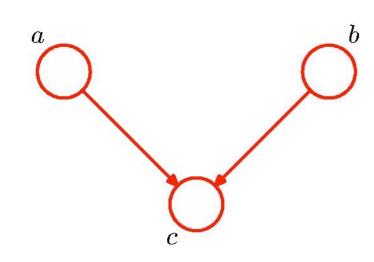
The Head-to-Head Node



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

a	b	p(c a,b)
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"

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: dsep(A, B|C)



D-Separation

Say: A, B, and C are non-intersecting subsets of

nodes

A patha node

a) the autail at the

b) the a the noc

•If all p

D-Separation is a property of graphs

and not of

probability

distributions

be d-separated from B by C.

Notation: dsep(A, B|C)

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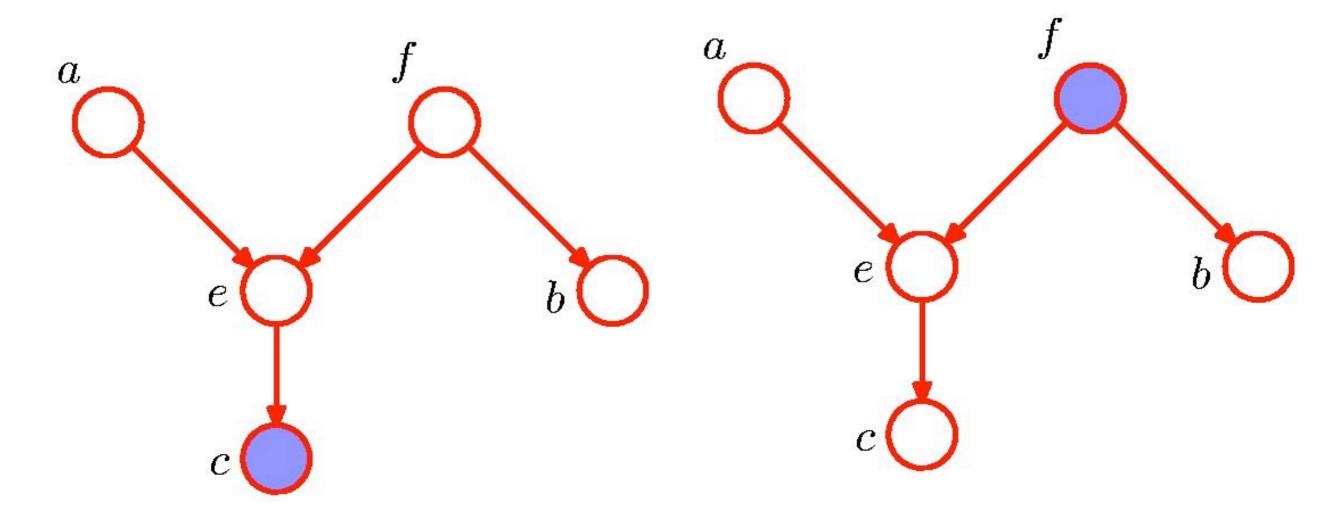
5

aid to





D-Separation: Example



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

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

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:

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

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:

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

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.

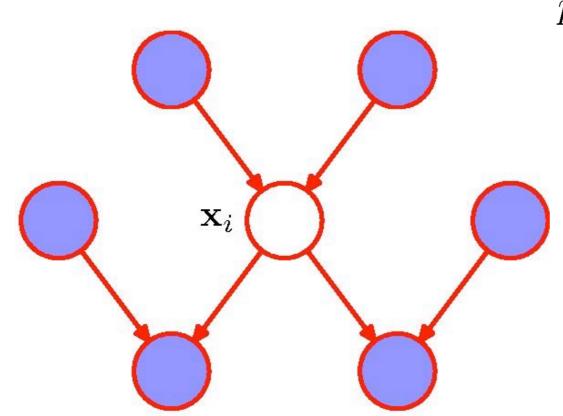
$$\forall A, B, C : A \perp \!\!\!\perp B \mid C \Leftrightarrow \text{dsep}(A, B, C)$$

A perfect map uniquely defines a probability distribution.



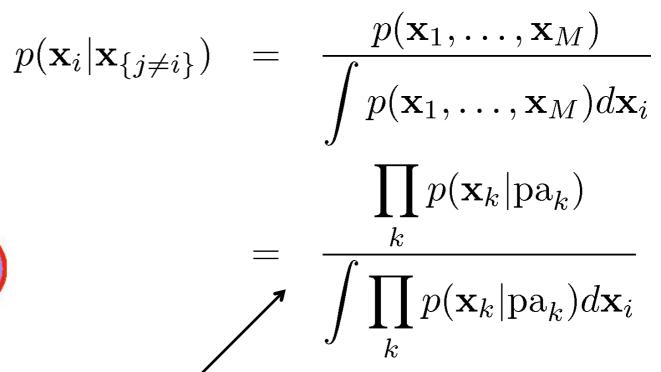
The Markov Blanket

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



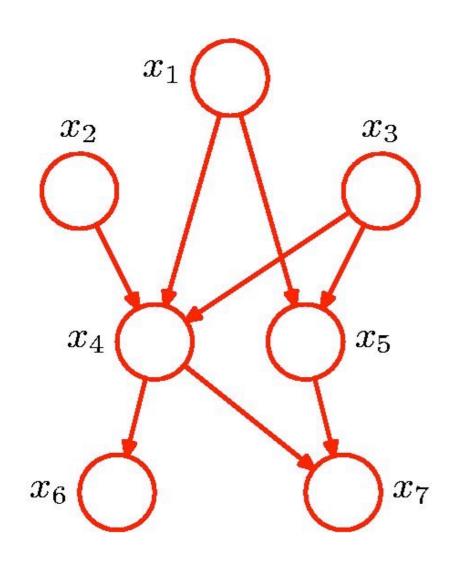
Markov blanket \mathcal{M}_i at

 \mathbf{x}_i : all parents, children and co-parents of \mathbf{x}_i .



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

Directed Graphical Models

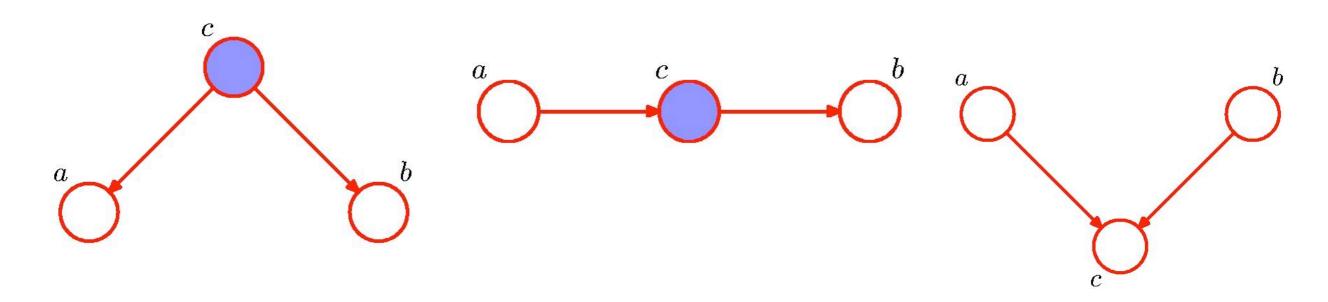


Directed graphical models can be used to represent probability distributions

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

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

Summary 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.



Directed vs. Undirected Graphs

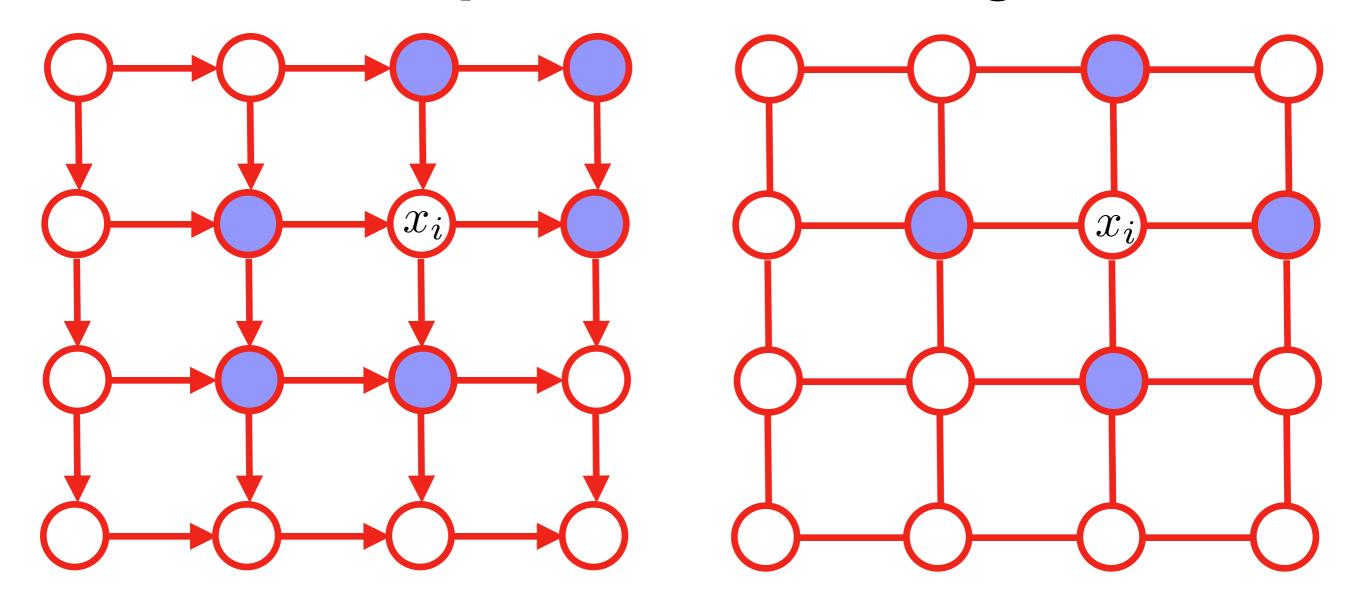
Using D-separation we can identify conditional independencies in directed graphical models, but:

- 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

Aim: Find a simpler formulation of d-separation!

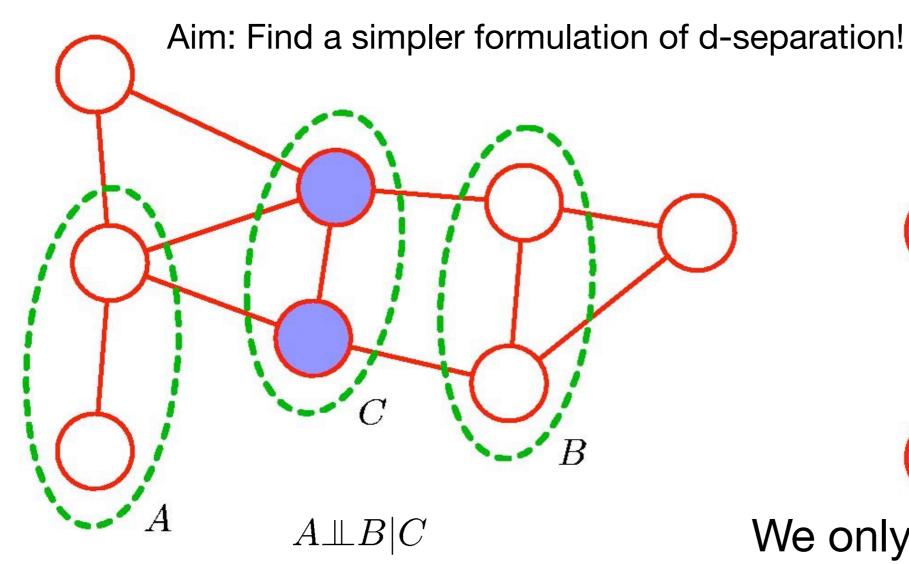


Markov Random Fields

Aim: Find a simpler formulation of d-separation! $A \perp \!\!\! \perp B | C$

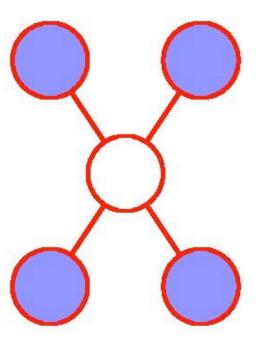
All paths from A to B go through C, i.e. C should block all paths.

Markov Random Fields



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

Markov Blanket



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

Factorization of MRFs

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

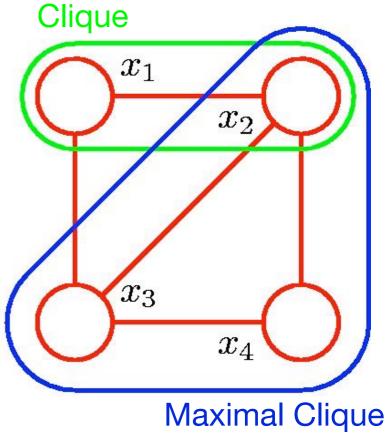
$$p(x_i, x_j \mid \mathbf{x}_{\setminus \{i,j\}}) = p(x_i \mid \mathbf{x}_{\setminus \{i,j\}}) p(x_j \mid \mathbf{x}_{\setminus \{i,j\}})$$

This means: each factor must contain only nodes that are pairwise connected

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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

$$p(\mathbf{x}) = \frac{\prod_{c \in \mathcal{C}} \psi_c(\mathbf{x}_c)}{\sum_{\mathbf{x}'} \prod_{c \in \mathcal{C}} \psi_c(\mathbf{x}'_c)} = \frac{1}{Z} \prod_{c \in \mathcal{C}} \psi_c(\mathbf{x}_c)$$
(4.1)

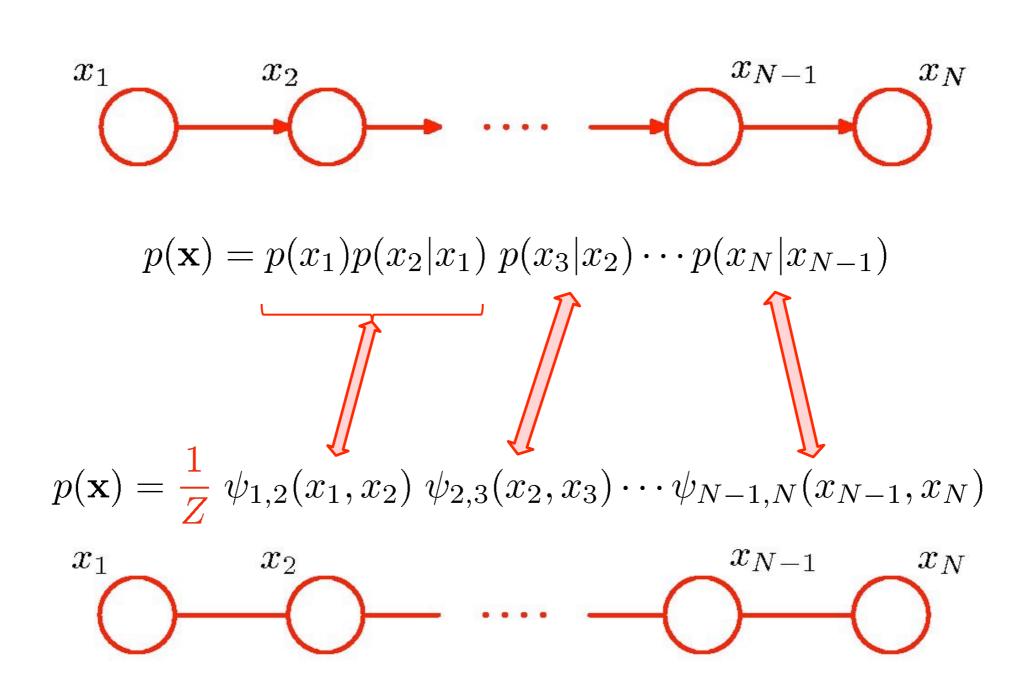
where C is the set of all (maximal) cliques and $\psi_c(\mathbf{x}_c)$ is a positive function of a given clique \mathbf{x}_C of nodes, called the **clique potential**. Z is called the **partition function**.

Theorem (Hammersley/Clifford): Any undirected model with associated clique potentials ψ_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.

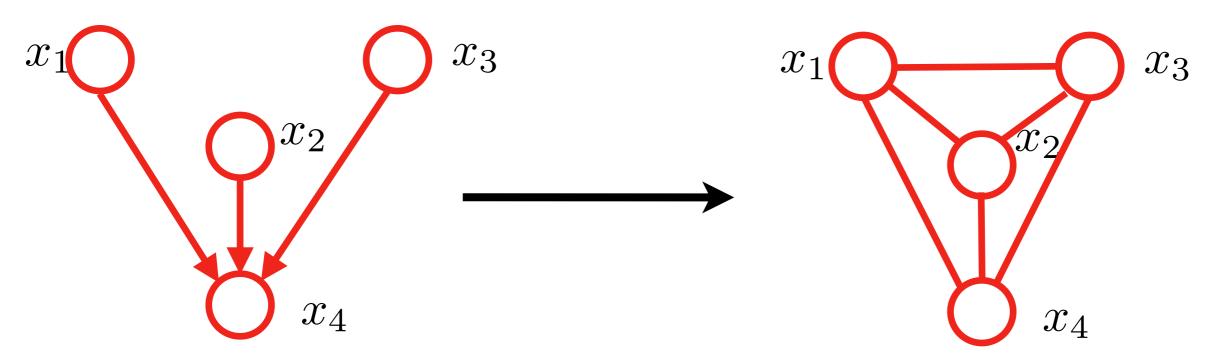


Converting Directed to Undirected Graphs (1)



In this case: Z=1

Converting Directed to Undirected Graphs (2)



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

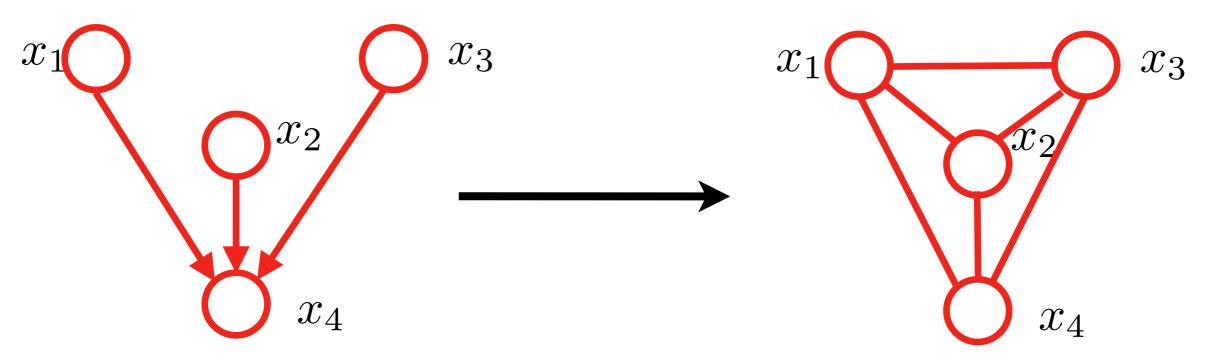
In general: conditional distributions in the directed graph are mapped to cliques in the undirected graph

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)



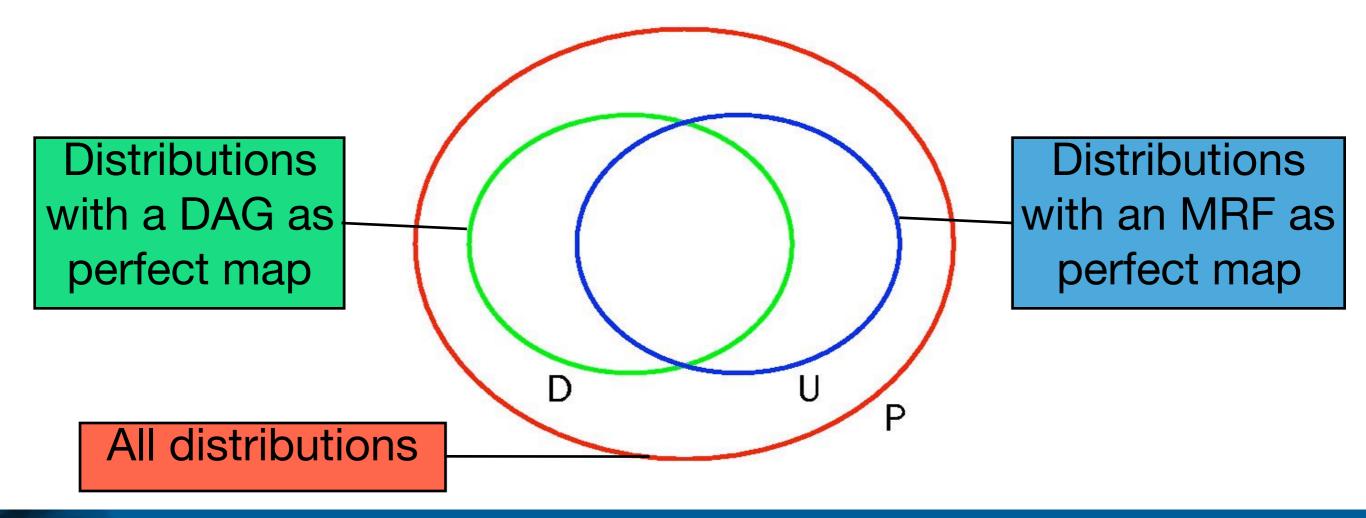
$$p(\mathbf{x}) = p(x_1)p(x_2)p(x_2)p(x_4 \mid x_1, x_2, x_3)$$
 $p(\mathbf{x}) = \phi(x_1, x_2, x_3, x_4)$

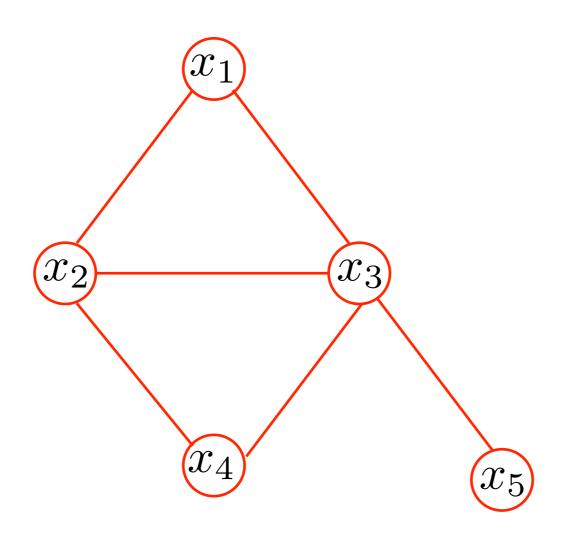
Problem: This process can remove conditional independence relations (inefficient)

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

Representability

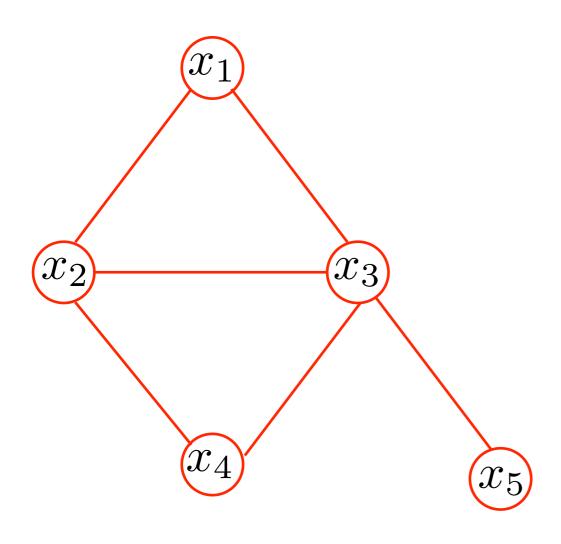
- As for DAGs, we can define an I-map, a D-map and a perfect map for MRFs.
- The set of all distributions for which a DAG exists that is a perfect map is different from that for MRFs.





If a distribution p satisfies all conditional independence relationships of this graph, then we can write p as

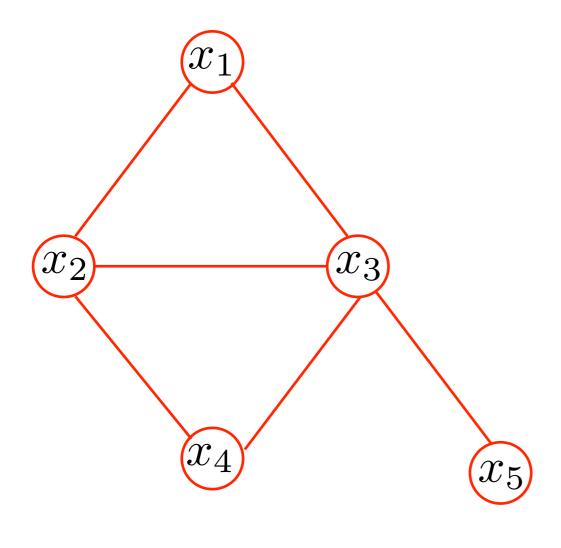
$$p(\mathbf{x}) = \frac{1}{Z}\psi_{123}(x_1, x_2, x_3)\psi_{234}(x_2, x_3, x_4)\psi_{35}(x_3, x_5)$$



How to define the potentials?

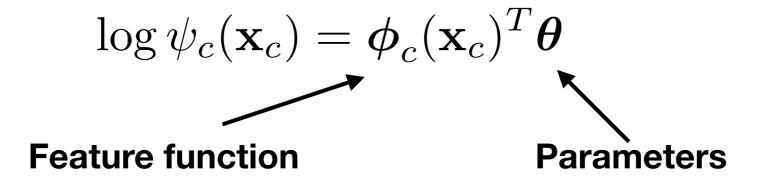
 Intuitively, the potential of a clique should be high, iff the joint probability of the corresponding random variables is high.

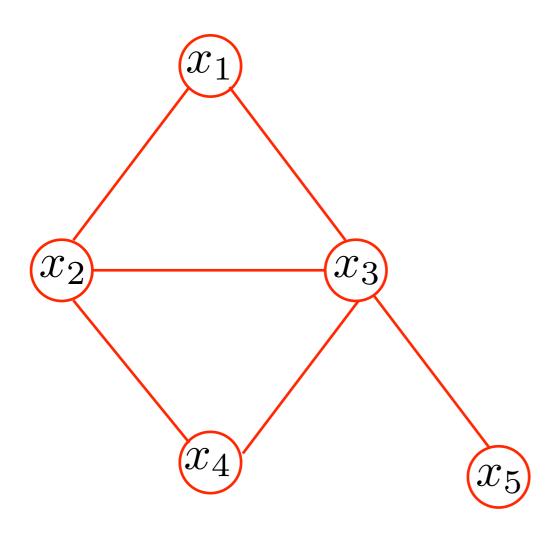
$$p(\mathbf{x}) = \frac{1}{Z} \psi_{123}(x_1, x_2, x_3) \psi_{234}(x_2, x_3, x_4) \psi_{35}(x_3, x_5)$$



How to define the potentials?

- Intuitively, the potential of a clique should be high, iff the joint probability of the corresponding random variables is high.
- In most cases the potential is defined using a log-linear model:





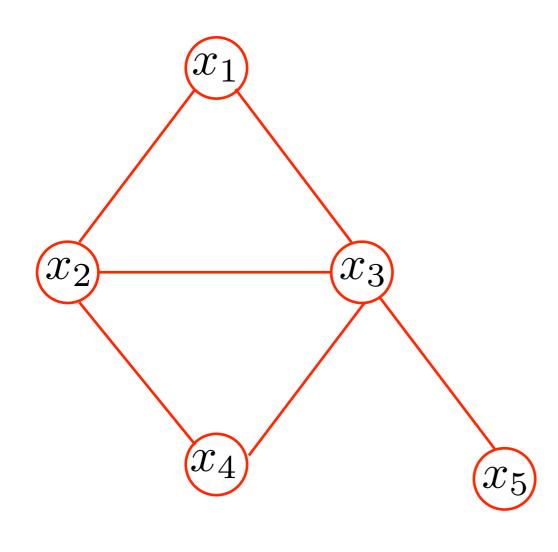
How to define the potentials?

- Intuitively, the potential of a clique should be high, iff the joint probability of the corresponding random variables is high.
- In most cases the potential is defined using a log-linear model

making the parameters explicit:

$$\log \psi_c(\mathbf{x}_c) = \boldsymbol{\phi}_c(\mathbf{x}_c)^T \boldsymbol{\theta}$$

$$\Rightarrow \log p(\mathbf{x} \mid \boldsymbol{\theta}) = \sum_{c \in \mathcal{C}} \boldsymbol{\phi}_c(\mathbf{x}_c)^T \boldsymbol{\theta} - \log Z(\boldsymbol{\theta})$$



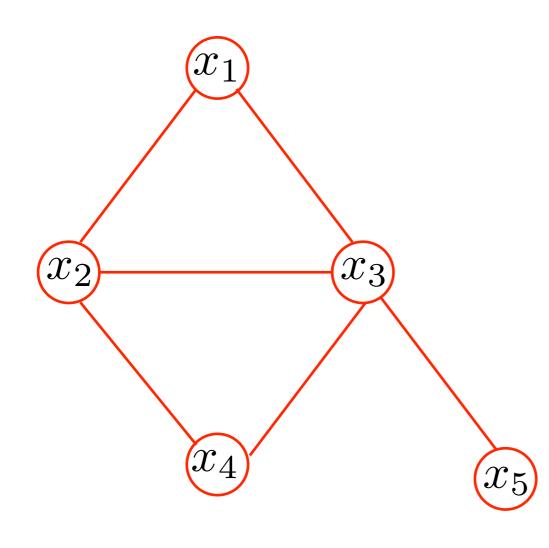
Using numbers, e.g.:

Let all variables be binary:

$$x_i \in \{0, 1\}$$

ullet We can define **features** ϕ

$$\phi_{ijk}(x_i, x_j, x_k) = \begin{cases} 1 & \text{if } x_n = 1 \ \forall n \in \{i, j, k\} \\ 0 & \text{otherwise} \end{cases}$$



Using numbers, e.g.:

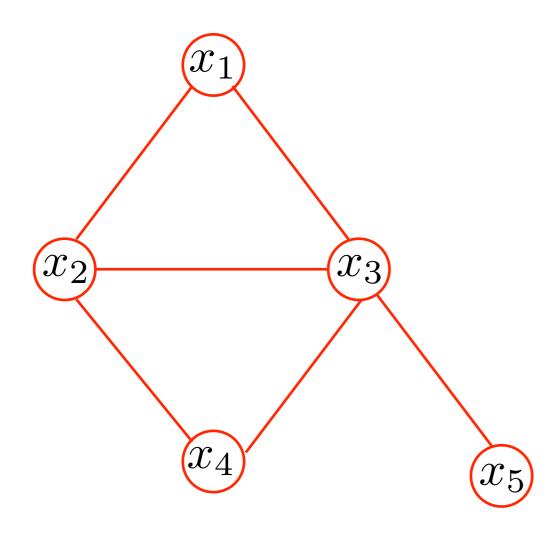
Let all variables be binary:

$$x_i \in \{0, 1\}$$

- We can define **features** ϕ
- and determine weights θ

$$\phi_{ijk}(x_i, x_j, x_k) = \begin{cases} 1 & \text{if } x_n = 1 \ \forall n \in \{i, j, k\} \\ 0 & \text{otherwise} \end{cases}$$

$$\boldsymbol{\theta} = (0\ 0\ 0\ 0\ 0\ 0\ 1)^T$$



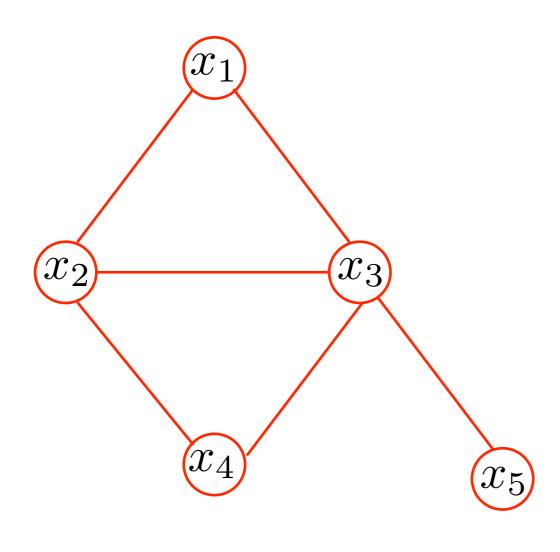
Using numbers, e.g.:

Let all variables be binary:

$$x_i \in \{0, 1\}$$

- We can define **features** ϕ
- and determine weights θ
- Then, we can compute the (log of the) joint probability for each realisation of the x_i

$$\log p(\mathbf{x} \mid \boldsymbol{\theta}) = \sum_{c \in \mathcal{C}} \boldsymbol{\phi}_c(\mathbf{x}_c)^T \boldsymbol{\theta} - \log Z(\boldsymbol{\theta})$$



Using numbers, e.g.:

- The same graph can also be interpreted as a binary MRF
- This a more specific representation, but it is less complex (and therefore more efficient)
- In Computer Vision, we almost always use **binary** MRFs; they are a specific case of general MRFs:

$$p(\mathbf{x}) = \frac{1}{Z}\psi_{12}(x_1, x_2)\psi_{13}(x_1, x_3)\psi_{23}(x_2, x_3)\psi_{24}(x_2, x_4)\psi_{34}(x_3, x_4)\psi_{35}(x_3, x_5)$$

Using Graphical Models

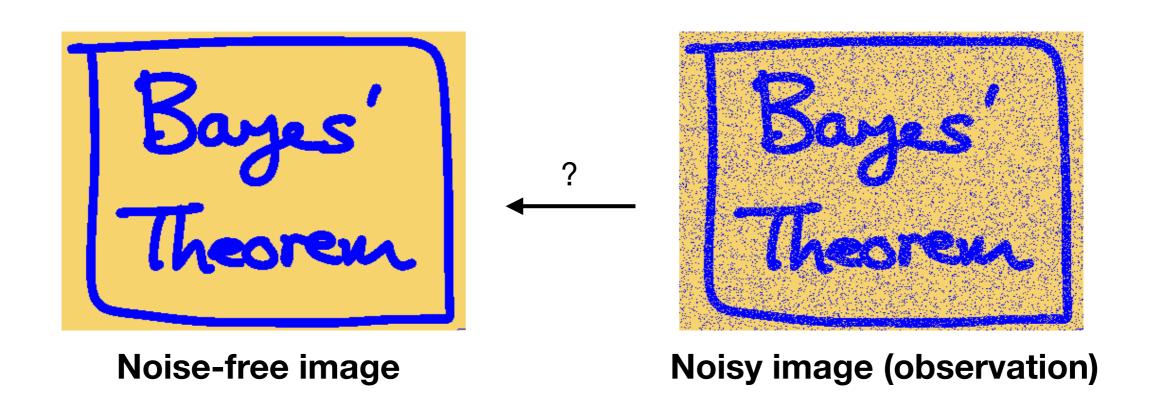
We can use a graphical model to do inference:

- We want to find $\arg \max_{\mathbf{x}} p(\mathbf{x})$
- 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.

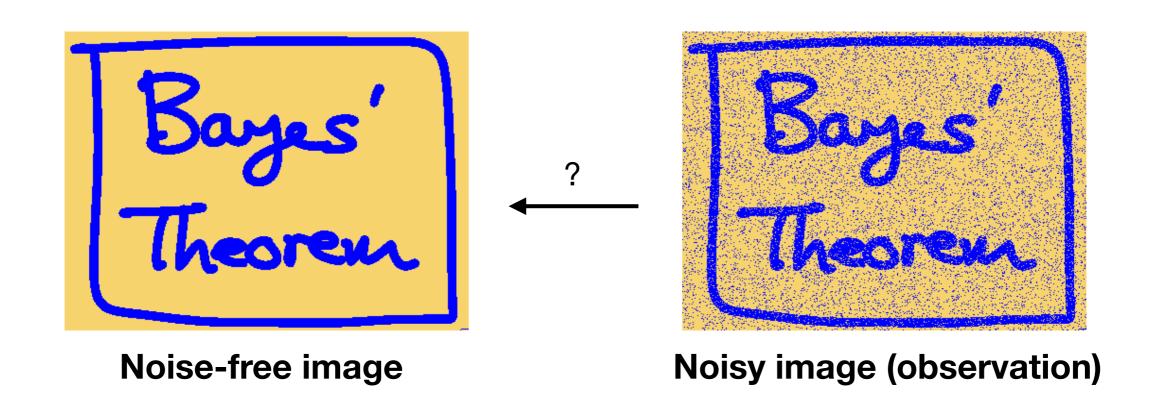
Question: How can inference be done with a graphical model?

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



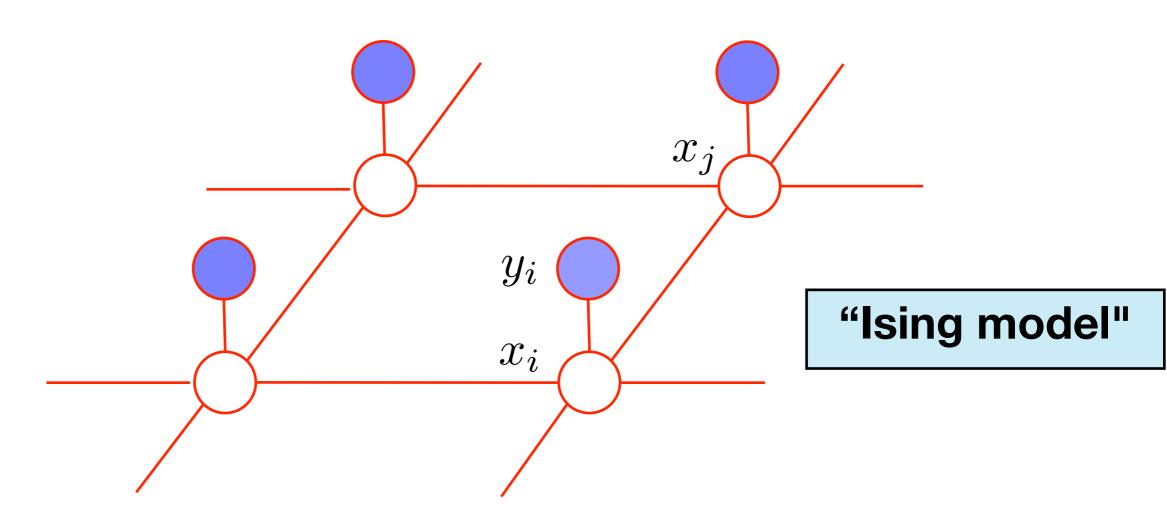


Aim: Recover the noise-free image from the noisy one We model the original image with variables $x_i \in \{-1, 1\}$ and the noisy image with pixel values $y_i \in \{-1, 1\}$



Aim: Recover the noise-free image from the noisy one We model the original image with variables $x_i \in \{-1,1\}$ and the noisy image with pixel values $y_i \in \{-1,1\}$ We consider the true pixel vales as **hidden** or **latent**





We define two simple edge features:

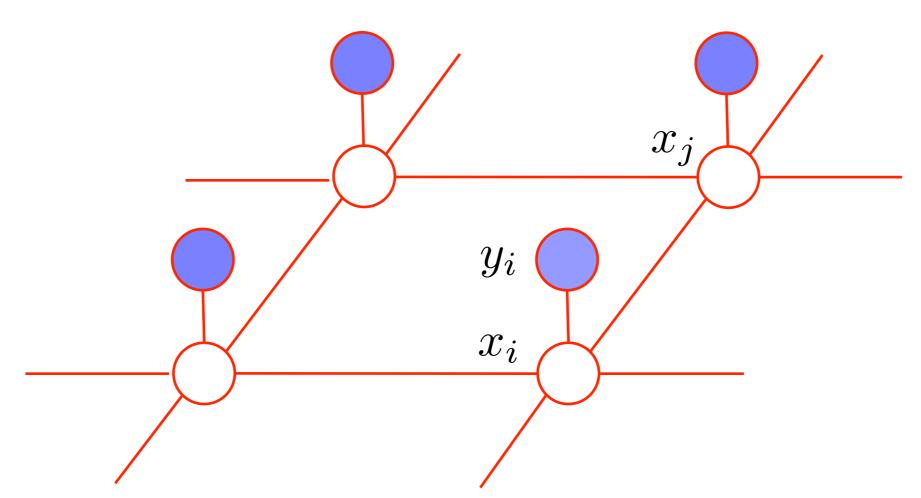
$$\phi(x_i, y_i) = x_i y_i \qquad \qquad \phi(x_i, x_j) = x_i x_j$$

These are multiplied by parameters β and η :

$$\log \psi(x_i, y_i) = \eta x_i y_i \qquad \log \psi(x_i, y_i) = \eta x_i y_i$$







With this, we can compute the joint:
$$p(\mathbf{x},\mathbf{y}\mid\eta,\beta) = \frac{1}{Z}\prod_{i}\exp(\eta x_{i}y_{i})\prod_{i,j}\exp(\beta x_{i}x_{j})$$

and its log:

$$\log p(\mathbf{x}, \mathbf{y} \mid \eta, \beta) = \eta \sum_{i} x_i y_i + \beta \sum_{i,j} x_i x_j - \log(Z)$$



$$\log p(\mathbf{x}, \mathbf{y} \mid \eta, \beta) = \eta \sum_{i} x_i y_i + \beta \sum_{i,j} x_i x_j - \log(Z)$$

Our aim now is to find the hidden states x_i such that this log of the joint is maximal (or at least very high). Simple approach is Iterated Conditional Modes (ICM):

- 1. Initialize all x_i by corresponding y_i
- 2. For all nodes x_i :
 - 1. set x_i to +1 and to -1 and evaluate $\log p(\mathbf{x}, \mathbf{y} \mid \eta, \beta)$
- 2. keep the value that gives higher log joint This will keep or increase the joint in every step The nodes can be visited in order or randomly

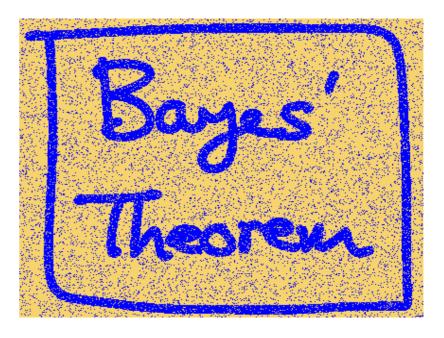




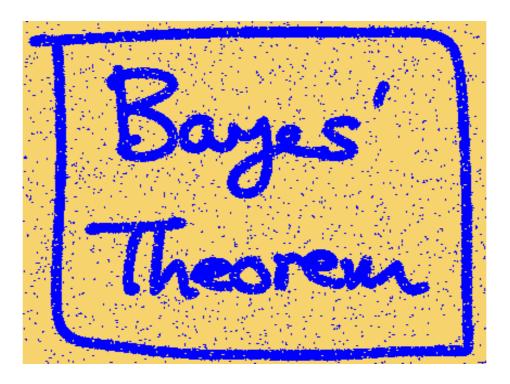
Result of ICM



Noise-free image



Noisy image (observation)



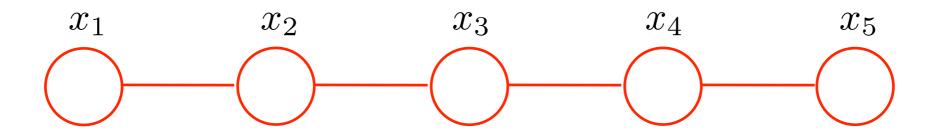
Result of ICM



General Inference in MRFs

- In general, we do not have such an easy model
- Therefore, we need more general inference methods for MRF
- The major aim is to exploit sparsity in the graphical model to make inference efficient





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 $p(x_3) = \sum \sum \sum p(\mathbf{x})$

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

In the general case with N nodes we have

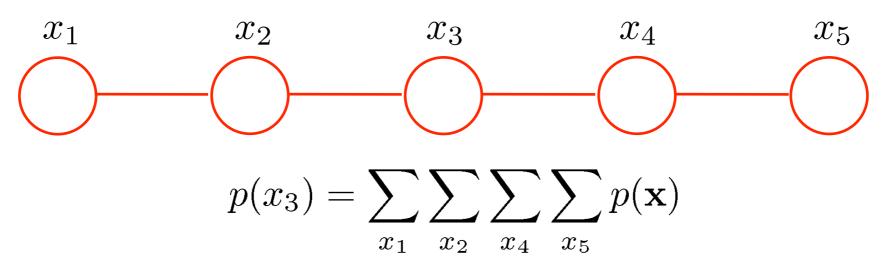
$$p(\mathbf{x}) = \frac{1}{Z} \psi_{1,2}(x_1, x_2) \psi_{2,3}(x_2, x_3) \cdots \psi_{N-1,N}(x_{N-1}, x_N)$$

and

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







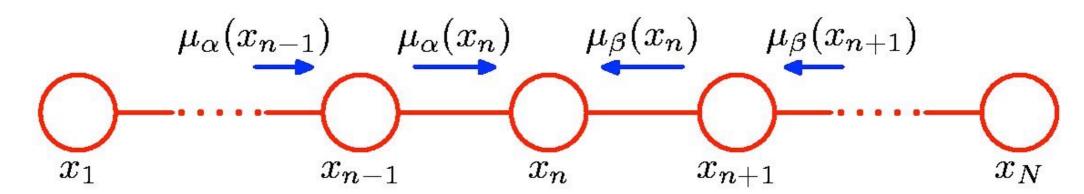
• This would mean K^N computations! A more efficient way is obtained by rearranging:

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

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

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

$$\mu_{\alpha}(x_3) \longleftarrow \text{Vectors of size K} \longrightarrow \mu_{\beta}(x_3)$$



In general, we have

$$p(x_n) = \frac{1}{Z} \left[\sum_{x_{n-1}} \psi_{n-1,n}(x_{n-1}, x_n) \cdots \left[\sum_{x_1} \psi_{1,2}(x_1, x_2) \right] \cdots \right]$$

$$\mu_{\alpha}(x_n)$$

$$\left[\sum_{x_{n+1}} \psi_{n,n+1}(x_n, x_{n+1}) \cdots \left[\sum_{x_N} \psi_{N-1,N}(x_{N-1}, x_N) \right] \cdots \right]$$

$$\mu_{\beta}(x_n)$$

The **messages** μ_{α} and μ_{β} can be computed recursively:

$$\mu_{\alpha}(x_{n}) = \sum_{x_{n-1}} \psi_{n-1,n}(x_{n-1}, x_{n}) \left[\sum_{x_{n-2}} \cdots \right]$$

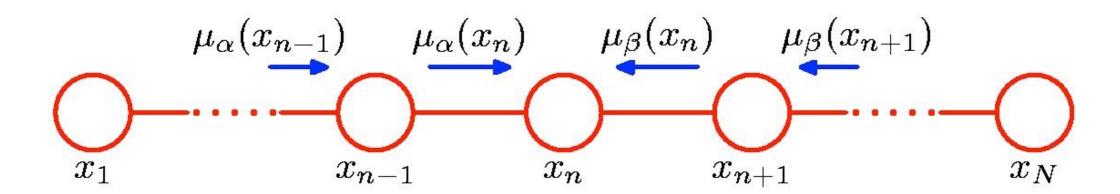
$$= \sum_{x_{n-1}} \psi_{n-1,n}(x_{n-1}, x_{n}) \mu_{\alpha}(x_{n-1}).$$

$$\mu_{\beta}(x_{n}) = \sum_{x_{n+1}} \psi_{n,n+1}(x_{n}, x_{n+1}) \left[\sum_{x_{n+2}} \cdots \right]$$

$$= \sum_{x_{n+1}} \psi_{n,n+1}(x_{n}, x_{n+1}) \mu_{\beta}(x_{n+1}).$$

Computation of μ_{α} starts at the first node and computation of μ_{β} starts at the last node.





• 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 $p(x_n)$

To compute local marginals:

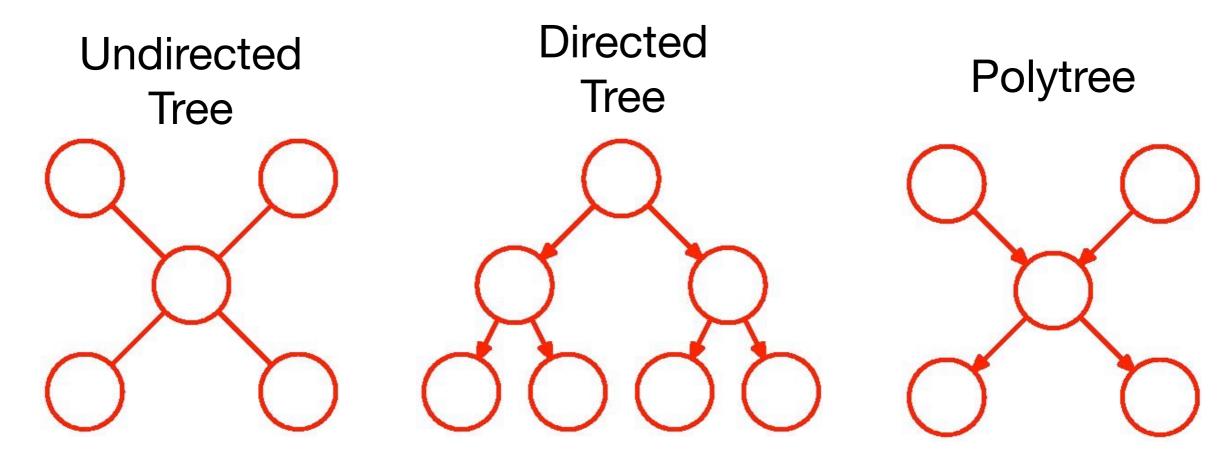
- •Compute and store all forward messages, $\mu_{\alpha}(x_n)$.
- •Compute and store all backward messages, $\mu_{\beta}(x_n)$
- •Compute Z once at a node x_m : $Z = \sum_{x_m} \mu_{\alpha}(x_m) \mu_{\beta}(x_m)$
- Compute

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

for all variables required.

More General Graphs

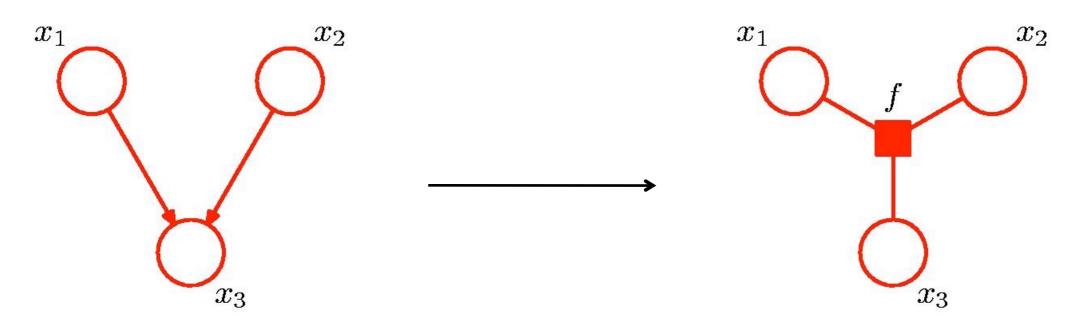
The message-passing algorithm can be extended to more general graphs:



It is then known as the sum-product algorithm. A special case of this is belief propagation.



- 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.



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

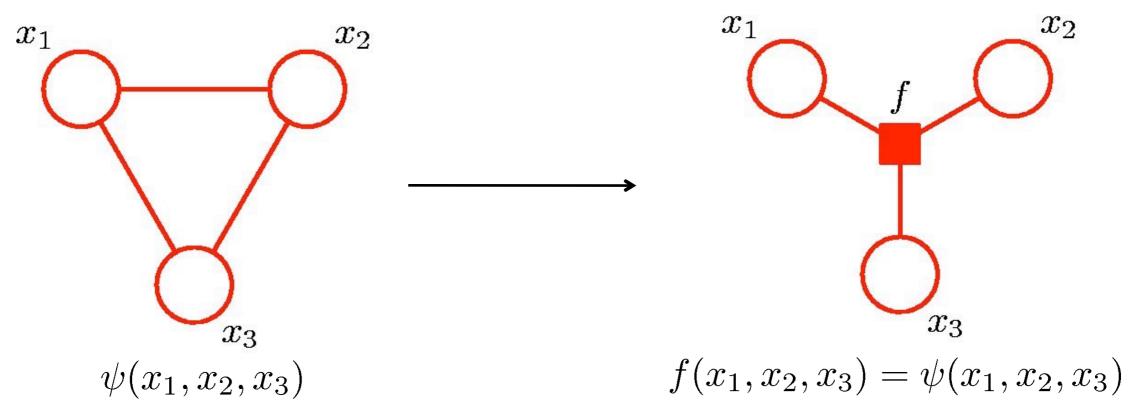
Directed graph

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

Factor graph



- 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.

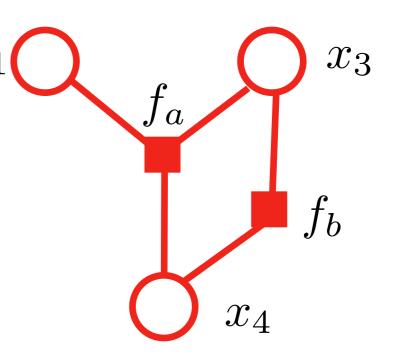


Undirected graph

Factor graph

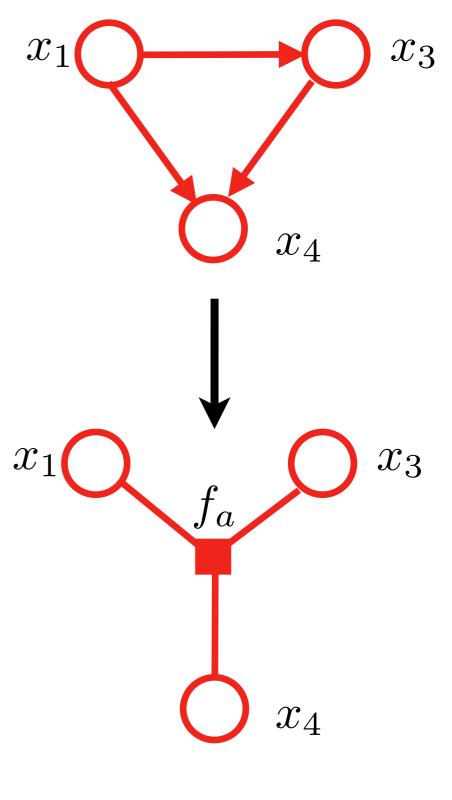
Factor graphs

- 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





- 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:

$$\mu_{f\to x}(x)=1$$
 (var) or $\mu_{x\to f}(x)=f(x)$ (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 y and features as continuous random variables 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 w are parameters learned from training data.

CRFs are discriminative and MRFs are generative



Conditional Random Fields

Derivation of the formula for CRFs:

$$p(\mathbf{y} \mid \mathbf{x}, \mathbf{w}) = \frac{p(\mathbf{y}, \mathbf{x} \mid \mathbf{w})}{p(\mathbf{x} \mid \mathbf{w})} = \frac{p(\mathbf{y}, \mathbf{x} \mid \mathbf{w})}{\sum_{y'} p(\mathbf{y'}, \mathbf{x} \mid \mathbf{w})} = \frac{\prod_{C} \phi_{C}(\mathbf{x}_{C}, \mathbf{y}_{C}; \mathbf{w})}{Z} \frac{Z}{\sum_{\mathbf{y'}} \prod_{C} \phi_{C}(\mathbf{x}_{C}, \mathbf{y'}_{C}; \mathbf{w})}$$

In the training phase, we compute parameters w that maximize the posterior:

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

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

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

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 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

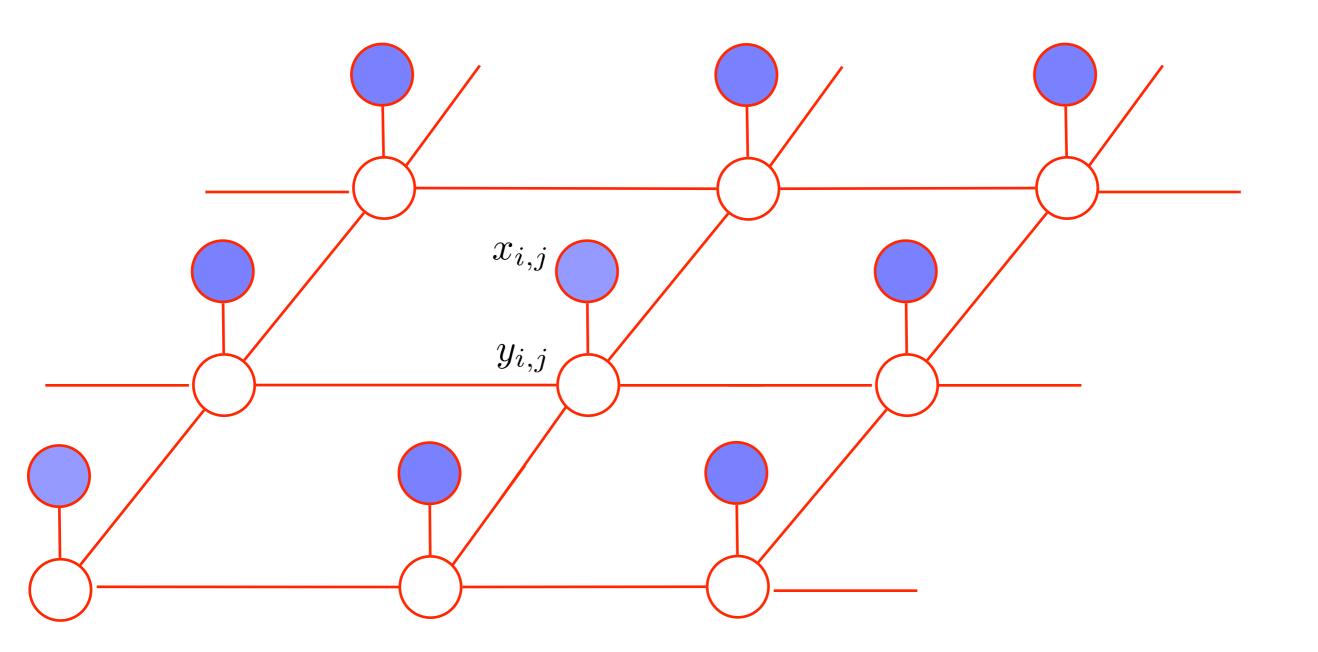
Markov blanket

 C_i : All cliques containing y_i

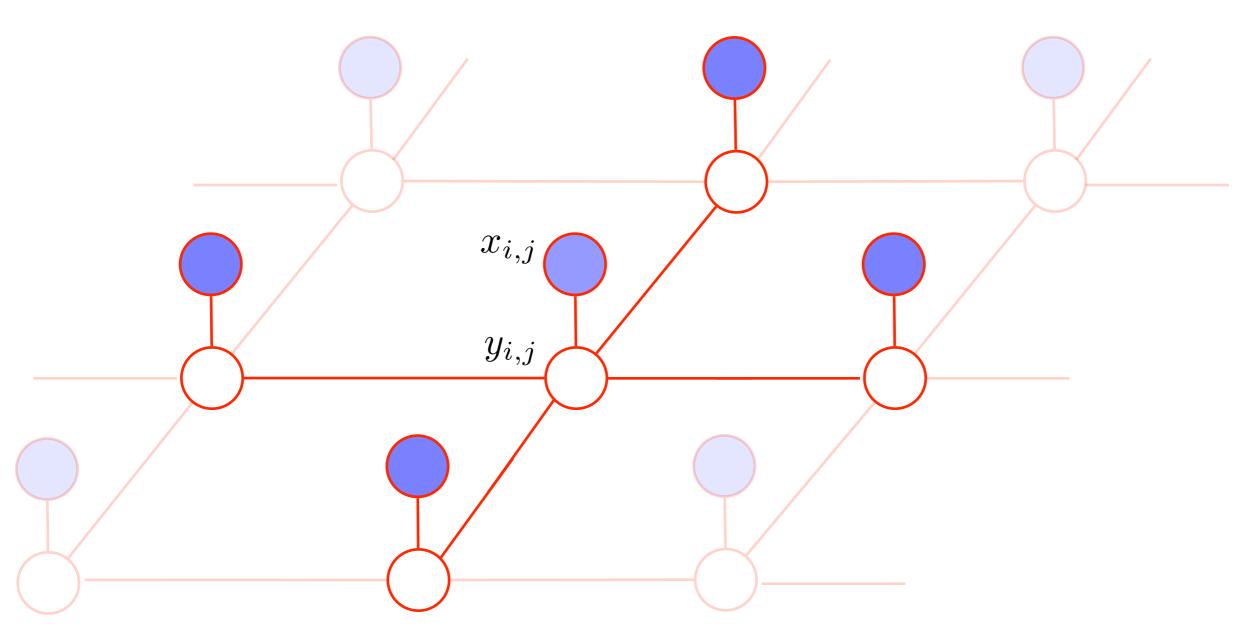
$$p(y_i^* \mid \mathcal{M}(y_i^*), \mathbf{x}^*, \mathbf{w}) = \frac{\prod_{C_i} \phi_{C_i}(\mathbf{x}_{C_i}^*, y_i^*, \mathbf{y}_{C_i}^*; \mathbf{w})}{\sum_{y_i'} \prod_{C_i} \phi_{C}(\mathbf{x}_{C_i}^*, y_i', \mathbf{y}_{C_i}^*; \mathbf{w})}$$



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

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

