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

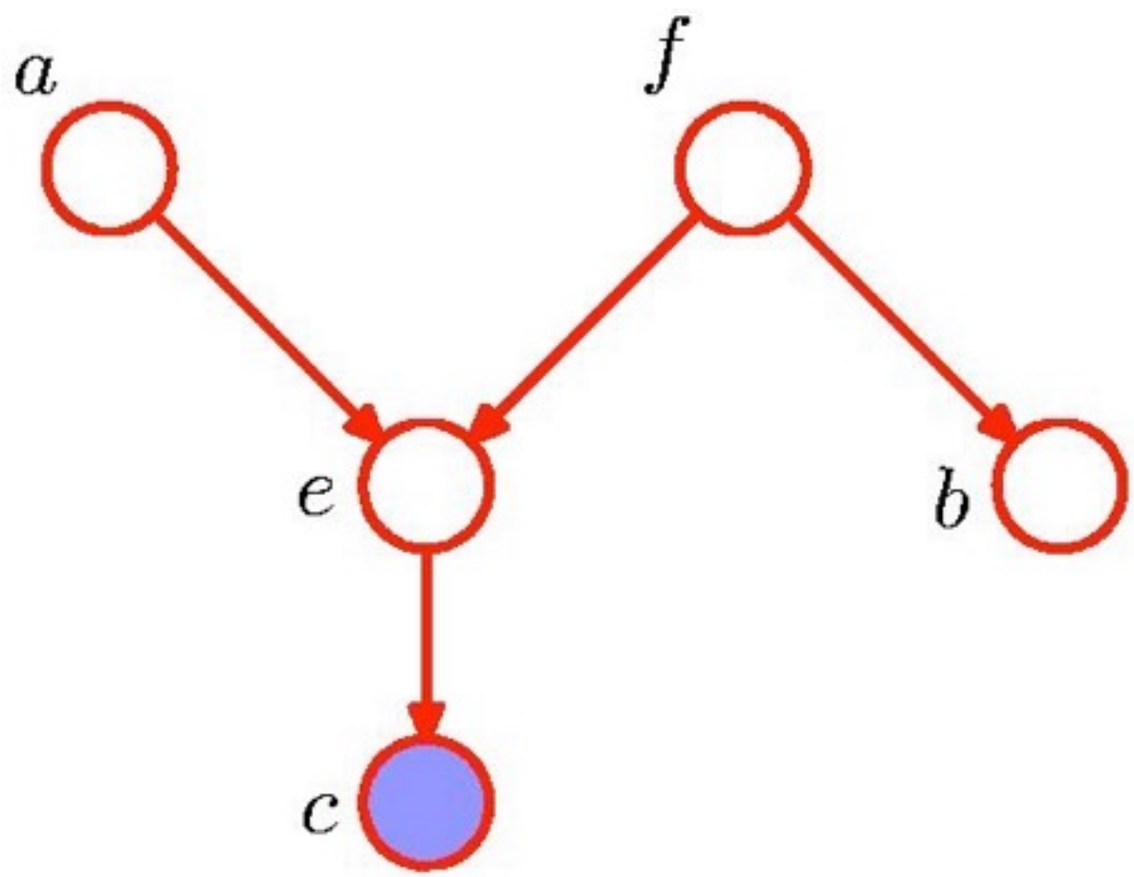
Say: A, B, and C are non-intersecting subsets of nodes in a directed graph.

- A path ... ntains a node ...
  a) the arrows ... **tail-to-tail** at the node ...
  b) the arrows ... neither the node ... C.
- If all paths ... said to be **d-separated** from B by C.

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

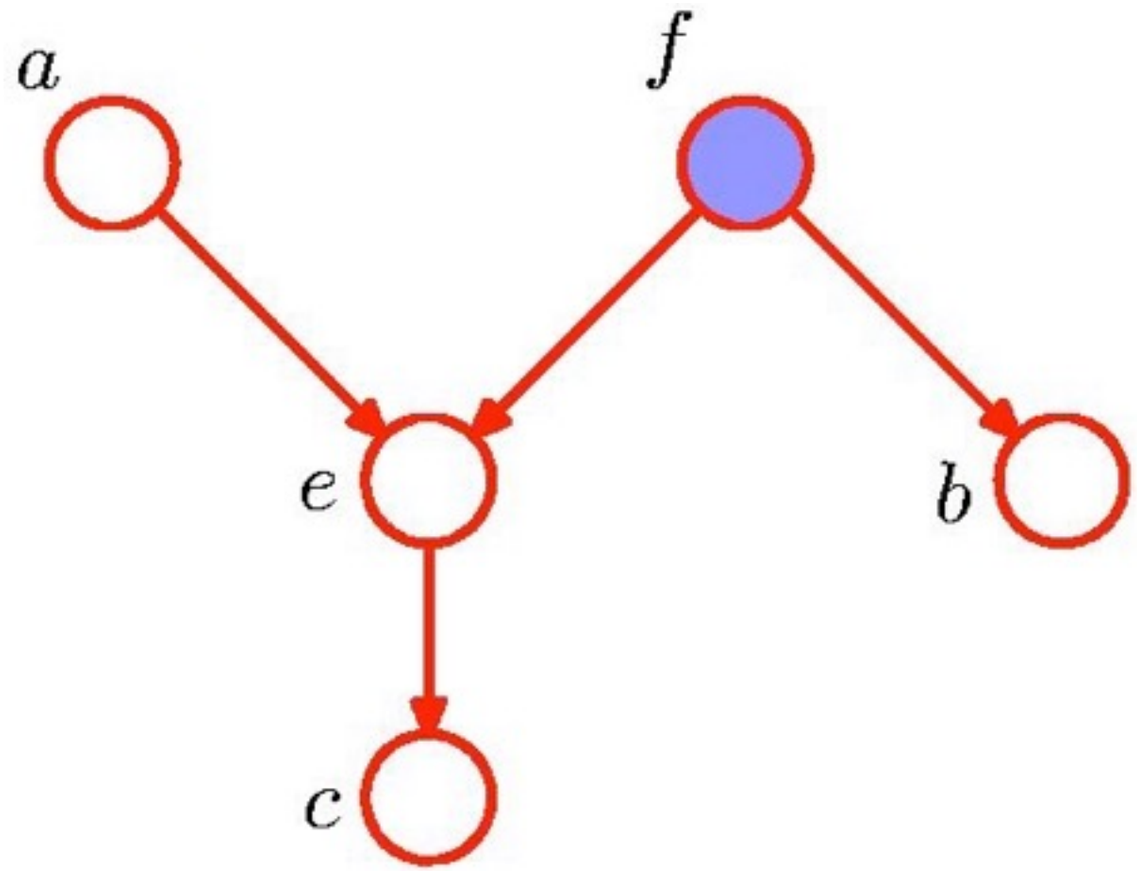
D-Separation is a property of graphs and not of probability distributions

D-Separation: Example



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

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



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

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

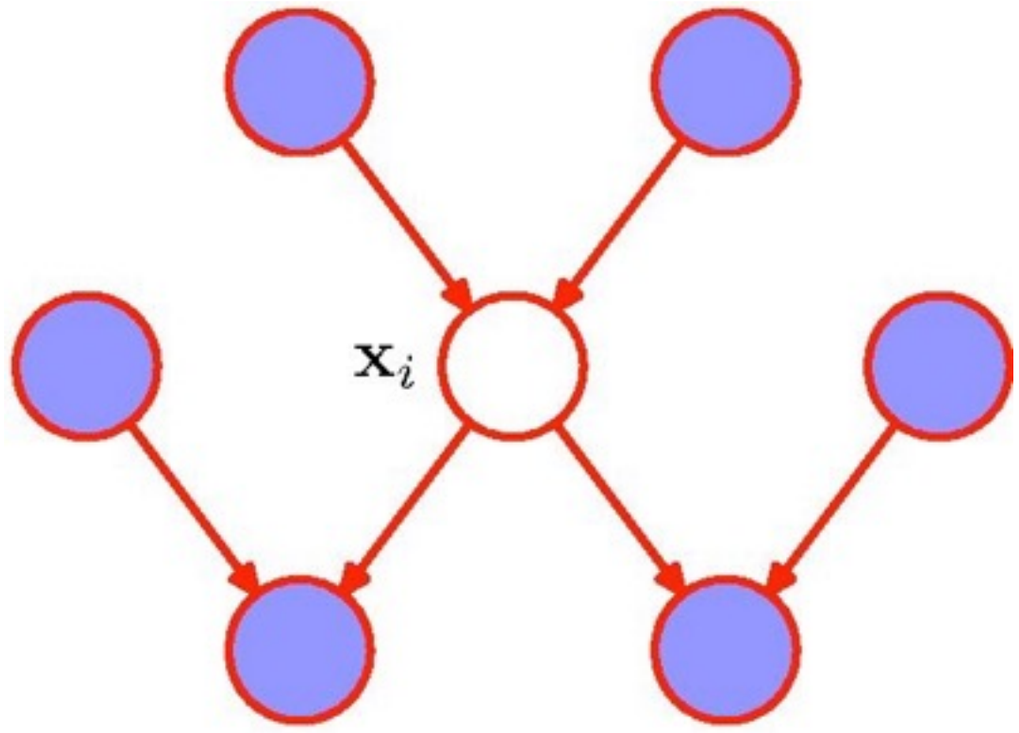
Definition 4.3: A graph G is called a **perfect map** for a distribution p if it is a D-map and an I-map of p.

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

A perfect map uniquely defines a probability distribution.

The Markov Blanket

Consider a distribution of a node $\boldsymbol{x}_i$ conditioned on all other nodes:



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

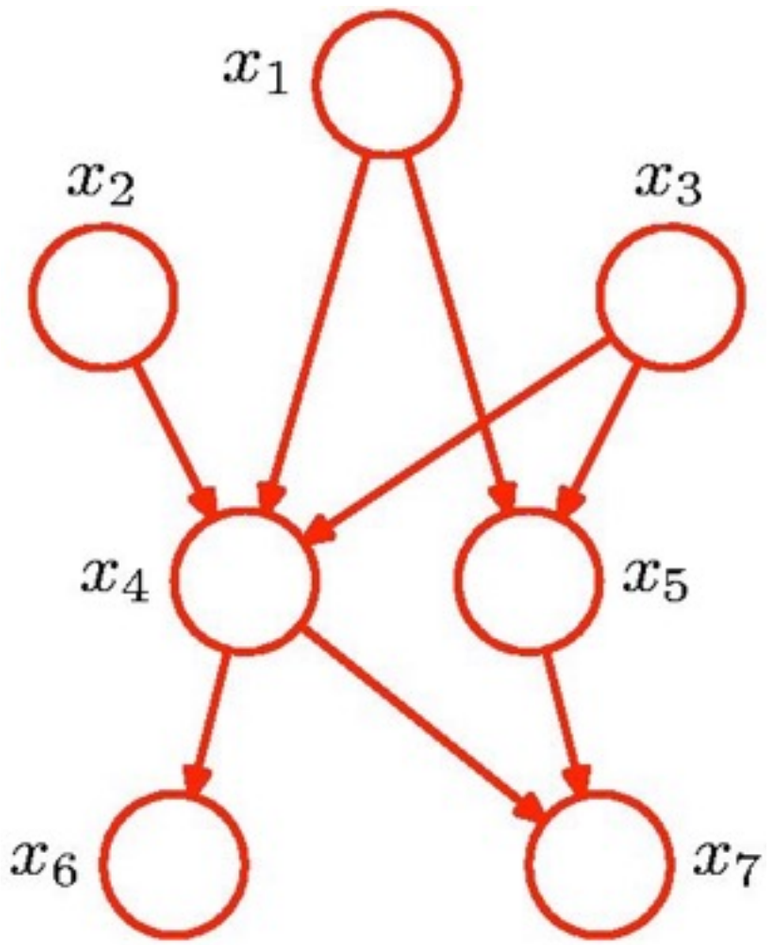
$$= \frac{\prod_k p(\mathbf{x}_k|\mathrm{pa}_k)}{\int \prod_k p(\mathbf{x}_k|\mathrm{pa}_k)d\mathbf{x}_i}$$

$$= p(\mathbf{x}_i \mid \mathbf{x}_{\mathcal{M}_i})$$

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.

Repetition: Directed Graphical Models

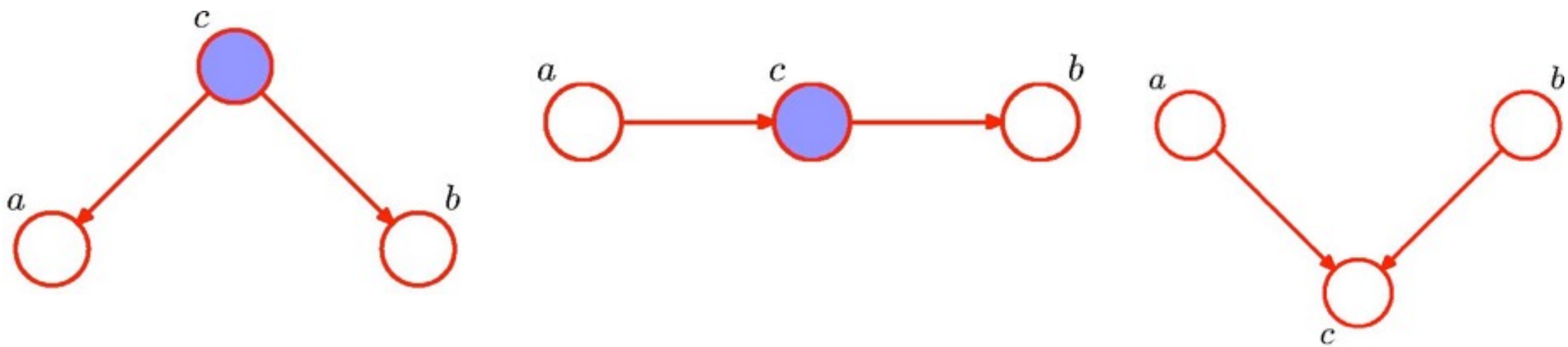


Directed graphical models can be used to represent **probability distributions**

This is useful to do **inference** and to **generate samples** from the distribution efficiently

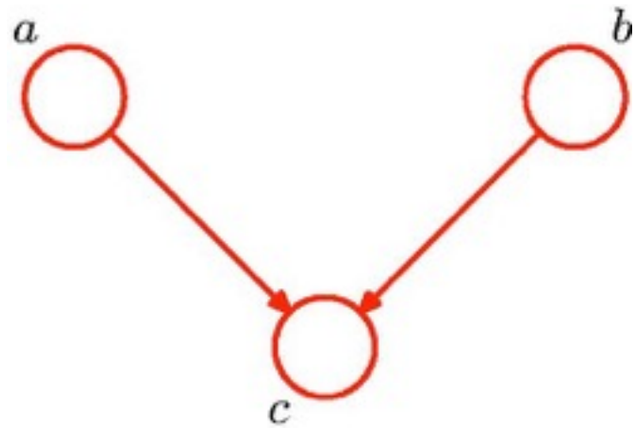
$$p(x_1, \ldots, x_7) = p(x_1)p(x_2)p(x_3)p(x_4|x_1, x_2, x_3)$$
$$p(x_5|x_1, x_3)p(x_6|x_4)p(x_7|x_4, x_5)$$

Repetition: D-Separation



- D-separation is a property of graphs that can be easily determined
- An I-map assigns every d-separation a c.i. rel
- A D-map assigns every c.i. rel a d-separation
- Every Bayes net determines a unique prob. dist.

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 $p(\neg c) = 0.315$

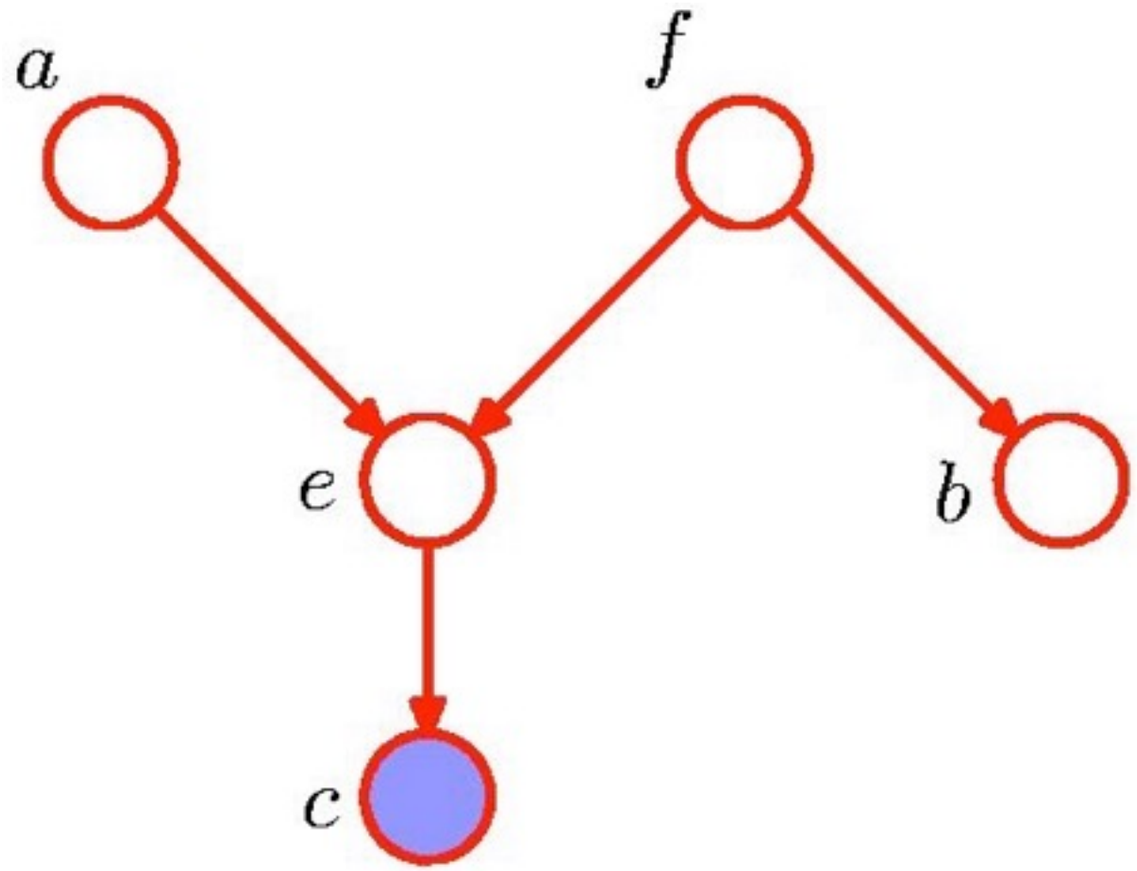
and $p(\neg c \mid \neg b) = 0.81$

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

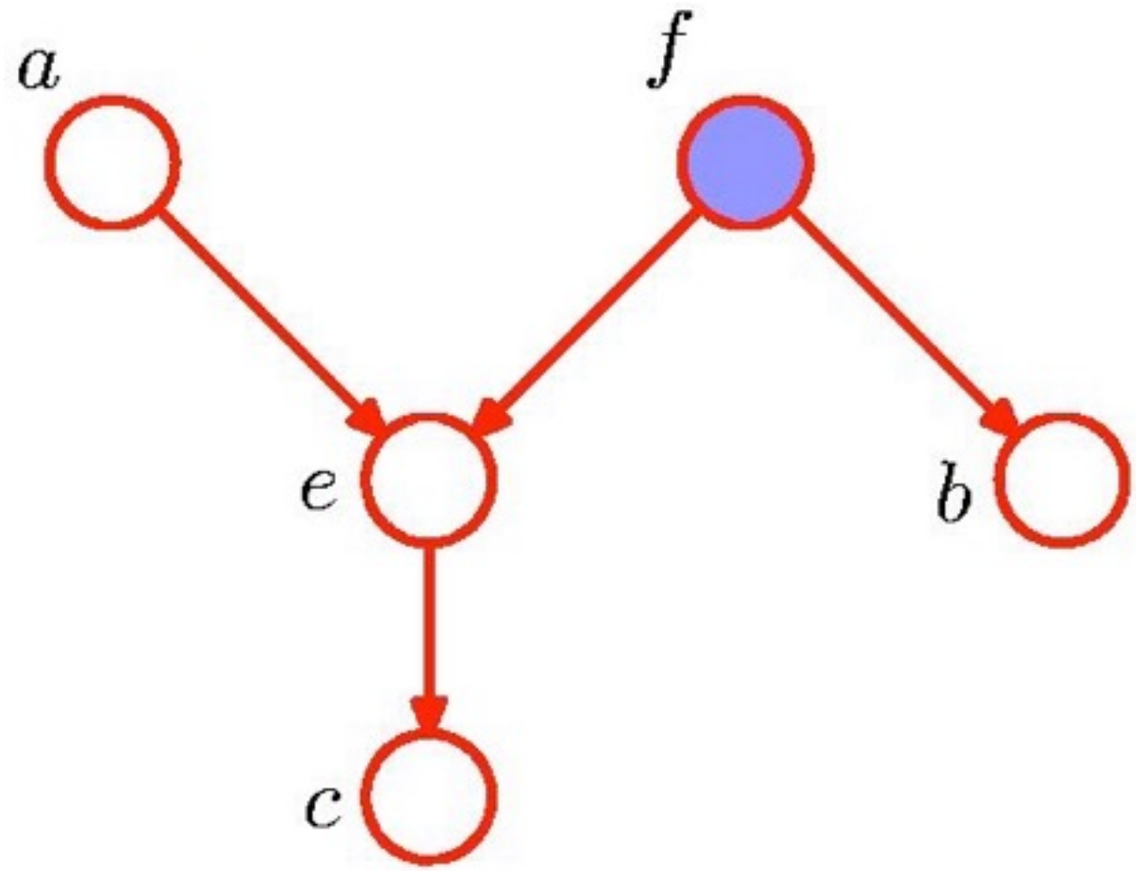
similarly: $p(\neg b \mid \neg c, \neg a) \approx 0.111$

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

Repetition: D-Separation



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



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

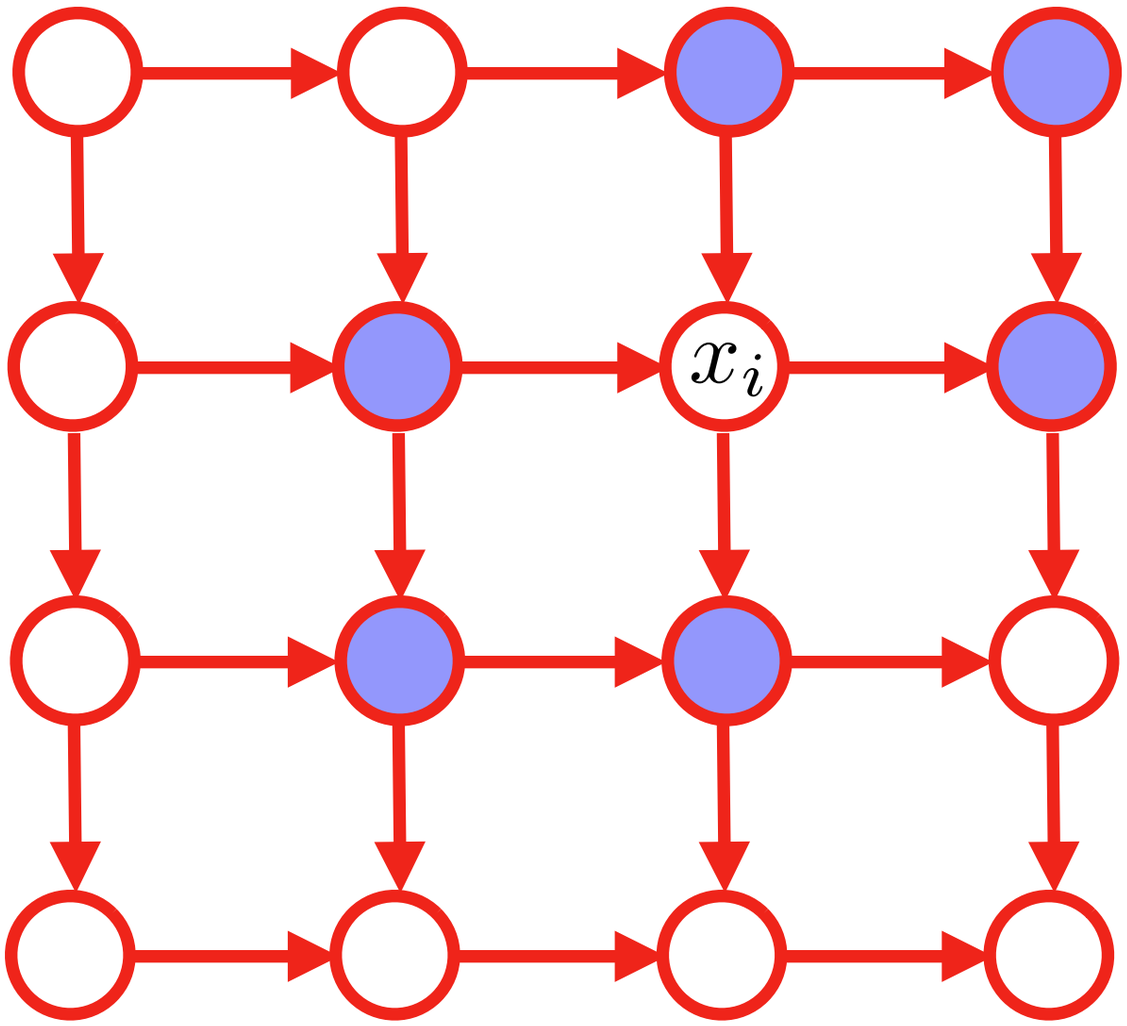
Directed vs. Undirected Graphs

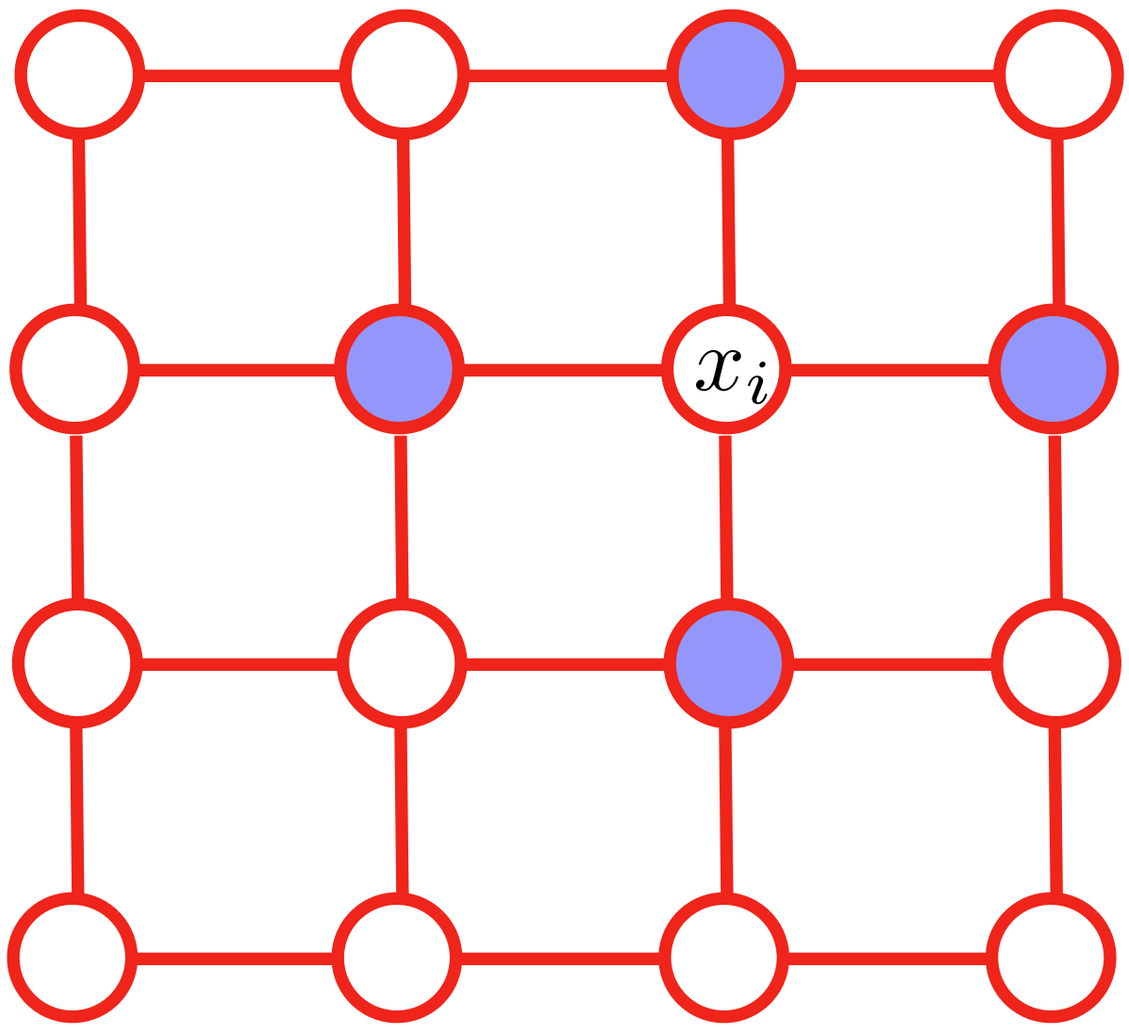
Using D-separation we can identify conditional independencies in directed graphical models, but:

- 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**

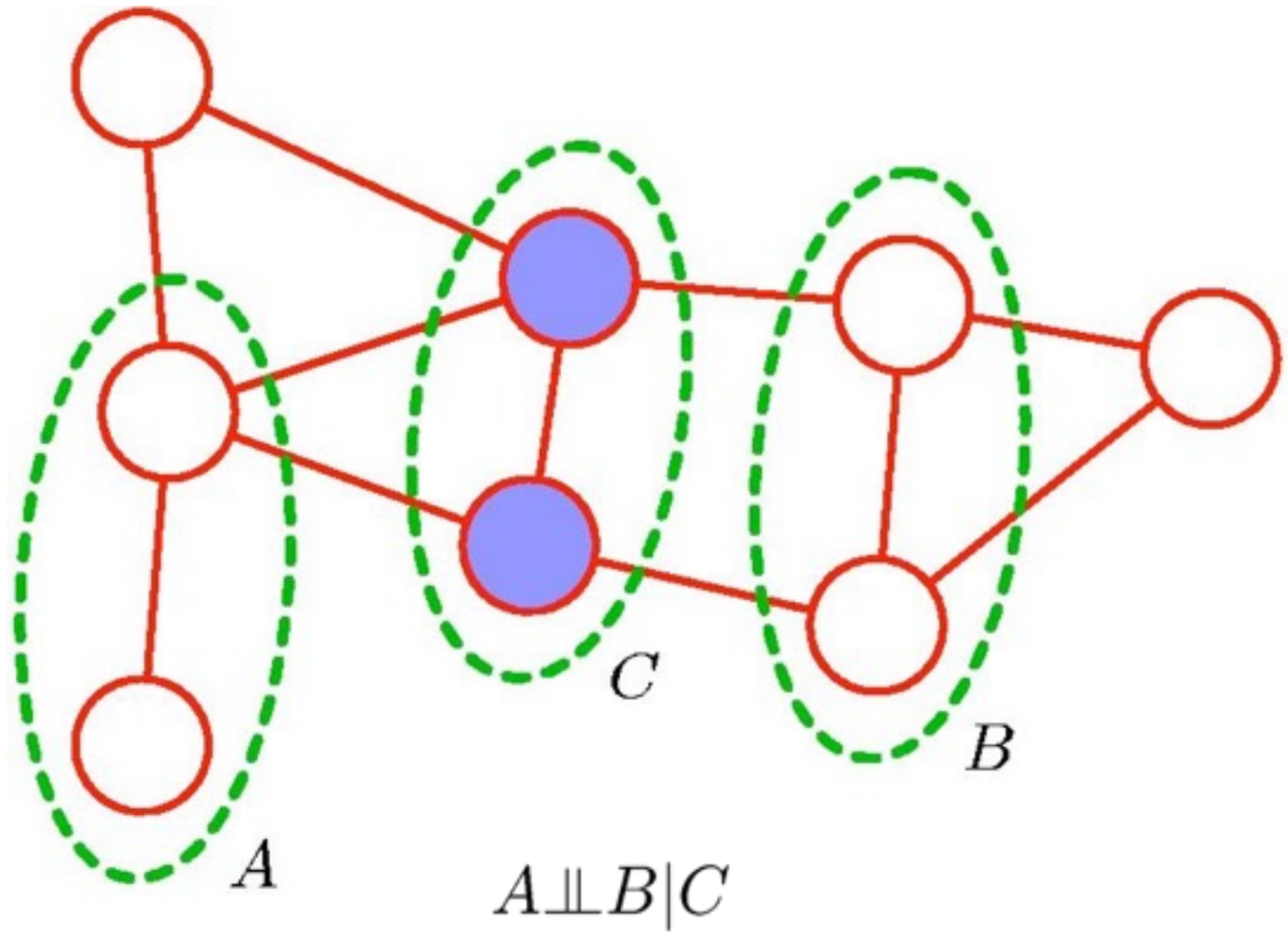
Example: Camera Image





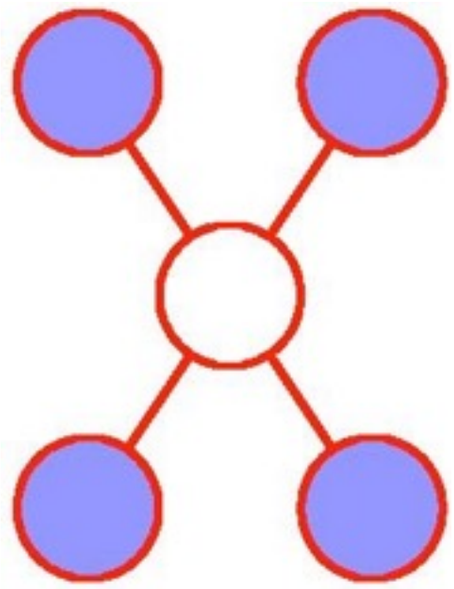
- directions are counter-intuitive for images
- Markov blanket is not just the direct neighbors when using a directed model

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

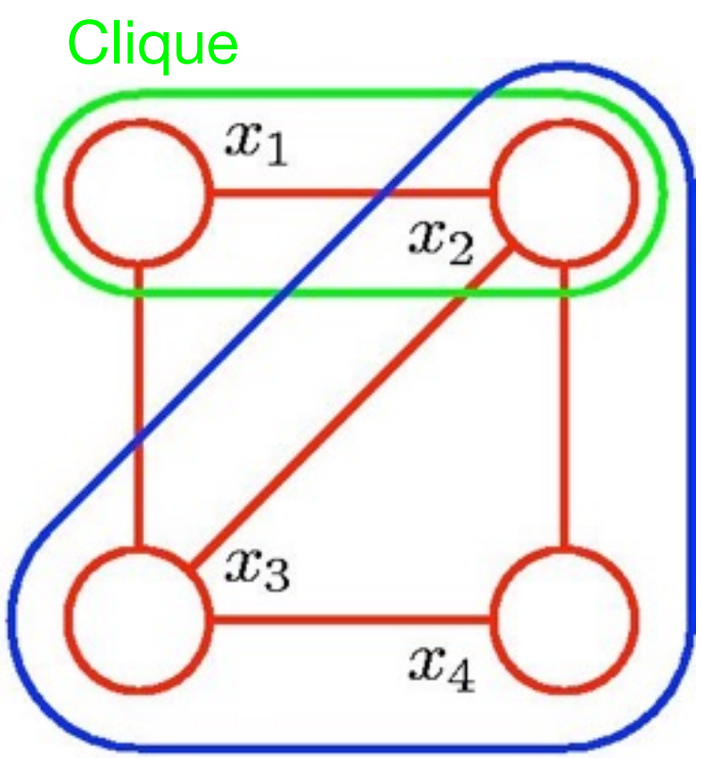
Any two nodes x_i and x_j that are not connected in an MRF are conditionally independent given all other nodes:

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

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.

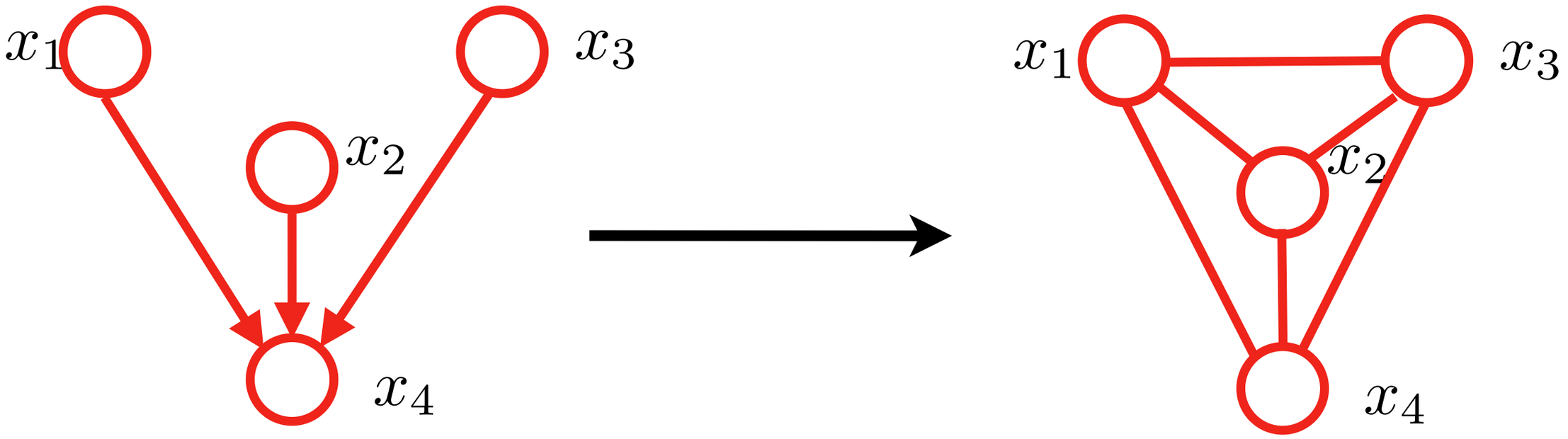
Converting Directed to Undirected Graphs (1)

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

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

In this case: Z=1

Converting Directed to Undirected Graphs (2)



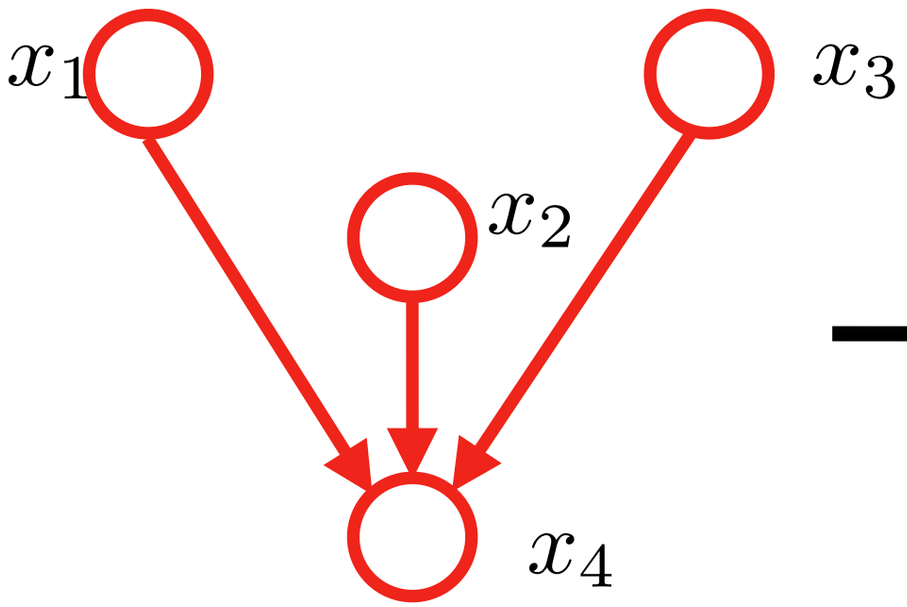
$$p(\mathbf{x}) = p(x_1)p(x_2)p(x_2)p(x_4 \mid x_1, x_2, x_3)$$

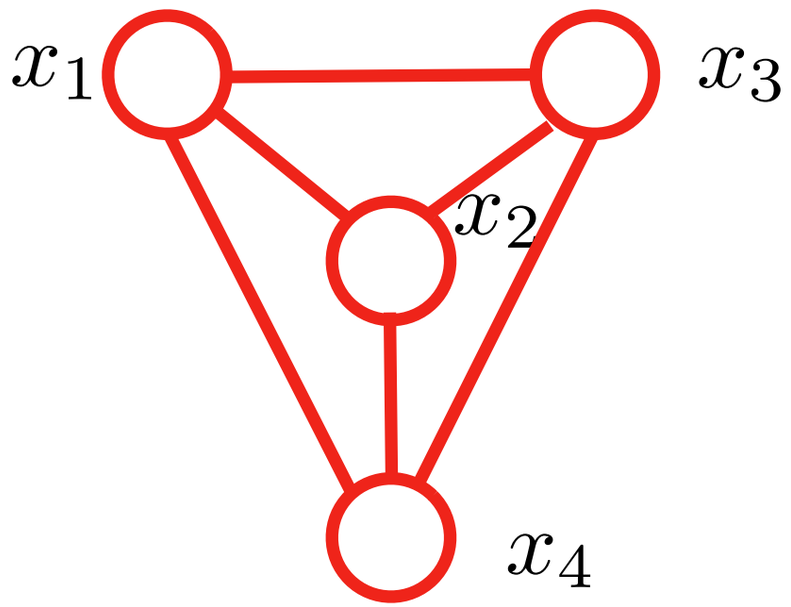
In general: conditional distributions in the directed graph are mapped to cliques in the undirected graph

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)





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

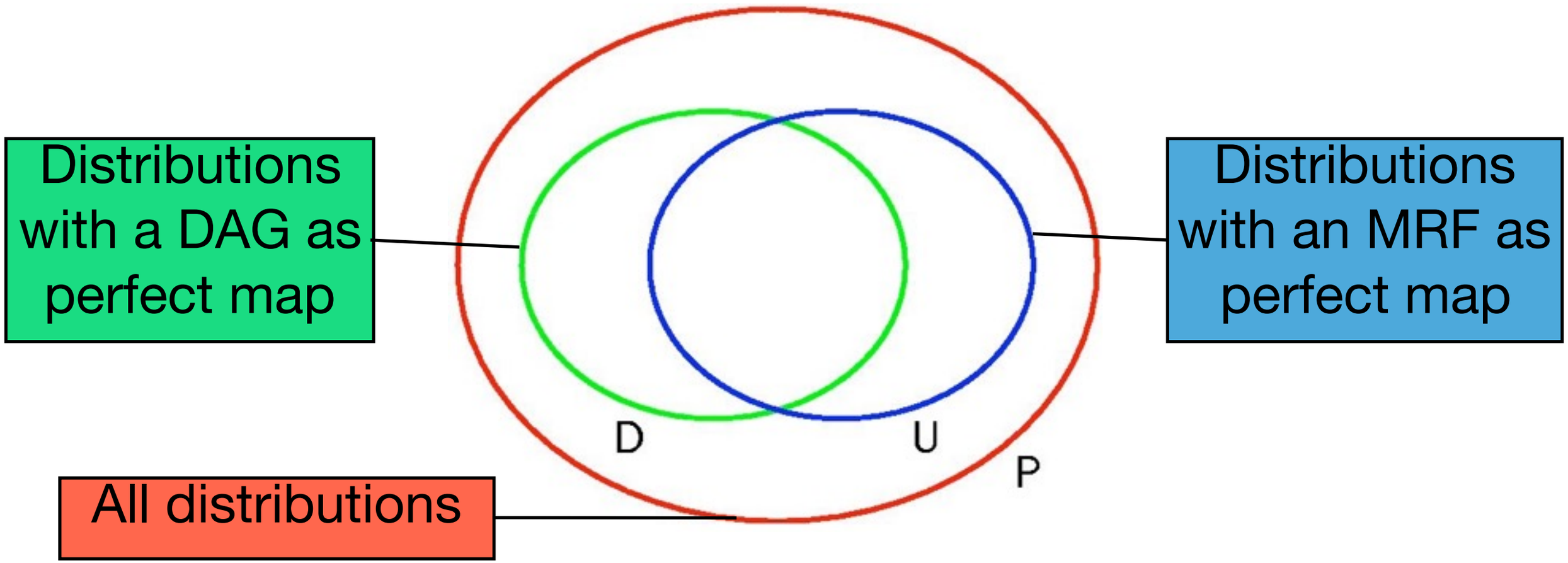
$$p(\mathbf{x}) = \phi(x_1, x_2, x_3, x_4)$$

Problem: This process can remove conditional independence relations (inefficient)

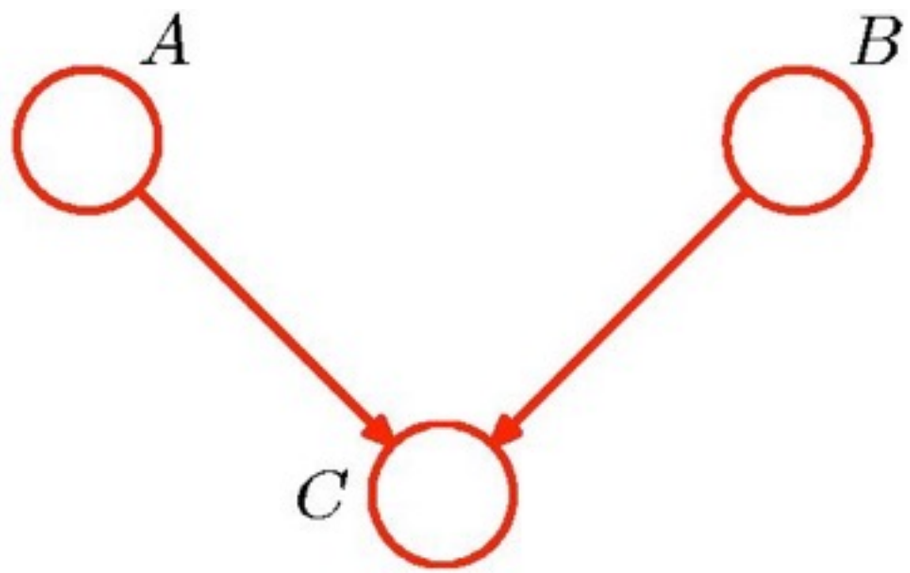
Generally: There is no one-to-one mapping between the distributions represented by directed and by undirected graphs.

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.

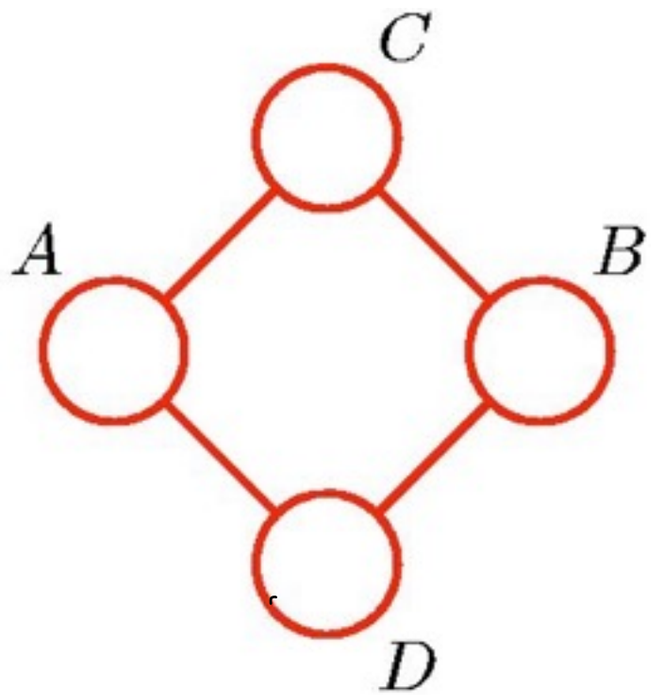


Directed vs. Undirected Graphs



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

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



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

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

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

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

Using Graphical Models

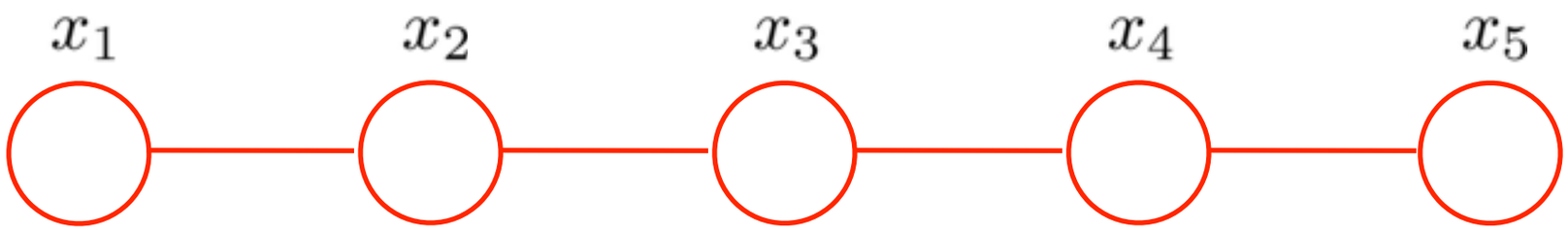
We can use a graphical model to do **inference**:

- Some nodes in the graph are **observed**, for others we want to find the posterior distribution
- Also, computing the local **marginal distribution** $p(x_n)$ at any node x_n can be done using inference.

Question: How can inference be done with a graphical model?

We will see that, when exploiting conditional independences, we can do efficient inference.

Inference on a Chain



The joint probability is given by

$$p(\mathbf{x}) = \frac{1}{Z}\psi_{1,2}(x_1, x_2)\psi_{2,3}(x_2, x_3)\psi_{3,4}(x_3, x_4)\psi_{4,5}(x_4, x_5)$$

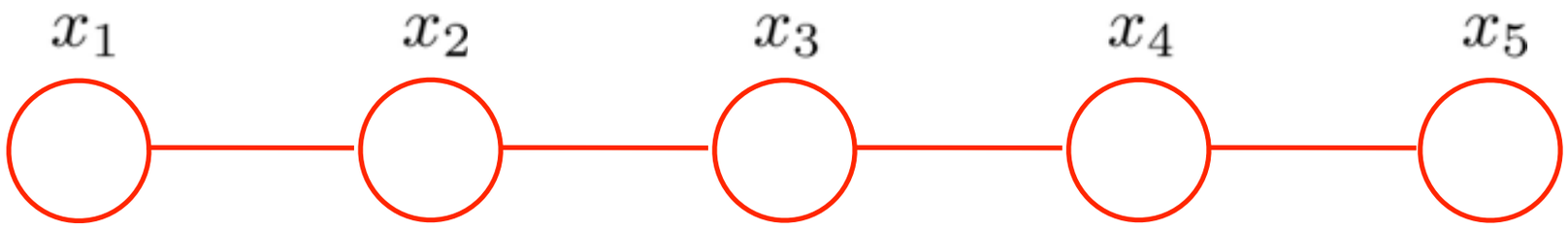
The marginal at x_3 is $$p(x_3) = \sum_{x_1}\sum_{x_2}\sum_{x_4}\sum_{x_5} p(\mathbf{x})$$

In the general case with N nodes we have

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

and $$p(x_n) = \sum_{x_1}\cdots\sum_{x_{n-1}}\sum_{x_{n+1}}\cdots\sum_{x_N} p(\mathbf{x})$$

Inference on a Chain



$$p(x_3) = \sum_{x_1}\sum_{x_2}\sum_{x_4}\sum_{x_5} p(\mathbf{x})$$

- This would mean K^N computations! A more efficient way is obtained by rearranging:

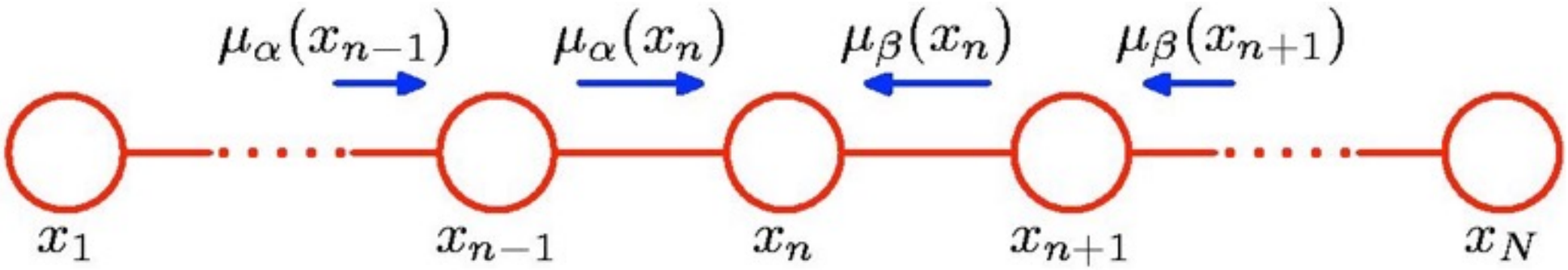
$$p(x_3) = \frac{1}{Z}\sum_{x_1}\sum_{x_2}\sum_{x_4}\sum_{x_5} \psi_{1,2}(x_1,x_2)\psi_{2,3}(x_2,x_3)\psi_{3,4}(x_3,x_4)\psi_{4,5}(x_4,x_5)$$

$$= \frac{1}{Z}\sum_{x_2}\sum_{x_1}\sum_{x_4}\sum_{x_5} \psi_{1,2}(x_1,x_2)\psi_{2,3}(x_2,x_3)\psi_{3,4}(x_3,x_4)\psi_{4,5}(x_4,x_5)$$

$$= \frac{1}{Z}\sum_{x_2}\psi_{2,3}(x_2,x_3)\sum_{x_1}\psi_{1,2}(x_1,x_2)\sum_{x_4}\psi_{3,4}(x_3,x_4)\sum_{x_5}\psi_{4,5}(x_4,x_5)$$

$\mu_\alpha(x_3)$ ← Vectors of size K → $\mu_\beta(x_3)$

Inference on a Chain



In general, we have

$$p(x_n) = \frac{1}{Z} \underbrace{\left[\sum_{x_{n-1}} \psi_{n-1,n}(x_{n-1}, x_n) \cdots \left[\sum_{x_1} \psi_{1,2}(x_1, x_2) \right] \cdots \right]}_{\mu_\alpha(x_n)} \underbrace{\left[\sum_{x_{n+1}} \psi_{n,n+1}(x_n, x_{n+1}) \cdots \left[\sum_{x_N} \psi_{N-1,N}(x_{N-1}, x_N) \right] \cdots \right]}_{\mu_\beta(x_n)}$$

Inference on a Chain

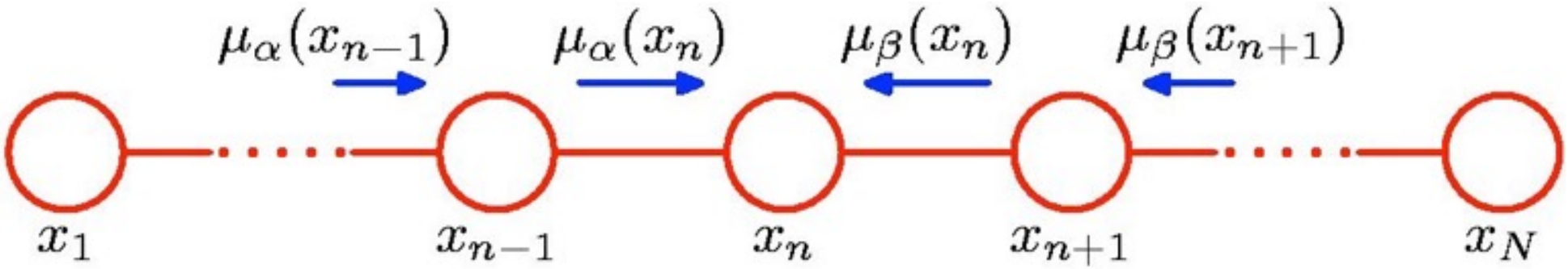
The **messages** μ_α and μ_β can be computed recursively:

$$\begin{aligned}
\mu_\alpha(x_n) &= \sum_{x_{n-1}} \psi_{n-1,n}(x_{n-1}, x_n) \left[\sum_{x_{n-2}} \cdots \right] \\
&= \sum_{x_{n-1}} \psi_{n-1,n}(x_{n-1}, x_n) \mu_\alpha(x_{n-1}).
\end{aligned}$$

$$\begin{aligned}
\mu_\beta(x_n) &= \sum_{x_{n+1}} \psi_{n,n+1}(x_n, x_{n+1}) \left[\sum_{x_{n+2}} \cdots \right] \\
&= \sum_{x_{n+1}} \psi_{n,n+1}(x_n, x_{n+1}) \mu_\beta(x_{n+1}).
\end{aligned}$$

Computation of μ_α starts at the first node and computation of μ_β starts at the last node.

Inference on a Chain



- The first values of μ_α and μ_β are:

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

- The partition function can be computed at any node:

$$Z = \sum_{x_n} \mu_\alpha(x_n)\mu_\beta(x_n)$$

- Overall, we have $O(NK^2)$ operations to compute the marginal $p(x_n)$

Inference on a Chain

To compute local marginals:

- Compute and store all forward messages, $\mu_\alpha(x_n)$.
- Compute and store all backward messages, $\mu_\beta(x_n)$
- Compute Z **once** at a node x_m: $Z = \sum_{x_m} \mu_\alpha(x_m)\mu_\beta(x_m)$
- Compute

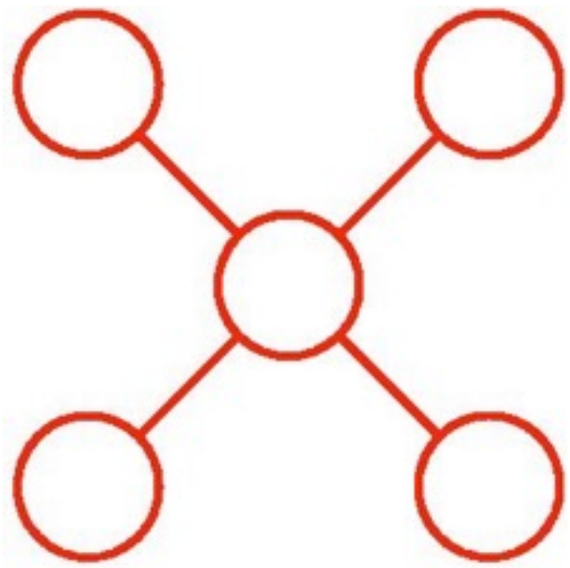
$$p(x_n) = \frac{1}{Z}\mu_\alpha(x_n)\mu_\beta(x_n)$$

for all variables required.

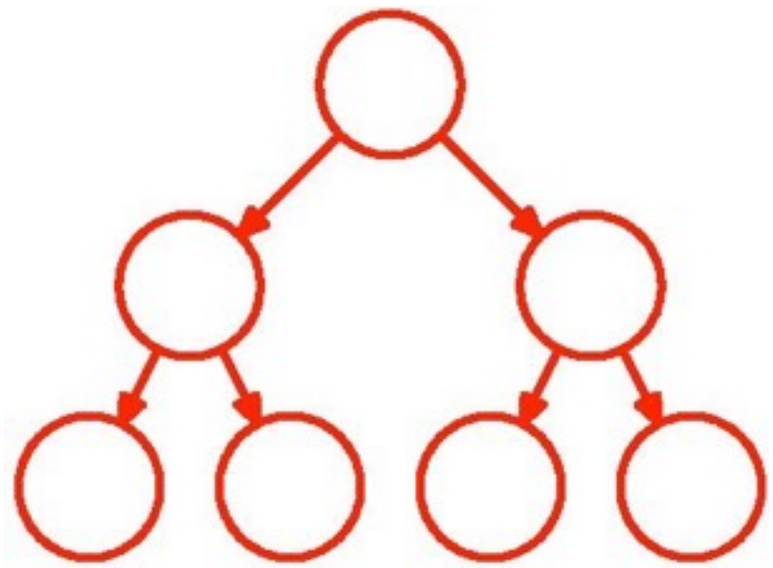
More General Graphs

The message-passing algorithm can be extended to more general graphs:

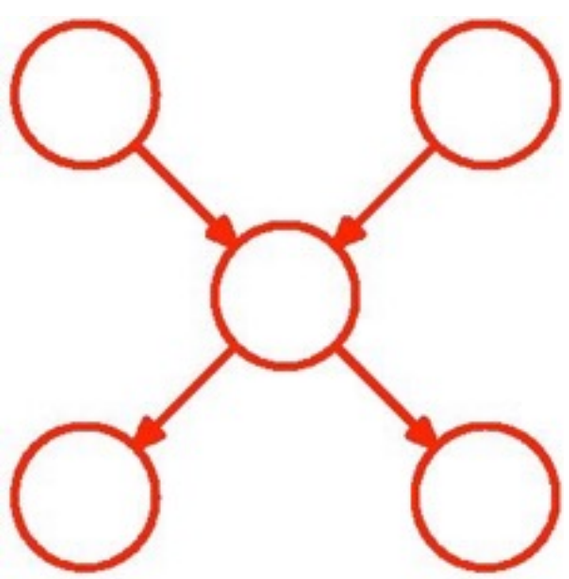
Undirected Tree



Directed Tree



Polytree

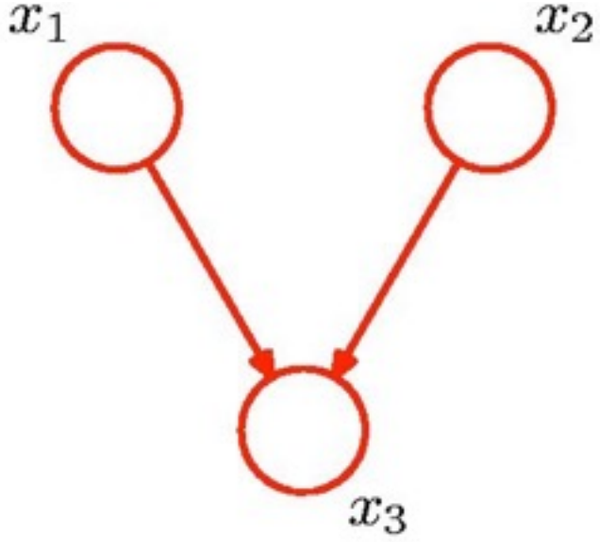


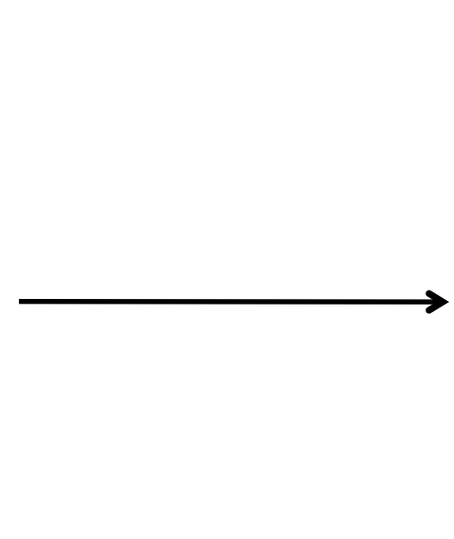
It is then known as the **sum-product algorithm.**

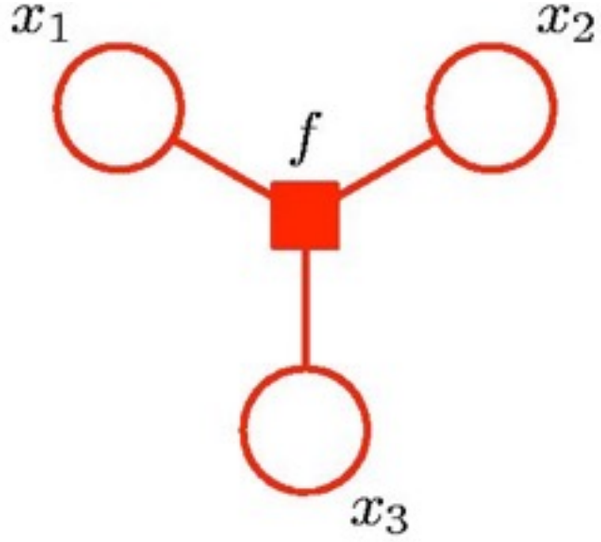
A special case of this is **belief propagation**.

Factor Graphs

- The Sum-product algorithm can be used to do inference on undirected and directed graphs.
- A representation that generalizes directed and undirected models is the **factor graph**.







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

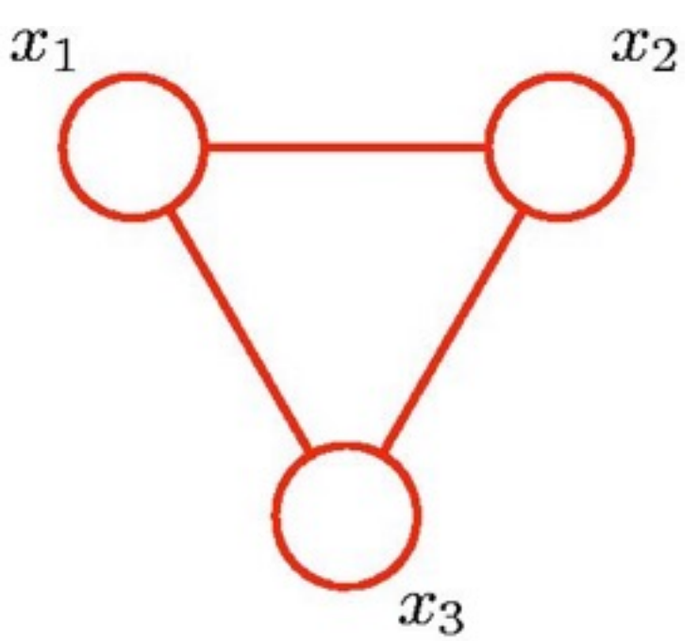
Directed graph

$$f(x_1, x_2, x_3) = p(x_1)p(x_2)p(x_3 \mid x_1, x_2)$$

Factor graph

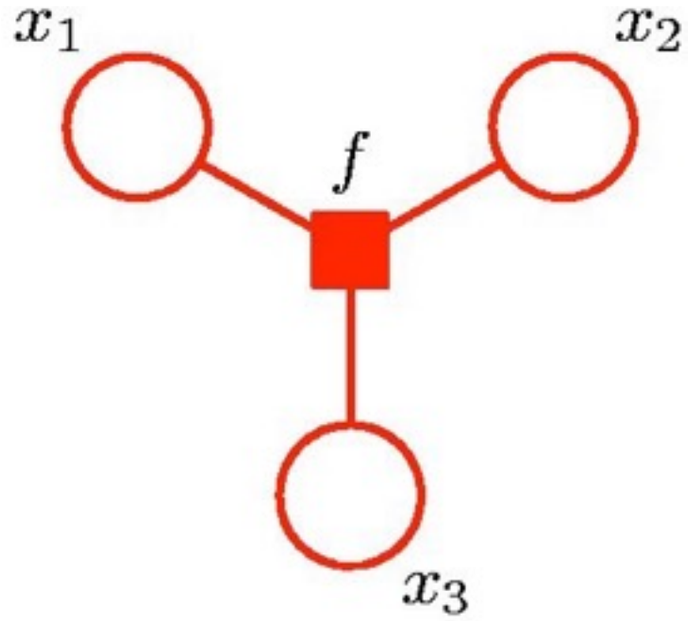
Factor Graphs

- The Sum-product algorithm can be used to do inference on undirected and directed graphs.
- A representation that generalizes directed and undirected models is the **factor graph**.



$$\psi(x_1, x_2, x_3)$$

Undirected graph



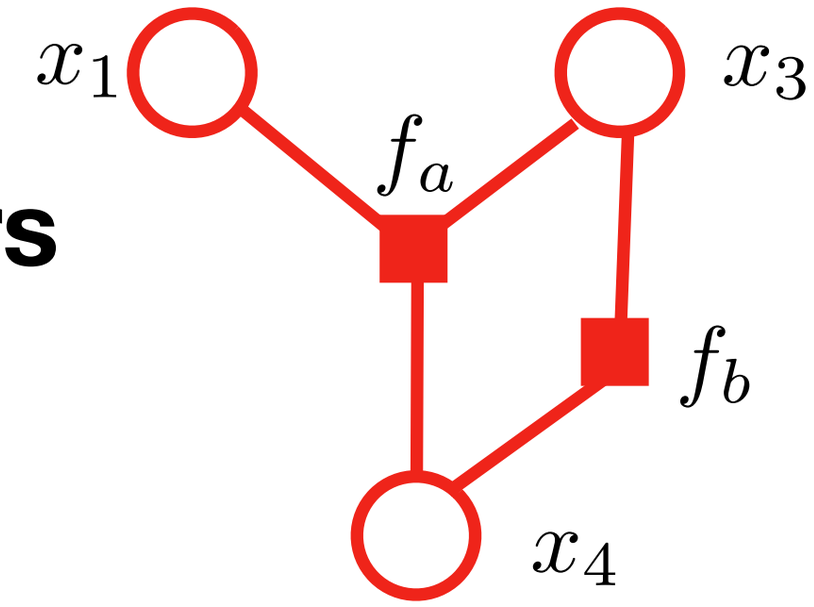
$$f(x_1, x_2, x_3) = \psi(x_1, x_2, x_3)$$

Factor graph

Factor Graphs

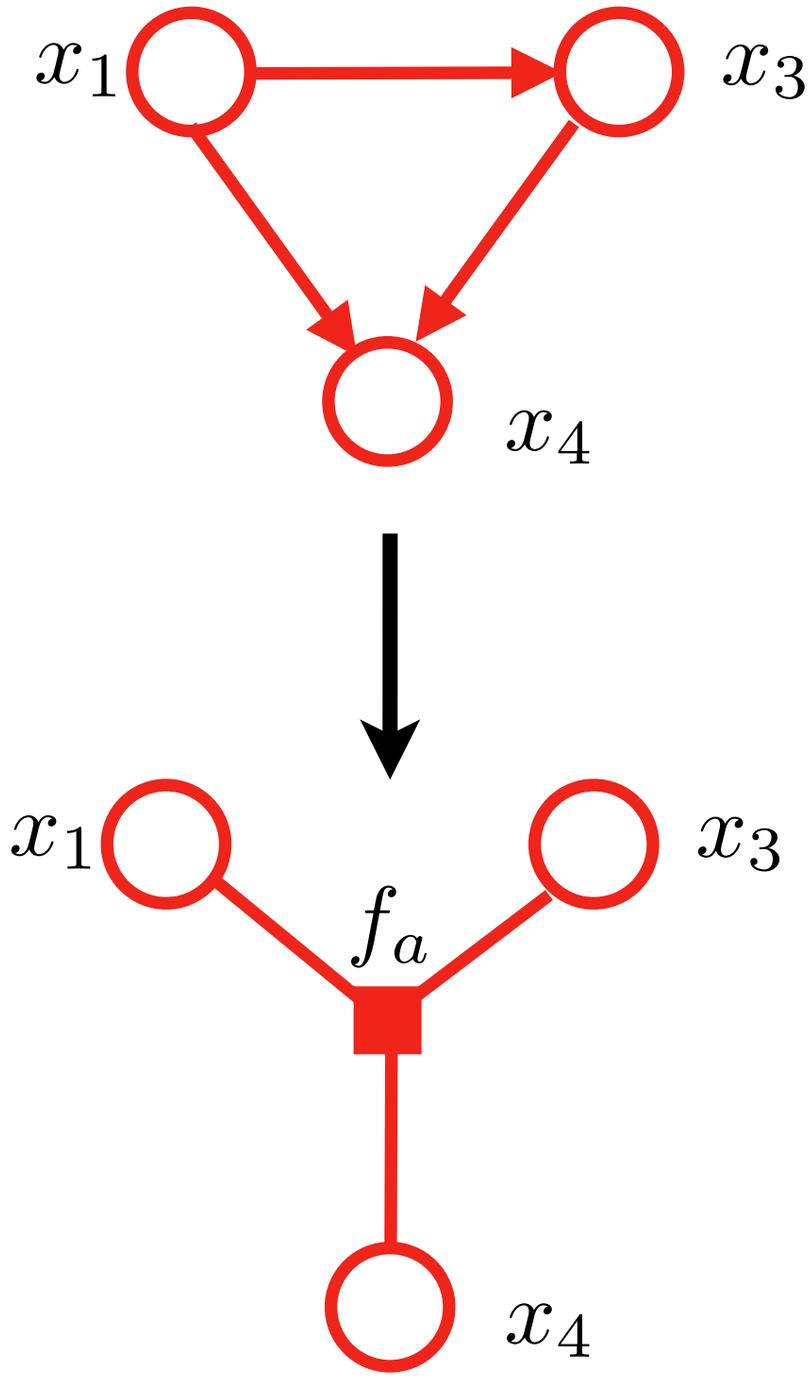
Factor graphs

- can contain **multiple factors** for the same nodes
- are more general than undirected graphs
- are **bipartite**, i.e. they consist of two kinds of nodes and all edges connect nodes of different kind



Factor Graphs

- Directed trees convert to tree-structured factor graphs
- The same holds for undirected trees
- Also: directed polytrees convert to tree-structured factor graphs
- And: Local cycles in a directed graph can be removed by converting to a factor graph



Sum-Product Inference in General Graphical Models

1. Convert graph (directed or undirected) into a **factor graph** (there are no cycles)
2. If the goal is to **marginalize** at node x, then consider x as a root node
3. Initialize the recursion at the leaf nodes as:

$$\mu_{f \to x}(x) = 1 \quad \text{(var) or} \quad \mu_{x \to f}(x) = f(x) \text{ (fac)}$$

4. Propagate messages from the leaves to x
5. Propagate messages from x to the leaves
6. Obtain marginals at every node by multiplying all incoming messages

Other Inference Algorithms

- Max-Sum algorithm: used to **maximize** the joint probability of all variables (no marginalization)
- Junction Tree algorithm: exact inference for general graphs (even with loops)
- Loopy belief propagation: approximate inference on general graphs (more efficient)

Special kind of undirected GM:

- Conditional Random fields (e.g.: classification)

Conditional Random Fields

- Another kind of undirected graphical model is known as **Conditional Random Field** (CRF).
- CRFs are used for classification where labels are represented as discrete random variables $\mathbf{y}$ and features as continuous random variables $\mathbf{x}$
- A CRF represents the conditional probability

$$p(\mathbf{y} \mid \mathbf{x}, \mathbf{w}) = \frac{\prod_C \phi_C(\mathbf{x}_C, \mathbf{y}_C; \mathbf{w})}{\sum_{\mathbf{y}'} \prod_C \phi_C(\mathbf{x}_C, \mathbf{y}'_C; \mathbf{w})}$$

  where $\mathbf{w}$ are parameters learned from training data.
- CRFs are **discriminative** and MRFs are **generative**

Conditional Random Fields

Derivation of the formula for CRFs:

$$p(\mathbf{y} \mid \mathbf{x}, \mathbf{w}) = \frac{p(\mathbf{y}, \mathbf{x} \mid \mathbf{w})}{p(\mathbf{x} \mid \mathbf{w})} = \frac{p(\mathbf{y}, \mathbf{x} \mid \mathbf{w})}{\sum_{y'} p(\mathbf{y}', \mathbf{x} \mid \mathbf{w})} = \frac{\prod_C \phi_C(\mathbf{x}_C, \mathbf{y}_C; \mathbf{w}) \quad Z}{Z \quad \sum_{\mathbf{y}'} \prod_C \phi_C(\mathbf{x}_C, \mathbf{y}'_C; \mathbf{w})}$$

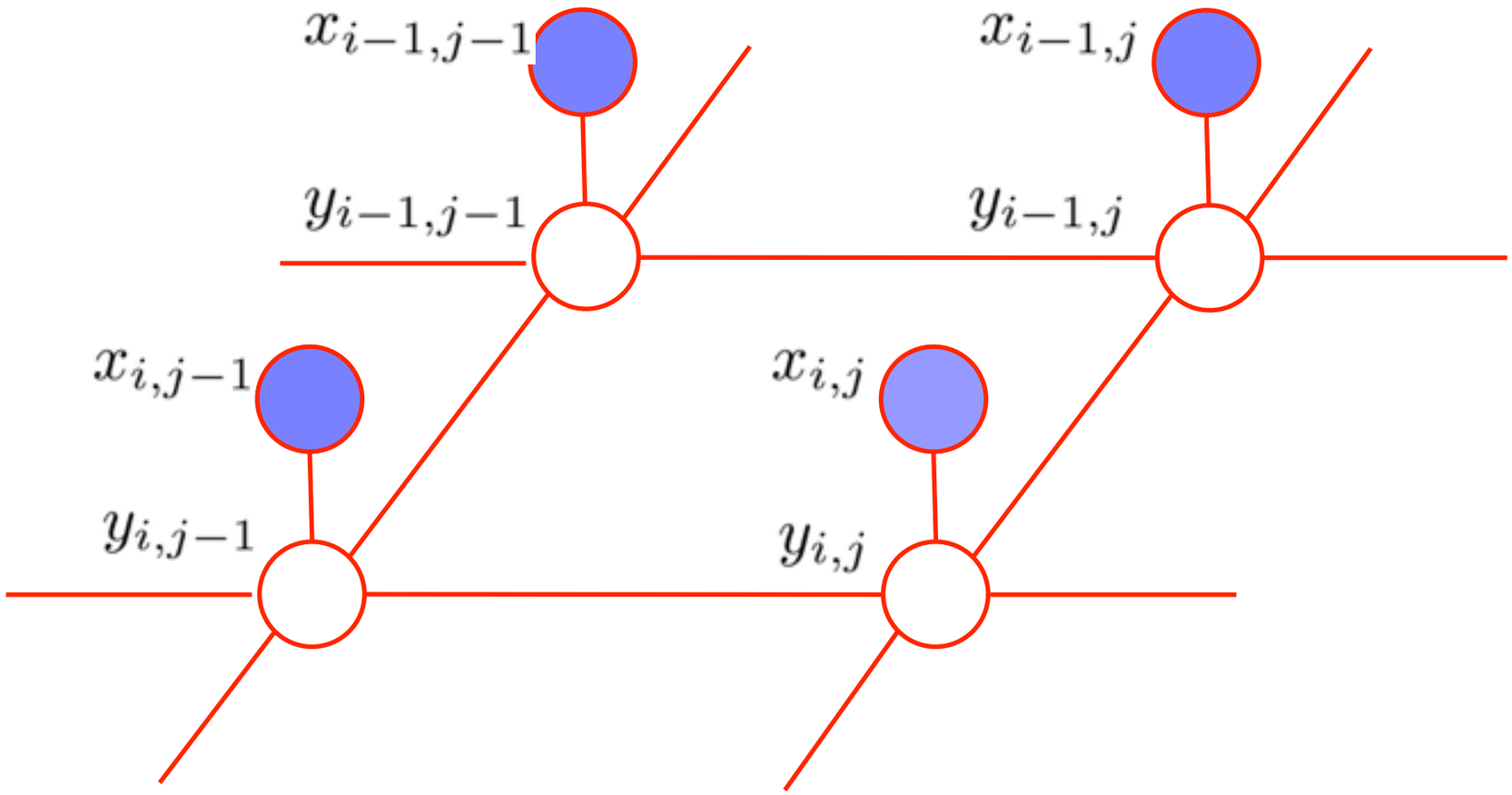
In the training phase, we compute parameters $\mathbf{w}$ that maximize the posterior:

$$\mathbf{w}^* = \arg\max_{\mathbf{w}} p(\mathbf{w} \mid \mathbf{x}^*, \mathbf{y}^*) \propto p(\mathbf{y}^* \mid \mathbf{x}^*, \mathbf{w}) p(\mathbf{w})$$

where $(\mathbf{x}^*, \mathbf{y}^*)$ is the training data and $p(\mathbf{w})$ is a Gaussian prior. In the inference phase we maximize

$$\arg\max_{\mathbf{y}} p(\mathbf{y} \mid \mathbf{x}, \mathbf{w}^*)$$

Conditional Random Fields



Typical example: **observed** variables $x_{i,j}$ are intensity values of pixels in an image and **hidden** variables $y_{i,j}$ are object labels

Note: the definition of $x_{i,j}$ and $y_{i,j}$ is different from the one in C.M. Bishop (pg.389)!

CRF Training

We minimize the negative log-posterior:

$$\mathbf{w}^* = \arg\min_{\mathbf{w}} \{-\ln p(\mathbf{w} \mid \mathbf{x}^*, \mathbf{y}^*)\} = \arg\min_{\mathbf{w}} \{-\ln p(\mathbf{y}^* \mid \mathbf{x}^*, \mathbf{w}) - \ln p(\mathbf{w})\}$$

Computing the likelihood is intractable, as we have to compute the partition function for each $\mathbf{w}$. We can approximate the likelihood using **pseudo-likelihood**:

$$p(\mathbf{y}^* \mid \mathbf{x}^*, \mathbf{w}) \approx \prod_i p(y_i^* \mid \mathcal{M}(y_i^*), \mathbf{x}^*, \mathbf{w})$$

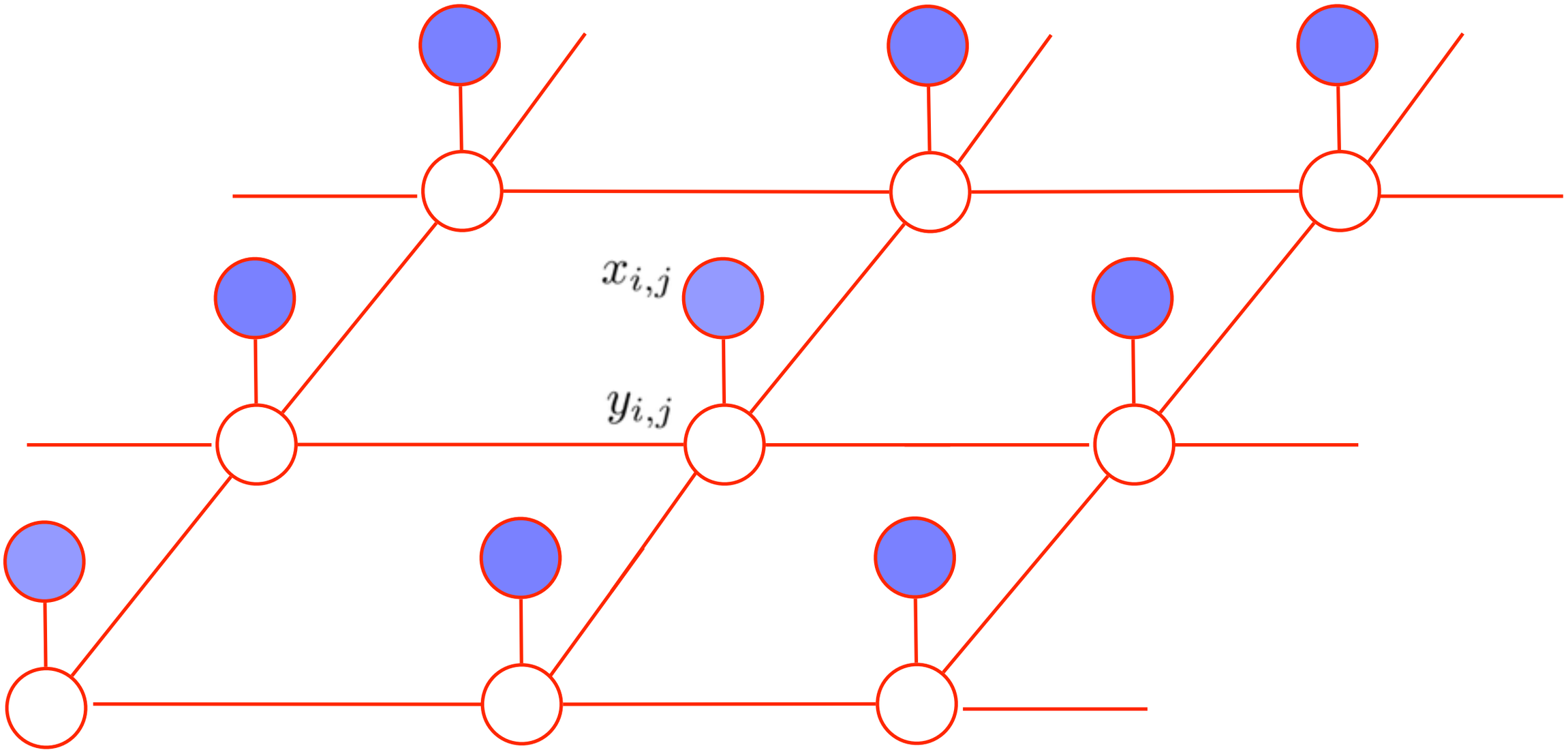
where

Markov blanket

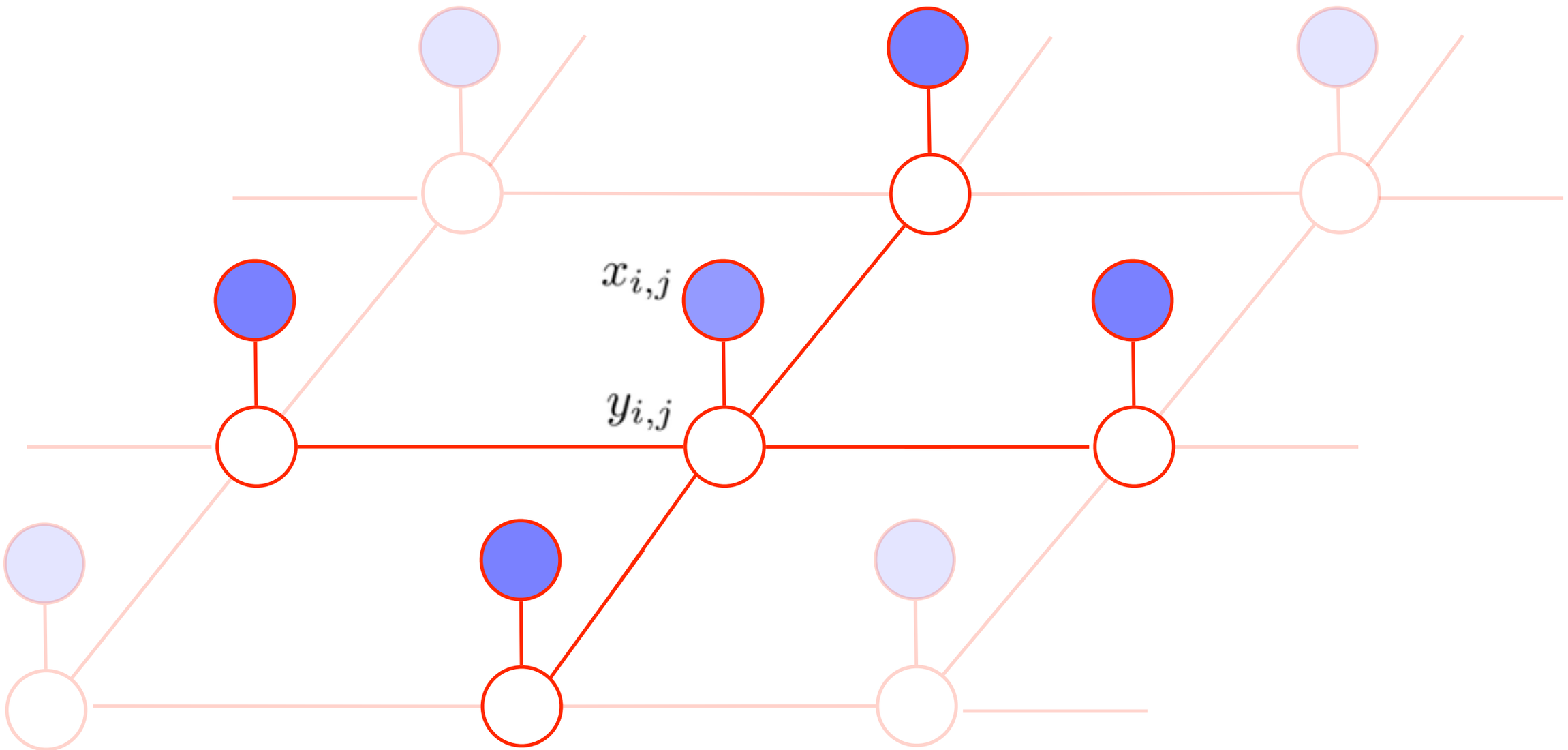
C_i: All cliques containing y_i

$$p(y_i^* \mid \mathcal{M}(y_i^*), \mathbf{x}^*, \mathbf{w}) = \frac{\prod_{C_i} \phi_{C_i}(\mathbf{x}_{C_i}^*, y_i^*, \mathbf{y}_{C_i}^*; \mathbf{w})}{\sum_{y_i'} \prod_{C_i} \phi_C(\mathbf{x}_{C_i}^*, y_i', \mathbf{y}_{C_i}^*; \mathbf{w})}$$

Pseudo Likelihood



Pseudo Likelihood



Pseudo-likelihood is computed only on the Markov blanket of y_i and its corresp. feature nodes.

Potential Functions

- The only requirement for the potential functions is that they are positive. We achieve that with:

$$\phi_C(\mathbf{x}_C, \mathbf{y}_C, \mathbf{w}) := \exp(\mathbf{w}^T f(\mathbf{x}_C, \mathbf{y}_C))$$

where f is a compatibility function that is large if the labels $\mathbf{y}_C$ fit well to the features $\mathbf{x}_C$.

- This is called the **log-linear model.**
- The function f can be, e.g. a local classifier

CRF Training and Inference

Training:

- Using pseudo-likelihood, training is efficient. We have to minimize:

$$L(\mathbf{w}) = -lpl(\mathbf{y}^* \mid \mathbf{x}^*, \mathbf{w}) + \frac{1}{2\sigma^2}\mathbf{w}^T\mathbf{w}$$

Log-pseudo-likelihood

Gaussian prior

- This is a convex function that can be minimized using gradient descent

Inference:

- Only approximatively, e.g. using loopy belief propagation

Summary

- Undirected models (aka Markov random fields) provide an intuitive representation of conditional independence
- An MRF is defined as a **factorization** over clique potentials and normalized globally
- Directed and undirected models have different representative power (no simple “containment”)
- Inference on undirected Markov chains is efficient using message passing
- Factor graphs are more general; exact inference can be done efficiently using sum-product