistic Graphical Models

The Bayes Filter (Rep.)

$$\mathrm{Bel}(x_t) = p(x_t \mid u_1, z_1, \ldots, u_t, z_t)$$

(Bayes) $$= \eta\, p(z_t \mid x_t, u_1, z_1, \ldots, u_t) p(x_t \mid u_1, z_1, \ldots, u_t)$$

(Markov) $$= \eta\, p(z_t \mid x_t) p(x_t \mid u_1, z_1, \ldots, u_t)$$

(Tot. prob.) $$= \eta\, p(z_t \mid x_t) \int p(x_t \mid u_1, z_1, \ldots, u_t, x_{t-1}) p(x_{t-1} \mid u_1, z_1, \ldots, u_t) dx_{t-1}$$

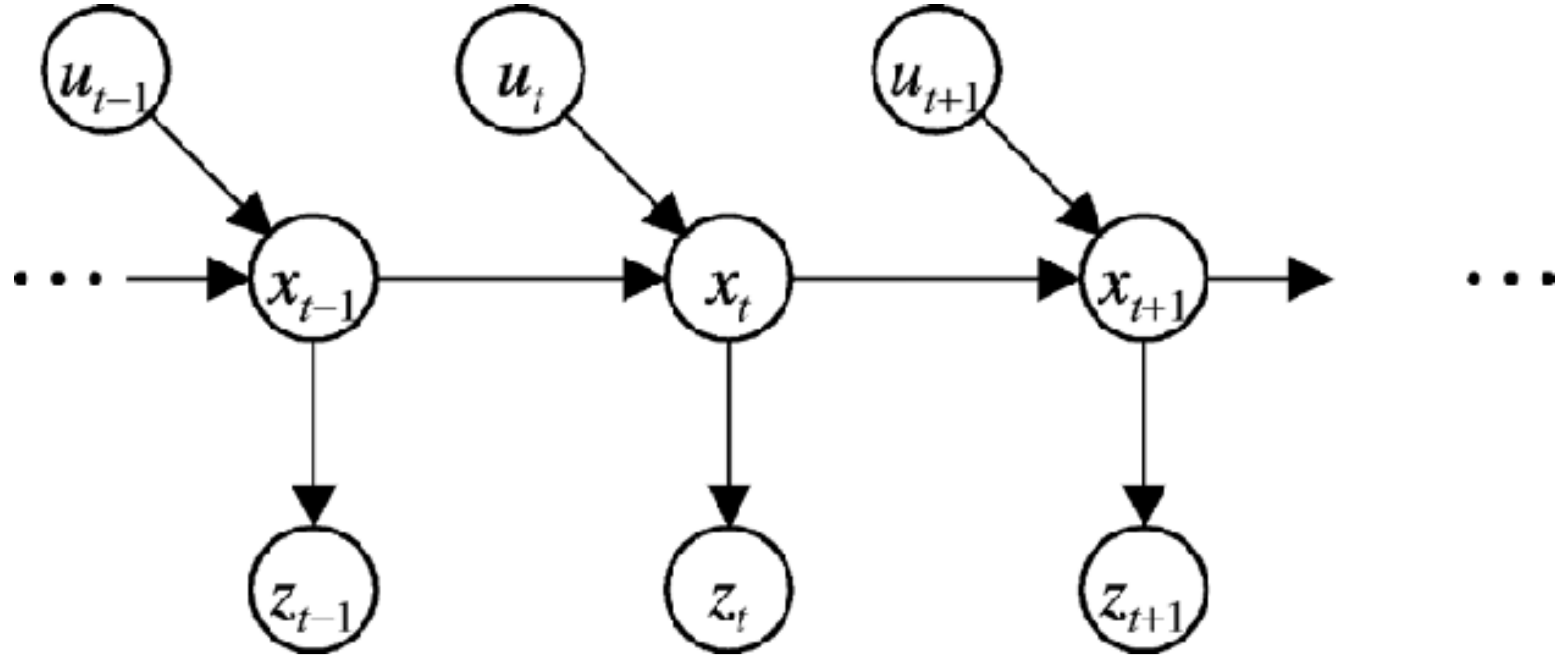
(Markov) $$= \eta\, p(z_t \mid x_t) \int p(x_t \mid u_t, x_{t-1}) p(x_{t-1} \mid u_1, z_1, \ldots, u_t) dx_{t-1}$$

(Markov) $$= \eta\, p(z_t \mid x_t) \int p(x_t \mid u_t, x_{t-1}) p(x_{t-1} \mid u_1, z_1, \ldots, z_{t-1}) dx_{t-1}$$

$$= \eta\, p(z_t \mid x_t) \int p(x_t \mid u_t, x_{t-1}) \mathrm{Bel}(x_{t-1}) dx_{t-1}$$

Graphical Representation (Rep.)

We can describe the overall process using a ***Dynamic Bayes Network***:



- This incorporates the following Markov assumptions:

$$p(z_t \mid x_{0:t}, u_{1:t}, z_{1:t}) = p(z_t \mid x_t) \quad \text{(measurement)}$$

$$p(x_t \mid x_{0:t-1}, u_{1:t}, z_{1:t}) = p(x_t \mid x_{t-1}, u_t) \quad \text{(state)}$$

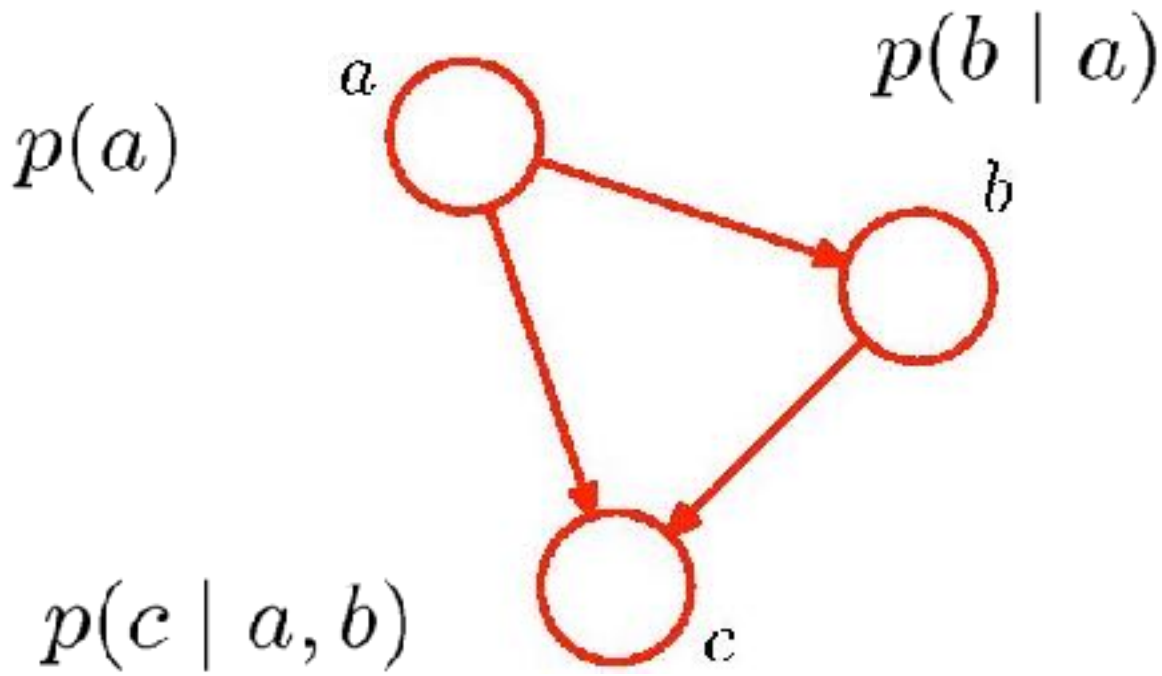
Definition

> A Probabilistic Graphical Model is a diagrammatic representation of a probability distribution.

- In a Graphical Model, random variables are represented as **nodes**, and statistical dependencies are represented using **edges** between the nodes.
- The resulting graph can have the following properties:
- Cyclic / acyclic
- Directed / undirected
- The simplest graphs are Directed Acyclic Graphs (DAG).

Simple Example

- Given: 3 random variables a, b, and c
- Joint prob: $p(a,b,c) = p(c|a,b)p(a,b) = p(c|a,b)p(b|a)p(a)$



Random variables can be discrete or continuous

A Graphical Model based on a DAG is called a **Bayesian Network**

Simple Example

- In general: K random variables $x_1, x_2, \ldots, x_K$
- Joint prob:

$$p(x_1, \ldots, x_K) = p(x_K | x_1, \ldots, x_{K-1}) \ldots p(x_2 | x_1) p(x_1)$$

- This leads to a fully connected graph.
- Note: The ordering of the nodes in such a fully connected graph is **arbitrary**. They all represent the joint probability distribution:

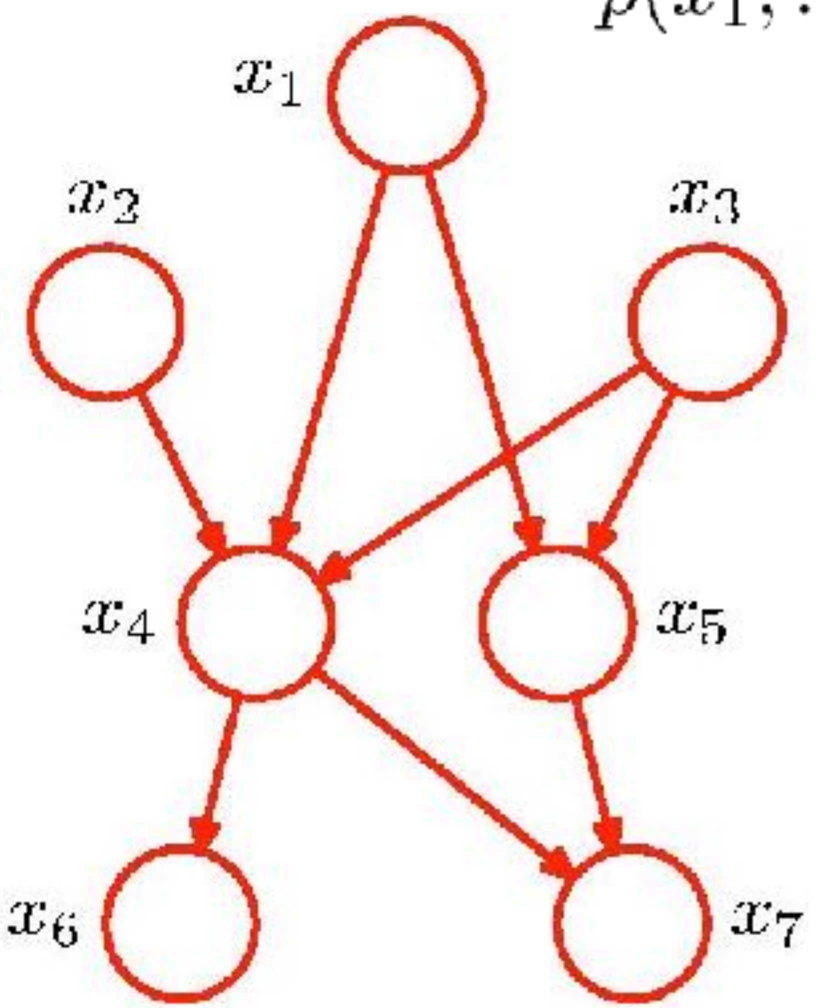
$$p(a, b, c) = p(a | b, c) p(b | c) p(c)$$

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

$$\vdots$$

Bayesian Networks

Statistical independence can be represented by the **absence** of edges. This makes the computation efficient.

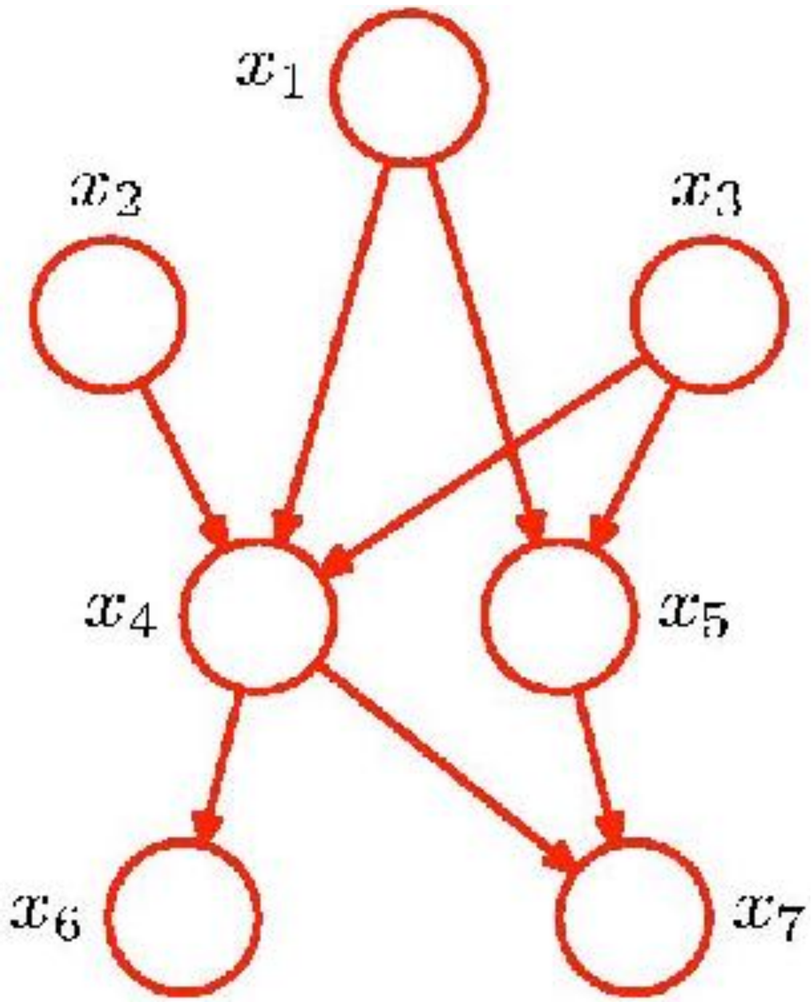


$$p(x_1, \ldots, x_7) = p(x_1)p(x_2)p(x_3)p(x_4|x_1, x_2, x_3)$$
$$p(x_5|x_1, x_3)p(x_6|x_4)p(x_7|x_4, x_5)$$

Intuitively: only x_1 and x_3 have an influence on x_5

Bayesian Networks

We can now define a mapping from graphical models to probabilistic formulations (factorisations) and back:



General Factorisation:

$$p(\mathbf{x}) = \prod_{k=1}^{K} p(x_k|\mathrm{pa}_k)$$

where

$pa_k \triangleq$ ancestors of p_k

and

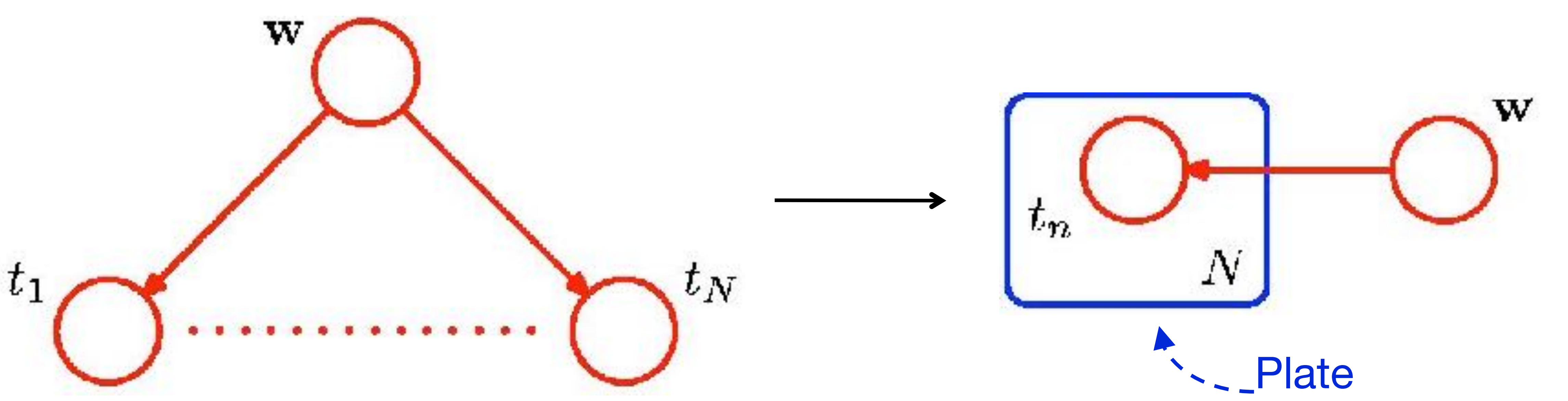
$$p(\mathbf{x}) = p(x_1, \ldots, x_K)$$

Note: Many different factorisations (and graphs) can represent the same distribution

Elements of Graphical Models

In case of a series of random variables with equal dependencies, we can subsume them using a **plate:**

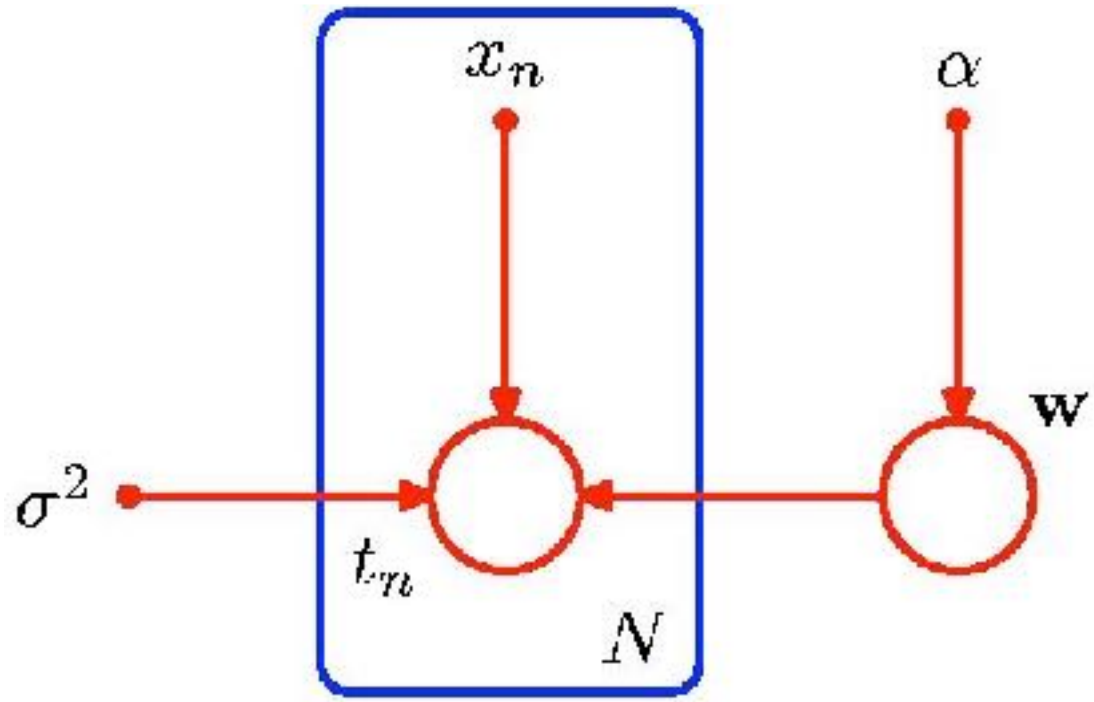
$$p(\mathbf{t}, \mathbf{w}) = p(\mathbf{w}) \prod_{n=1}^{N} p(t_n | \mathbf{w})$$



Elements of Graphical Models (2)

We distinguish between **input** variables and explicit **hyper-parameters**:

$$p(\mathbf{t}, \mathbf{w} | \mathbf{x}, \alpha, \sigma^2) = p(\mathbf{w}|\alpha) \prod_{n=1}^{N} p(t_n | \mathbf{w}, x_n, \sigma^2).$$

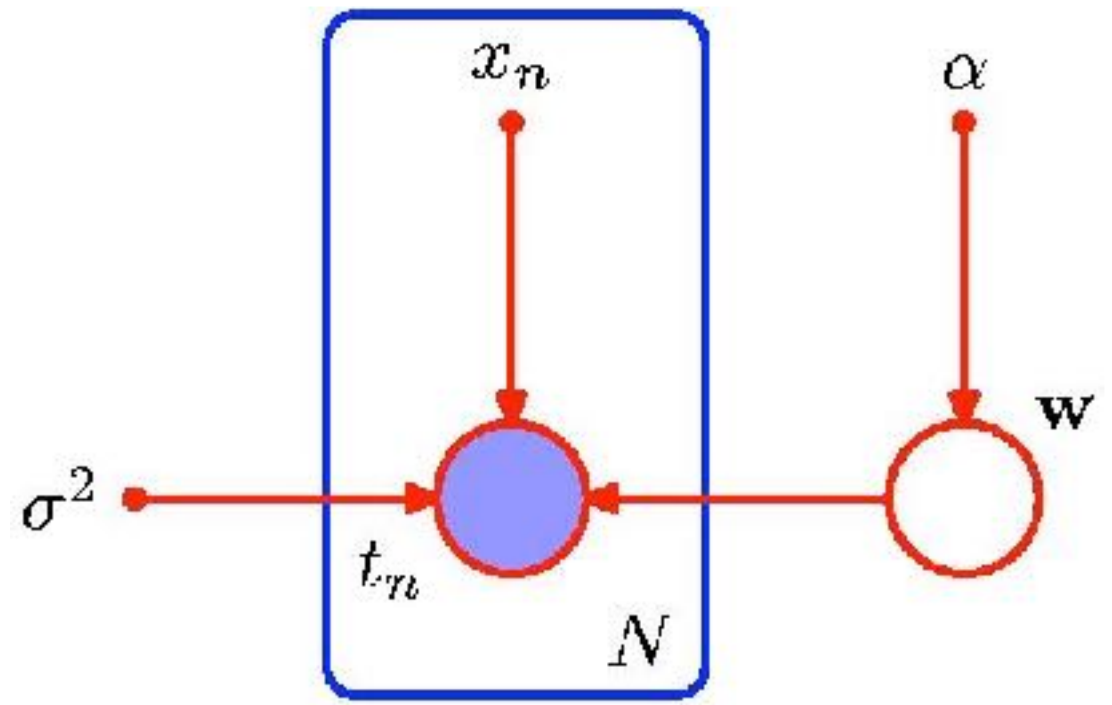


Elements of Graphical Models (3)

We distinguish between **observed** variables and **hidden** variables:

$$p(\mathbf{w}|\mathbf{t}) \propto p(\mathbf{w}) \prod_{n=1}^{N} p(t_n|\mathbf{w})$$

(deterministic parameters omitted in formula)



Example: Regression as a Graphical Model

Aim: Find a general expression to compute the **predictive distribution**: $p(\hat{t} \mid \hat{x}, \mathbf{x}, \mathbf{t})$

Notation:
$\hat{t} = t^*$

Bishop vs. Rasmussen

This expression should

- model all conditional independencies
- explicitly incorporate all parameters (also the deterministic ones)

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Bishop vs. Rasmussen

This expression should

- model all conditional independencies
- explicitly incorporate all parameters (also the deterministic ones)

$$p(\hat{t} \mid \hat{x}, \mathbf{x}, \mathbf{t}, \alpha, \sigma^2) = \int p(\hat{t}, \mathbf{w} \mid \hat{x}, \mathbf{x}, \mathbf{t}, \alpha, \sigma^2) d\mathbf{w}$$

$$= \int \frac{p(\hat{t}, \mathbf{w}, \mathbf{t} \mid \hat{x}, \mathbf{x}, \alpha, \sigma^2)}{p(\mathbf{t} \mid \hat{x}, \mathbf{x}, \alpha, \sigma^2)} d\mathbf{w} \quad \propto \int p(\hat{t}, \mathbf{w}, \mathbf{t} \mid \hat{x}, \mathbf{x}, \alpha, \sigma^2) d\mathbf{w}$$

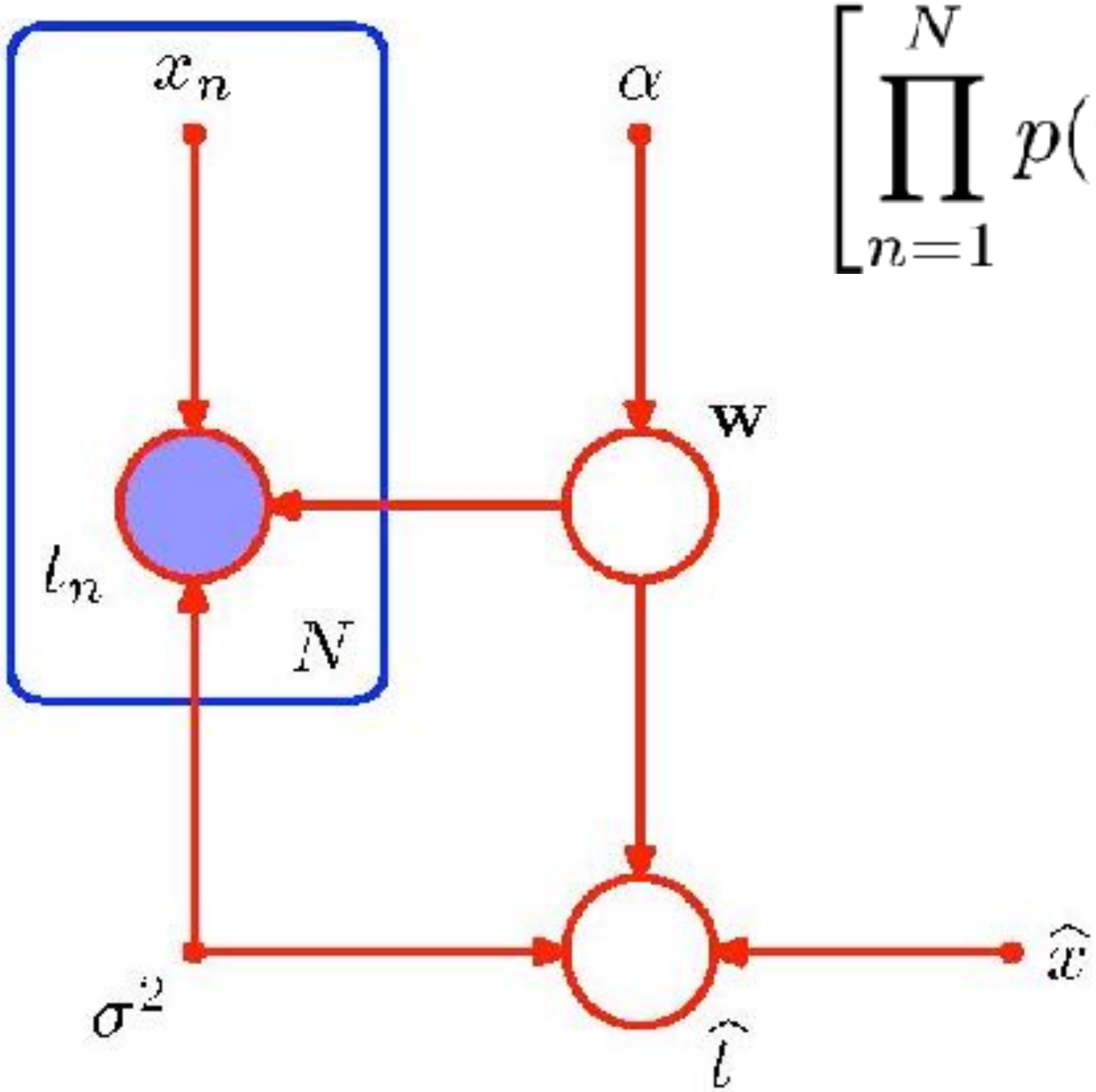
Regression as a Graphical Model

Regression: Prediction of a new target value $\hat{t}$

Notation:
$\hat{t} = t^*$

$$p(\hat{t}, \mathbf{t}, \mathbf{w} \mid \hat{x}, \mathbf{x}, \alpha, \sigma^2) =$$

$$\left[\prod_{n=1}^{N} p(t_n \mid x_n, \mathbf{w}, \sigma^2)\right] p(\mathbf{w} \mid \alpha) p(\hat{t} | \hat{x}, \mathbf{w}, \sigma^2)$$



Here: conditioning on all deterministic parameters

Using this, we can obtain the **predictive distribution:**

$$p(\widehat{t} | \widehat{x}, \mathbf{x}, \mathbf{t}, \alpha, \sigma^2) \propto \int p(\widehat{t}, \mathbf{t}, \mathbf{w} | \widehat{x}, \mathbf{x}, \alpha, \sigma^2) \, \mathrm{d}\mathbf{w}$$

Example: Discrete Variables

- Two dependent variables: $K^2 - 1$ parameters

Here: $K = 2$

x_1	$p(x_1)$
1	0.2
~~2~~	~~0.8~~

$K-1$

x_1	x_2	$p(x_2 \mid x_1)$
1	1	0.25
~~1~~	~~2~~	~~0.75~~
2	1	0.1
~~2~~	~~2~~	~~0.9~~

$K-1$

$K-1$

$K(K-1)$

$$K - 1 + K(K-1) = K^2 - 1$$

- Independent joint distribution: $2(K - 1)$ parameters

$$K - 1 + K - 1 = 2(K-1)$$

Discrete Variables: General Case

In a general joint distribution with M variables we need to store $K^M - 1$ parameters

If the distribution can be described by this graph:

then we have only $K - 1 + (M - 1)\, K(K - 1)$ parameters.

This graph is called a **Markov chain** with M nodes.

The number of parameters grows only **linearly** with the number of variables.

Independence (Rep.)

Definition 1.4: Two random variables X and Y are *independent* iff: $p(x, y) = p(x)p(y)$

For independent random variables X and Y we have:

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

Notation: $x \perp\!\!\!\perp y \mid \emptyset$

Independence does **not** imply conditional independence!

The same is true for the opposite case.

Conditional Independence (Rep.)

Definition 1.5: Two random variables X and Y are *conditional independent* given a third random variable Z iff:

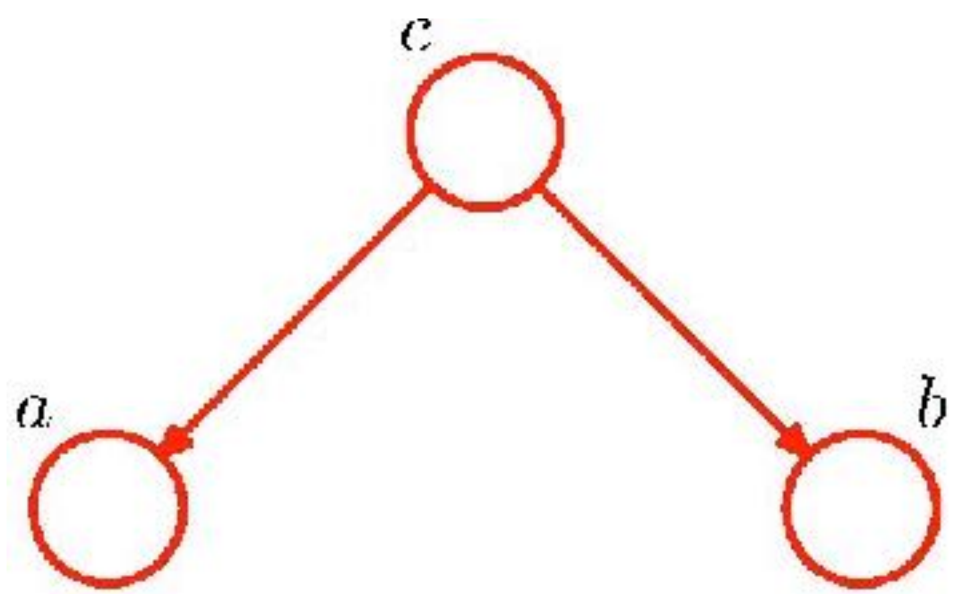
$$p(x, y \mid z) = p(x \mid z)p(y \mid z)$$

This is equivalent to:

$$p(x \mid z) = p(x \mid y, z) \quad \text{and}$$
$$p(y \mid z) = p(y \mid x, z)$$

Notation: $x \perp\!\!\!\perp y \mid z$

Conditional Independence: Example 1



This graph represents the probability distribution:

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

Marginalizing out *c* on both sides gives

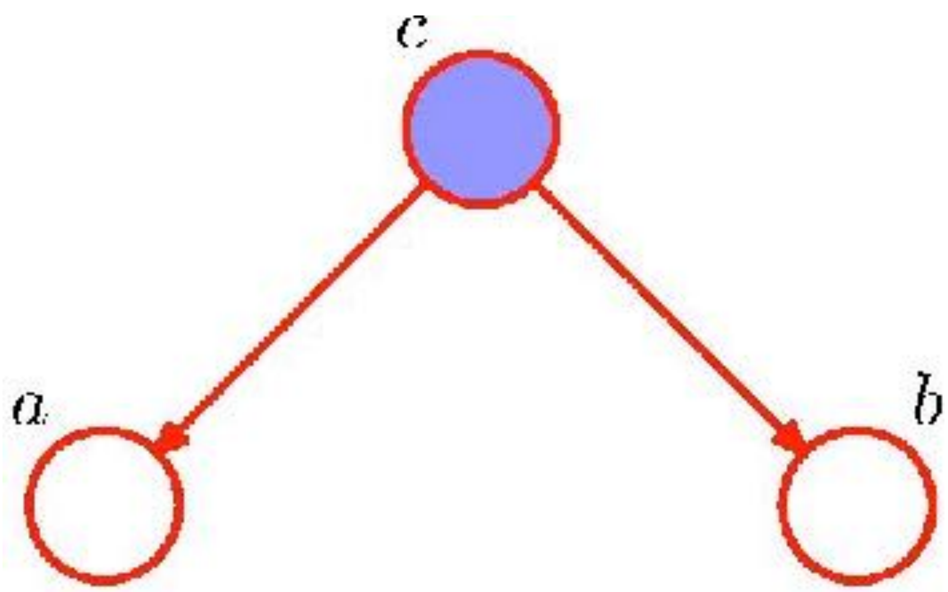
$$p(a, b) = \sum_c p(a|c)p(b|c)p(c)$$

This is in general not equal to $p(a)p(b)$.

Thus: a and b are not independent: $a \not\perp\!\!\!\perp b \mid \emptyset$

Conditional Independence: Example 1

Now, we condition on c (it is assumed to be known):

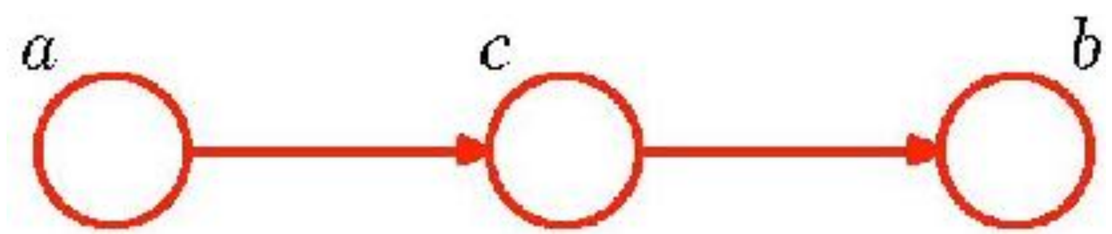


$$p(a, b|c) = \frac{p(a, b, c)}{p(c)} = p(a|c)p(b|c)$$

Thus: a and b are conditionally independent given c: $a \perp\!\!\!\perp b \mid c$

We say that the node at c is a **tail-to-tail node** on the path between a and b

Conditional Independence: Example 2



This graph represents the distribution:

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

Again, we marginalize over c:

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

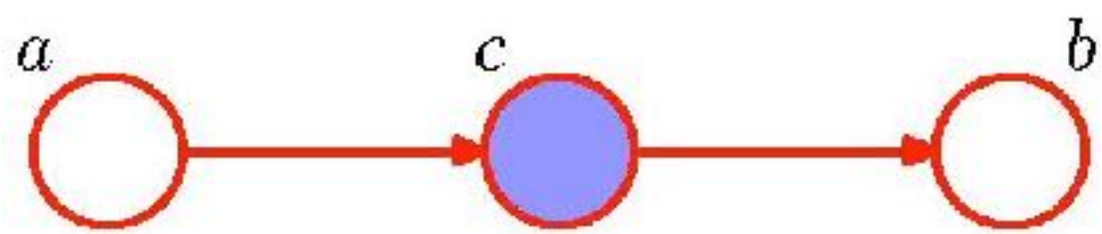
$$= p(a)\sum_c \frac{p(c,a)p(b,c,a)}{p(a)p(c,a)} = p(a)\sum_c p(b,c \mid a)$$

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

And we obtain: $a \not\perp\!\!\!\perp b \mid \emptyset$

Conditional Independence: Example 2

As before, now we condition on c :



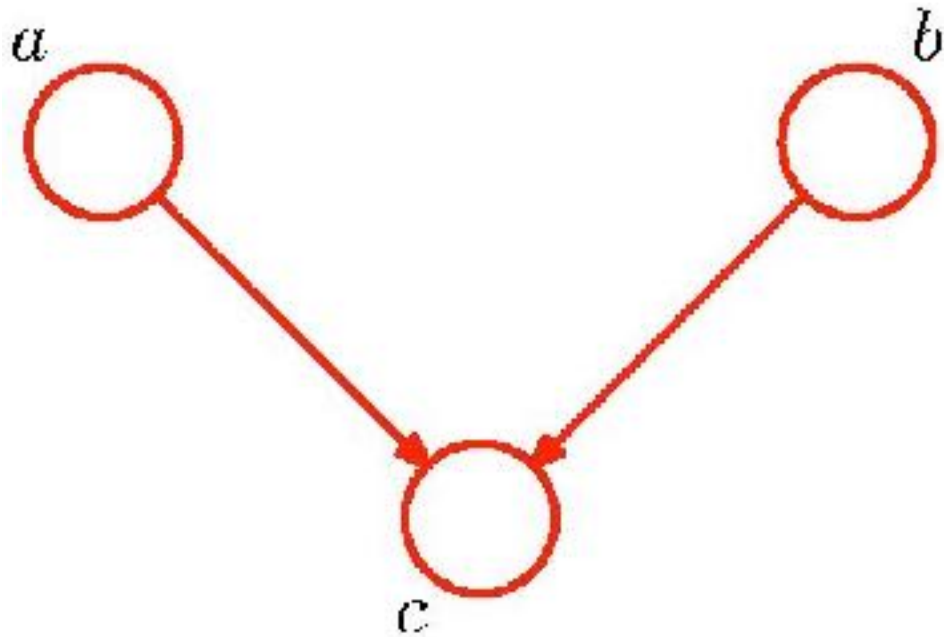
$$\begin{aligned} p(a,b|c) &= \frac{p(a,b,c)}{p(c)} \\ &= \frac{p(a)p(c|a)p(b|c)}{p(c)} \\ &= p(a|c)p(b|c) \end{aligned}$$

And we obtain: $a \perp\!\!\!\perp b \mid c$

We say that the node at c is a **head-to-tail node** on the path between a and b.

Conditional Independence: Example 3

Now consider this graph:



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

using:

$$\sum_c p(a, b, c) = p(a)p(b) \sum_c p(c \mid a, b)$$

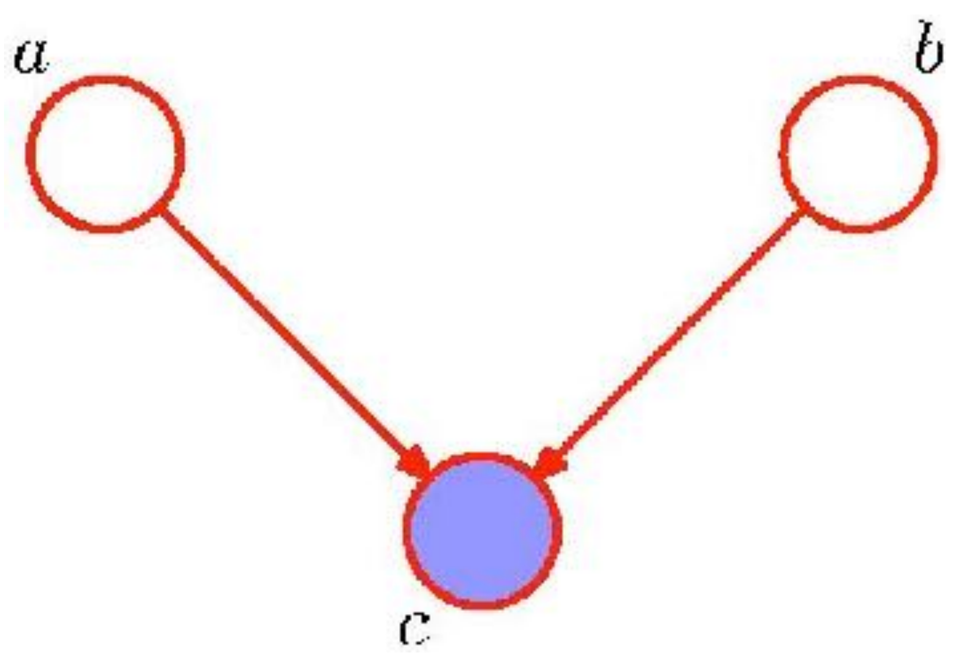
we obtain:

$$p(a, b) = p(a)p(b)$$

And the result is: $a \perp\!\!\!\perp b \mid \emptyset$

Conditional Independence: Example 3

Again, we condition on c



$$p(a,b|c) = \frac{p(a,b,c)}{p(c)} = \frac{p(a)p(b)p(c|a,b)}{p(c)}$$

This results in: $a \not\perp\!\!\!\perp b \mid c$

We say that the node at c is a **head-to-head node** on the path between a and b.

To Summarize

- When does the graph represent (conditional) independence?

  Tail-to-tail case: if we condition on the tail-to-tail node

  Head-to-tail case: if we cond. on the head-to-tail node

  Head-to-head case: if we do **not** condition on the head-to-head node (and neither on any of its descendants)

In general, this leads to the notion of **D-separation** for directed graphical models.

D-Separation

Say: A, B, and C are non-intersecting subsets of nodes in a directed graph.

A path from A to B is **blocked** by C if it contains a node such that either

a) the arrows on the path meet either **head-to-tail** or **tail-to-tail** at the node, and the node is **in** the set C, or

b) the arrows meet **head-to-head** at the node, and neither the node, nor any of its descendants, are in the set C.

If all paths from A to B are blocked, A is said to be **d-separated** from B by C.

Notation: $\mathrm{dsep}(A, B|C)$

D-Separation

Say: A, B, and C are non-intersecting subsets of nodes in a directed graph.

- A path ... ntains a nod...

a) the a... **tail-to-tail** at t...

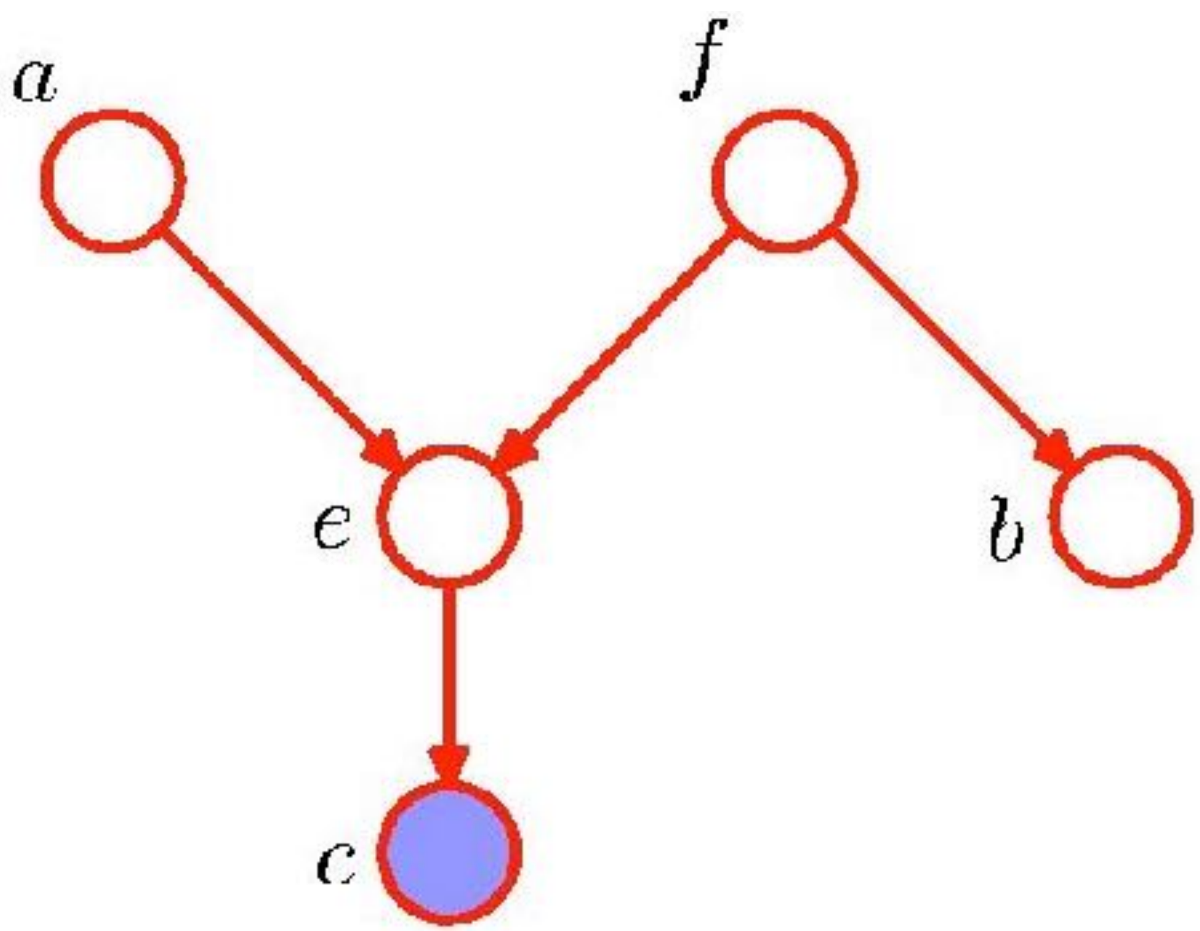
b) the a... neither the nod... C.

- If all p... aid to be **d-separated** from B by C.

Notation: $\mathrm{dsep}(A, B | C)$

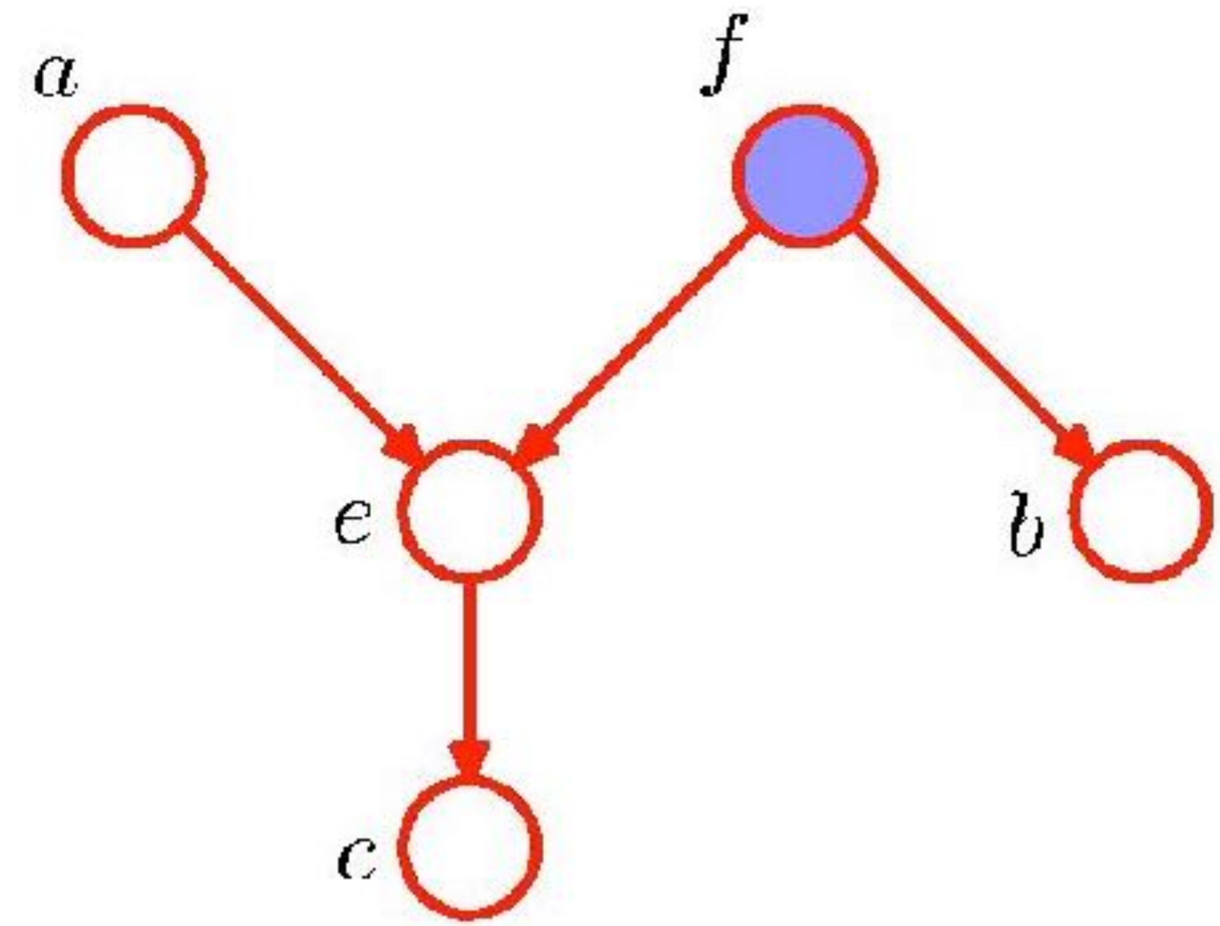
D-Separation is a property of graphs and not of probability distributions

D-Separation: Example



$\neg\mathrm{dsep}(a, b|c)$

We condition on a descendant of e, i.e. it does not block the path from a to b.



$\mathrm{dsep}(a, b|f)$

We condition on a tail-to-tail node on the only path from a to b, i.e f blocks the path.

I-Map

Definition 4.1: A graph G is called an **I-map** for a distribution p if every D-separation of G corresponds to a conditional independence relation satisfied by p:

$$\forall A, B, C : \mathrm{dsep}(A, B, C) \Rightarrow A \perp\!\!\!\perp B \mid C$$

Example: The fully connected graph is an I-map for any distribution, as there are no D-separations in that graph.

D-Map

Definition 4.2: A graph G is called an **D-map** for a distribution p if for every conditional independence relation satisfied by p there is a D-separation in G :

$$\forall A, B, C : A \perp\!\!\!\perp B \mid C \Rightarrow \mathrm{dsep}(A, B, C)$$

Example: The graph without any edges is a D-map for any distribution, as all pairs of subsets of nodes are D-separated in that graph.

Perfect Map

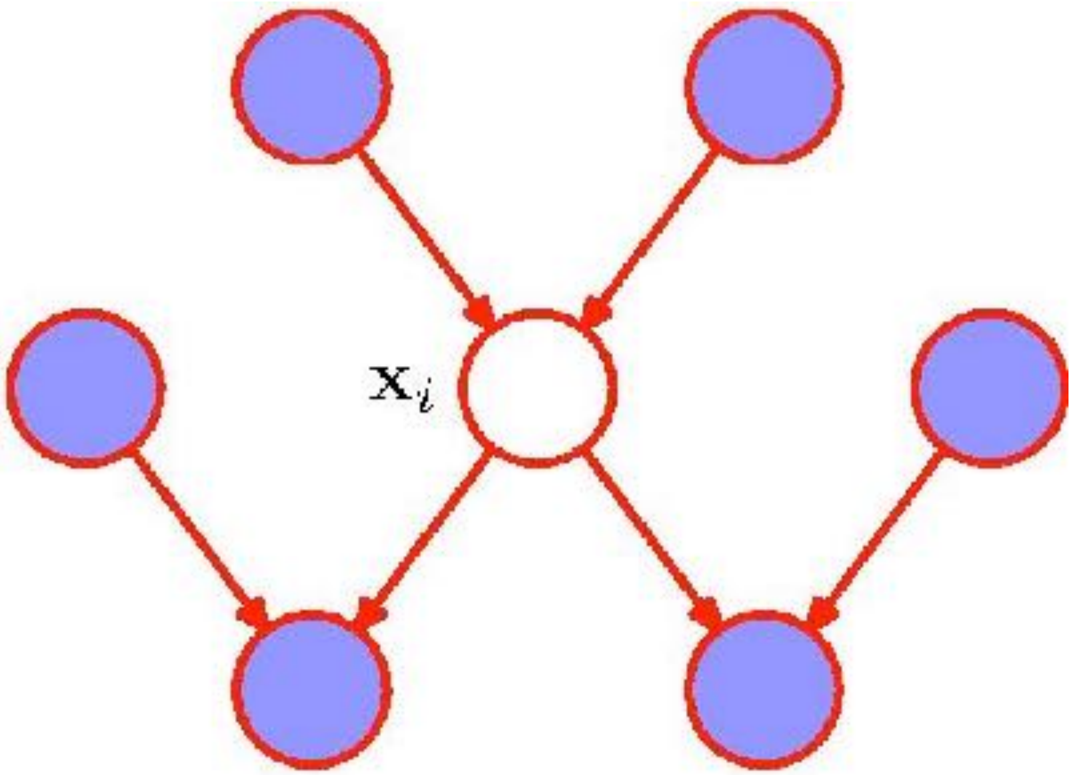
Definition 4.3: A graph G is called a **perfect map** for a distribution p if it is a D-map and an I-map of p.

$$\forall A, B, C : A \perp\!\!\!\perp B \mid C \Leftrightarrow \mathrm{dsep}(A, B, C)$$

A perfect map uniquely defines a probability distribution.

The Markov Blanket

Consider a distribution of a node x_i conditioned on all other nodes:

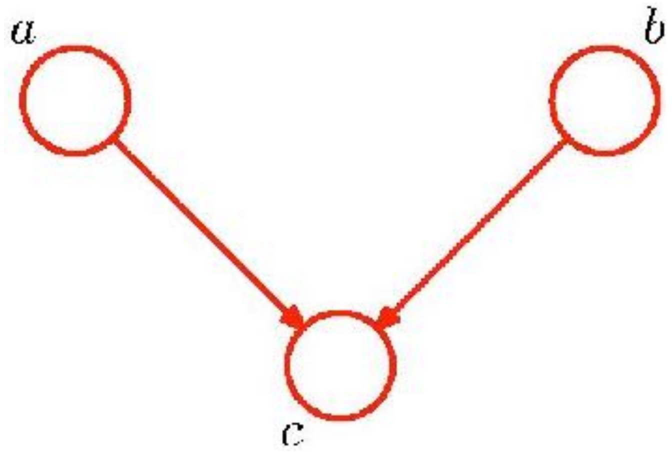


$$p(\mathbf{x}_i|\mathbf{x}_{\{j\neq i\}}) = \frac{p(\mathbf{x}_1,\ldots,\mathbf{x}_M)}{\int p(\mathbf{x}_1,\ldots,\mathbf{x}_M)d\mathbf{x}_i} = \frac{\prod_k p(\mathbf{x}_k|\mathrm{pa}_k)}{\int \prod_k p(\mathbf{x}_k|\mathrm{pa}_k)d\mathbf{x}_i}$$

Markov blanket $\mathcal{M}_i$ at $\mathbf{x}_i$: all parents, children and co-parents of $\mathbf{x}_i$.

Factors independent of $\mathbf{x}_i$ cancel between numerator and denominator.

In-depth: The Head-to-Head Node



$p(a) = 0.9 \qquad p(b) = 0.9$

a	b	$p(c)$
1	1	0.8
1	0	0.2
0	1	0.2
0	0	0.1

Example:

a: Battery charged (0 or 1)

b: Fuel tank full (0 or 1)

c: Fuel gauge says full (0 or 1)

We can compute $p(\neg c) = 0.315$

and $p(\neg c \mid \neg b) = 0.81$

and obtain $p(\neg b \mid \neg c) \approx 0.257$

similarly: $p(\neg b \mid \neg c, \neg a) \approx 0.111$

"a **explains** c **away**"

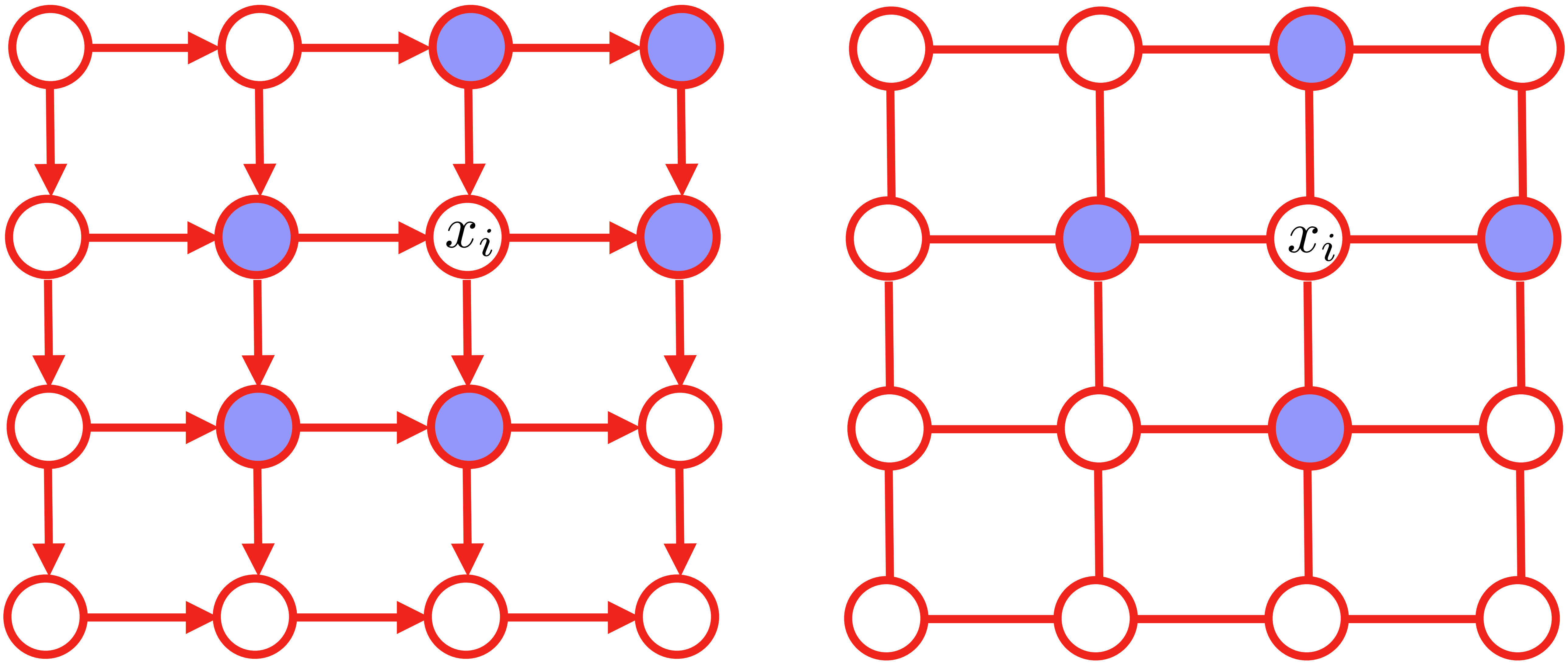
Directed vs. Undirected Graphs

Using D-separation we can identify conditional independencies in directed graphical models, but:

- Is there a simpler, more intuitive way to express conditional independence in a graph?
- Can we find a representation for cases where an „ordering“ of the random variables is inappropriate (e.g. the pixels in a camera image)?

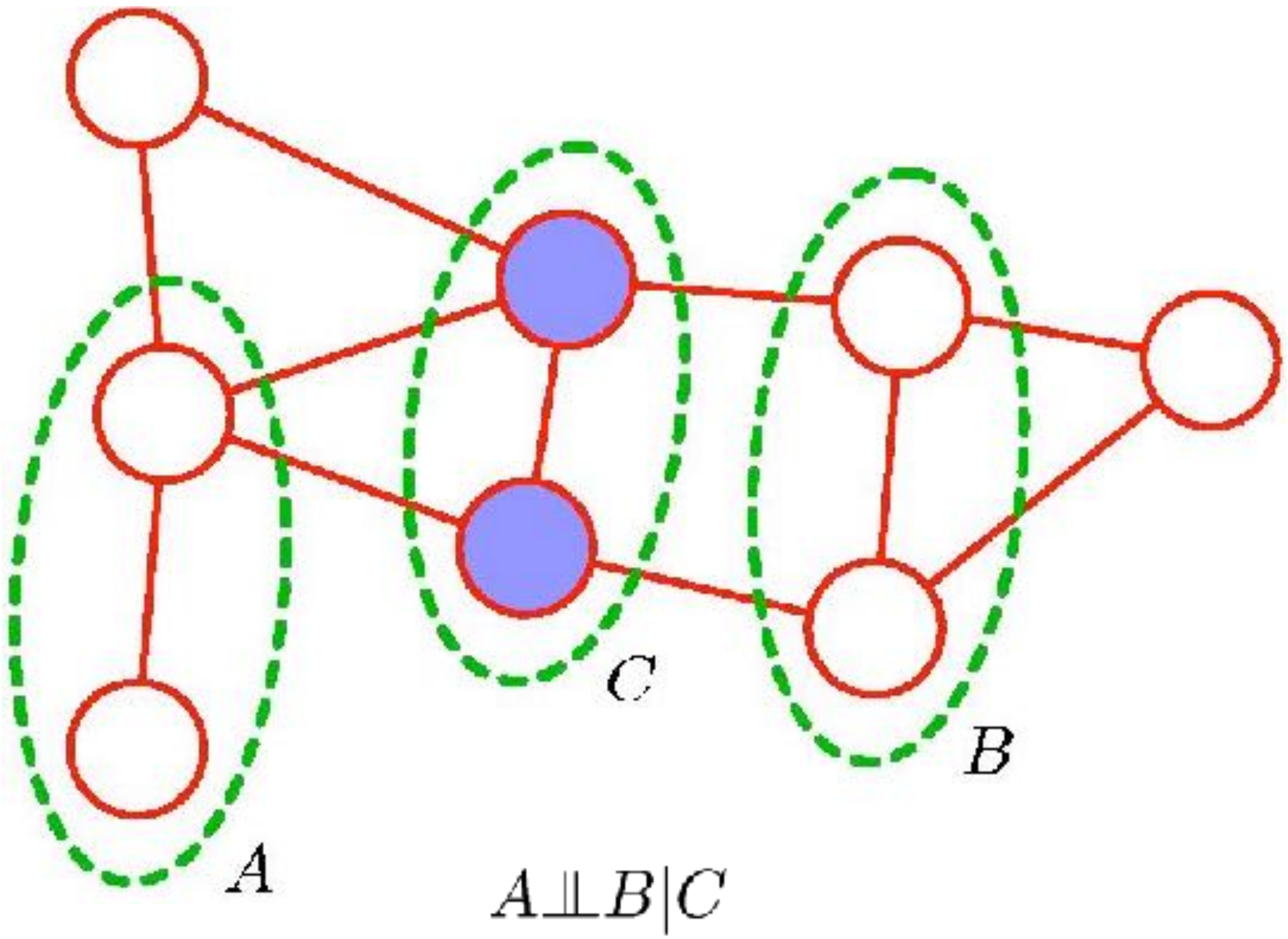
Yes, we can: by removing the directions of the edges we obtain an Undirected Graphical Model, also known as a **Markov Random Field**

Example: Camera Image



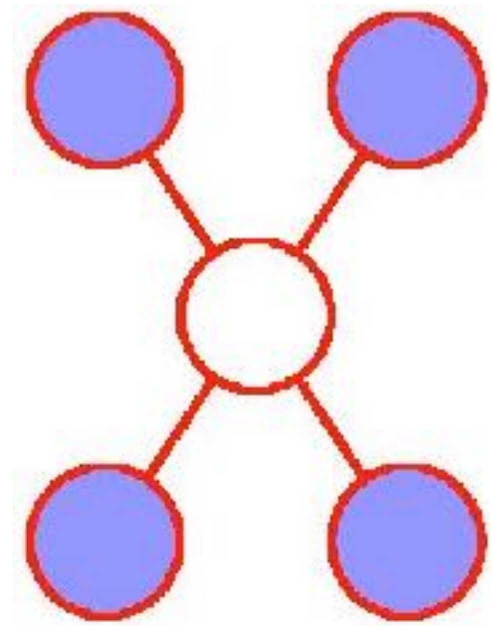
- directions are counter-intuitive for images
- Markov blanket is not just the direct neighbors when using a directed model

Markov Random Fields



All paths from A to B go through C, i.e. C blocks all paths.

Markov Blanket



We only need to condition on the **direct neighbors** of $\mathbf{x}$ to get c.i., because these already block every path from $\mathbf{x}$ to any other node.

Factorization of MRFs

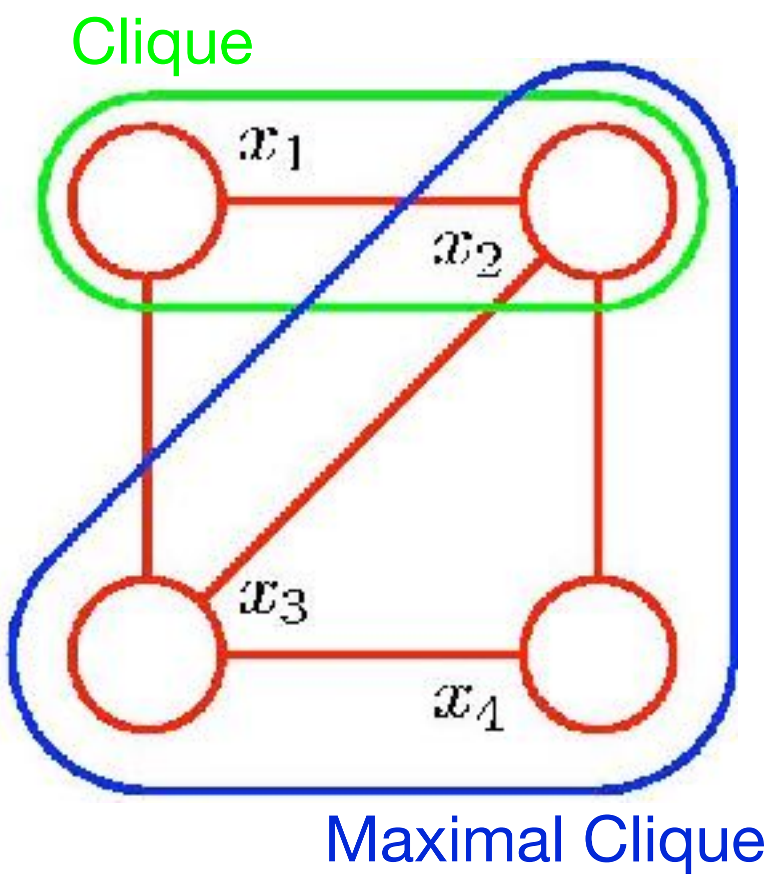
Any two nodes x_i and x_j that are not connected in an MRF are conditionally independent given all other nodes:

$$p(x_i, x_j \mid \mathbf{x}_{\setminus\{i,j\}}) = p(x_i \mid \mathbf{x}_{\setminus\{i,j\}})p(x_j \mid \mathbf{x}_{\setminus\{i,j\}})$$

In turn: each factor contains only nodes that are connected

This motivates the consideration of cliques in the graph:

- A **clique** is a fully connected subgraph.
- A **maximal** clique can not be extended with another node without loosing the property of full connectivity.



Factorization of MRFs

In general, a Markov Random Field is factorized as

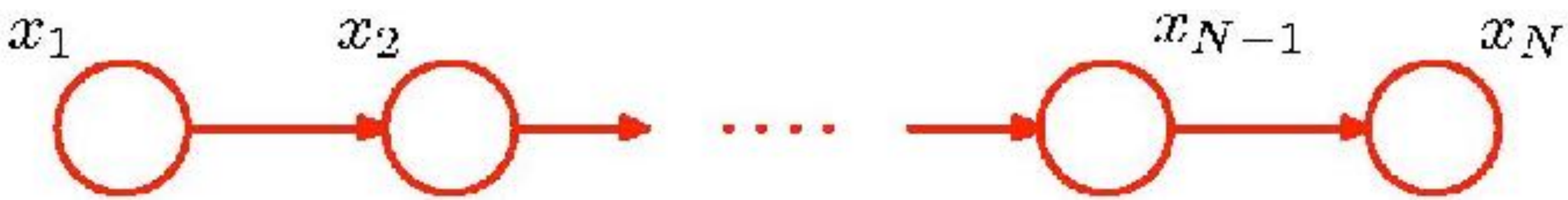
$$p(\mathbf{x}) = \frac{\prod_C \phi_C(\mathbf{x}_C)}{\sum_{\mathbf{x}'} \prod_C \phi_C(\mathbf{x}'_C)} = \frac{1}{Z} \prod_C \phi_C(\mathbf{x}_C) \qquad (4.1)$$

where C is the set of all (maximal) cliques and Φ_C is a positive function of a given clique $\mathbf{x}_C$ of nodes, called the **clique potential**. Z is called the **partition function**.

Theorem (Hammersley/Clifford): Any undirected model with associated clique potentials Φ_C is a perfect map for the probability distribution defined by Equation (4.1).

As a conclusion, all probability distributions that can be factorized as in (4.1), can be represented as an MRF.

Converting Directed to Undirected Graphs (1)

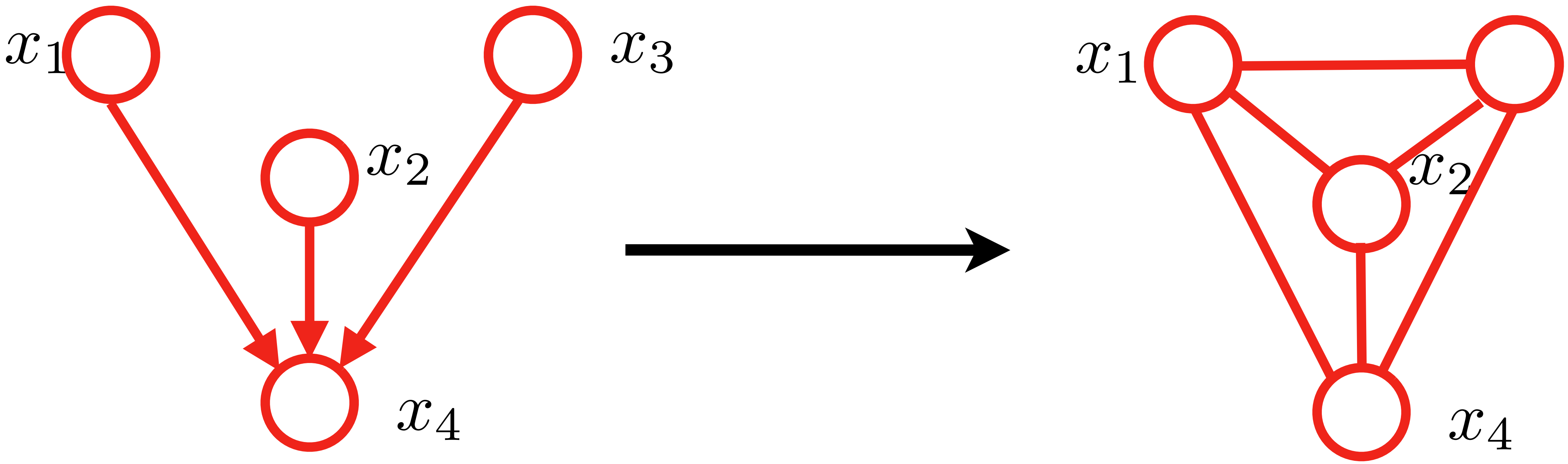


$$p(\mathbf{x}) = p(x_1)p(x_2|x_1)\,p(x_3|x_2)\cdots p(x_N|x_{N-1})$$

$$p(\mathbf{x}) = \frac{1}{Z}\psi_{1,2}(x_1,x_2)\,\psi_{2,3}(x_2,x_3)\cdots\psi_{N-1,N}(x_{N-1},x_N)$$

In this case: Z=1

Converting Directed to Undirected Graphs (2)



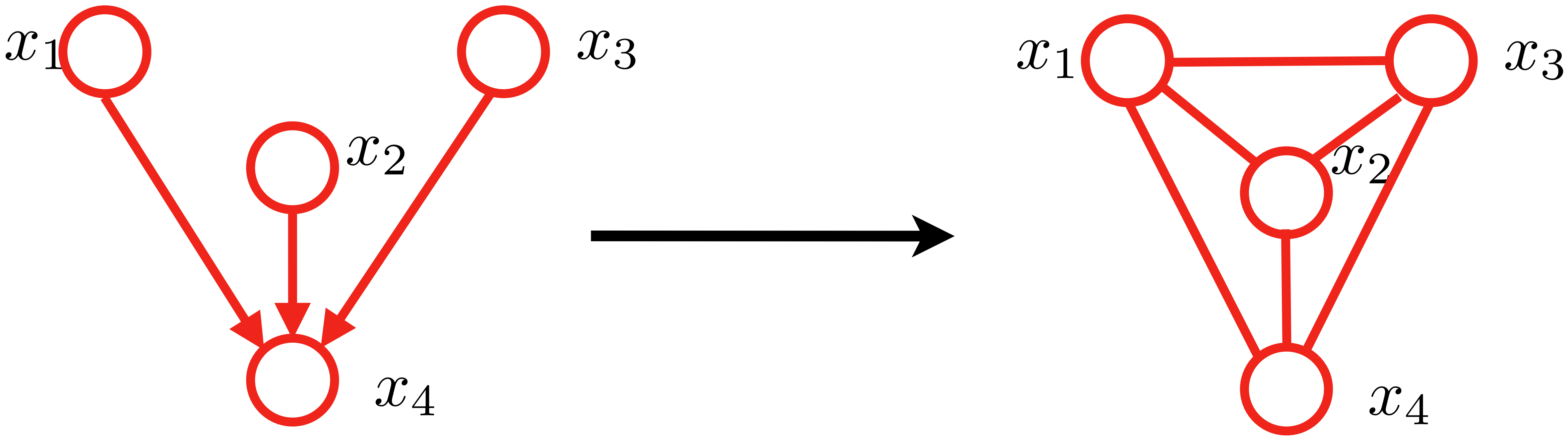
$$p(\mathbf{x}) = p(x_1)p(x_2)p(x_3)p(x_4 \mid x_1, x_2, x_3)$$

In general: conditional distributions in the directed graph are mapped to cliques in the undirected graph

However: the variables are **not** conditionally independent given the head-to-head node

Therefore: Connect all parents of head-to-head nodes with each other (**moralization**)

Converting Directed to Undirected Graphs (2)



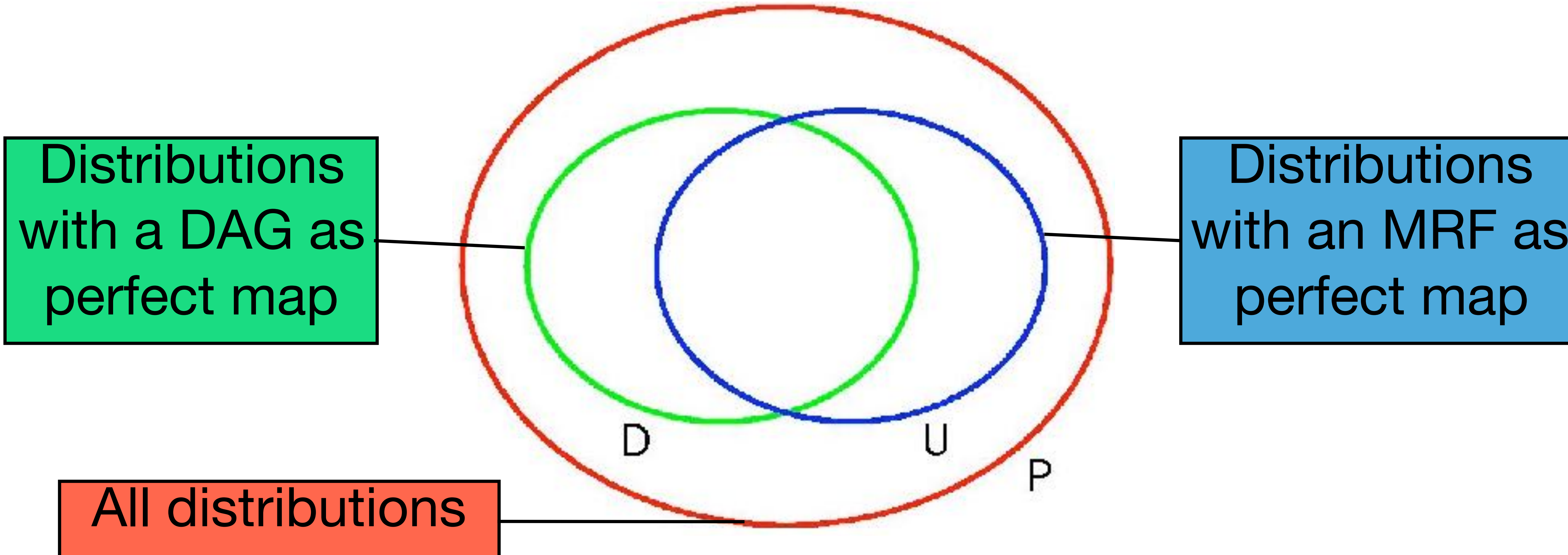
$p(\mathbf{x}) = p(x_1)p(x_2)p(x_3)p(x_4 \mid x_1, x_2, x_3)$ $\quad$ $p(\mathbf{x}) = \phi(x_1, x_2, x_3, x_4)$

Problem: This process can remove conditional independence relations, making the model too complex

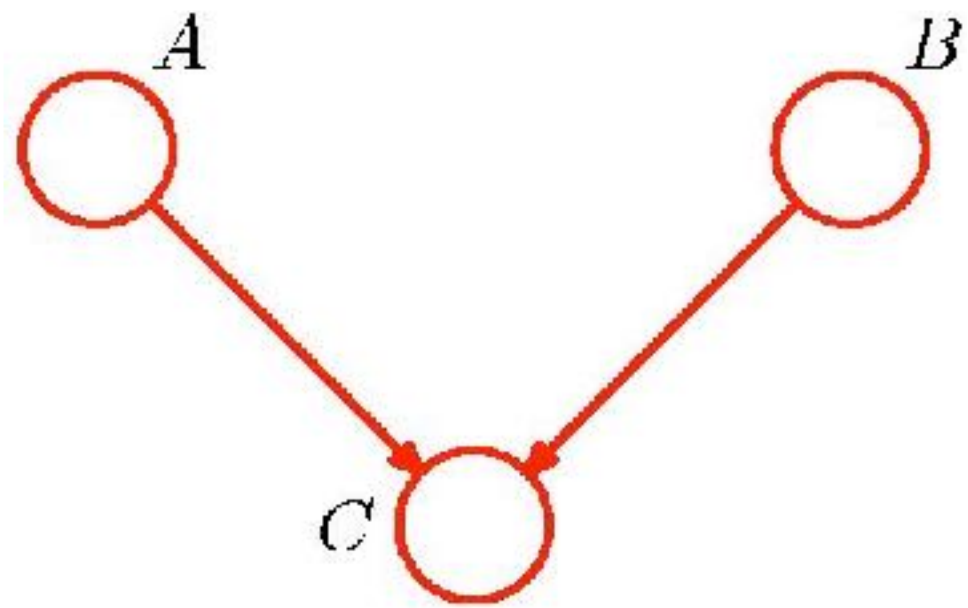
Generally: There is no one-to-one mapping between the distributions represented by directed and by undirected graphs.

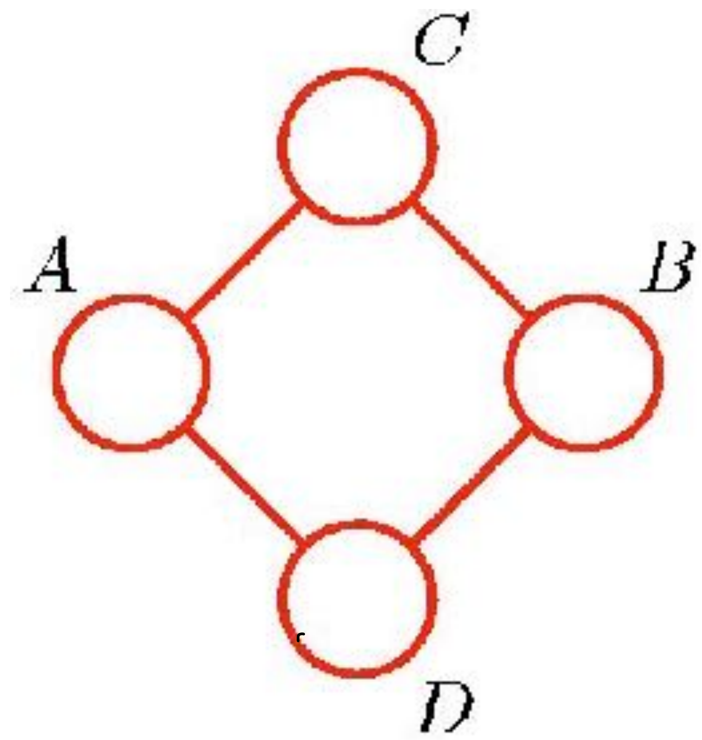
Representability

- As for DAGs, we can define an I-map, a D-map and a perfect map for MRFs.
- The set of all distributions for which a DAG exists that is a perfect map is different from that for MRFs.



Directed vs. Undirected Graphs





$$A \perp\!\!\!\perp B \mid \emptyset$$

$$A \not\!\perp\!\!\!\perp B \mid C$$

$$A \not\!\perp\!\!\!\perp B \mid \emptyset$$

$$A \perp\!\!\!\perp B \mid C \cup D$$

$$C \perp\!\!\!\perp D \mid A \cup B$$

Both distributions can not be represented in the other framework (directed/undirected) with all conditional independence relations.