CS60050: Machine Learning

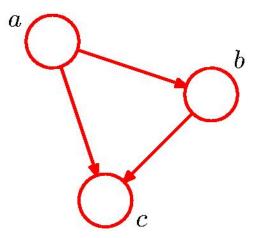
Graphical Models

Sourangshu Bhattacharya

BAYESIAN NETWORKS

Bayesian Networks

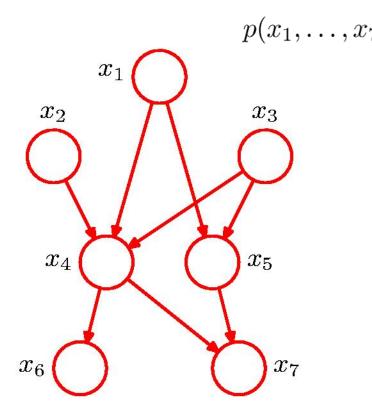
• Directed Acyclic Graph (DAG)



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

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

Bayesian Networks

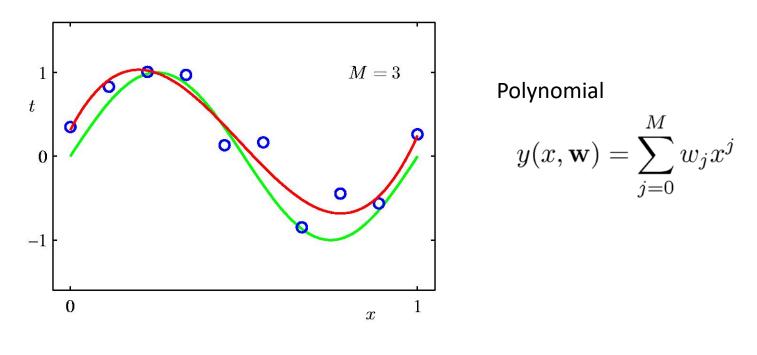


 $p(x_1, \dots, x_7) = p(x_1)p(x_2)p(x_3)p(x_4|x_1, x_2, x_3)$ $p(x_5|x_1, x_3)p(x_6|x_4)p(x_7|x_4, x_5)$

General Factorization

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

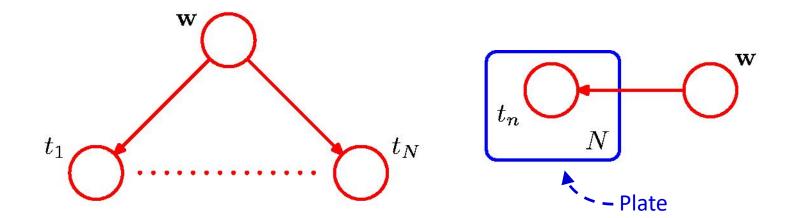
Bayesian Curve Fitting (1)



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

Bayesian Curve Fitting (2)

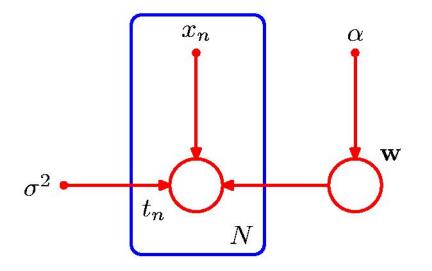
$$p(\mathbf{t}, \mathbf{w}) = p(\mathbf{w}) \prod_{n=1}^{N} p(t_n | y(\mathbf{w}, x_n))$$



Bayesian Curve Fitting (3)

• Input variables and explicit hyperparameters

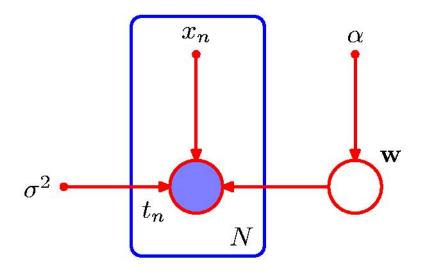
$$p(\mathbf{t}, \mathbf{w} | \mathbf{x}, \alpha, \sigma^2) = p(\mathbf{w} | \alpha) \prod_{n=1}^N p(t_n | \mathbf{w}, x_n, \sigma^2).$$



Bayesian Curve Fitting—Learning

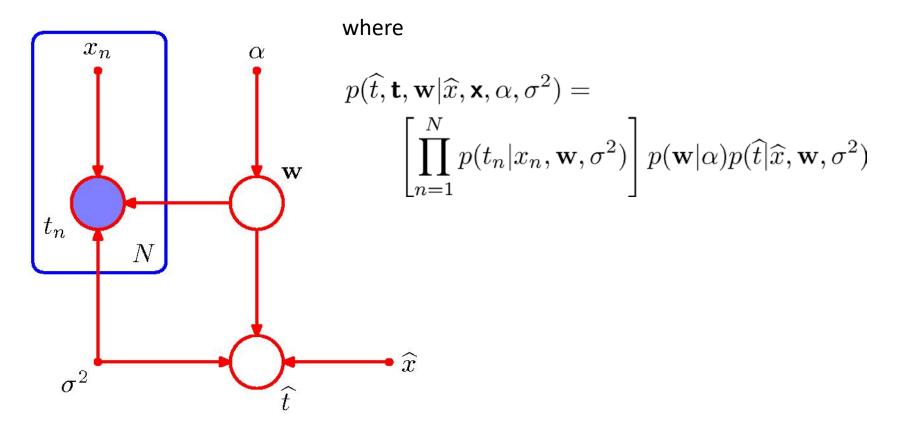
• Condition on data

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



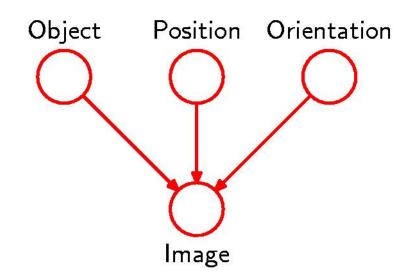
Bayesian Curve Fitting—Prediction

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



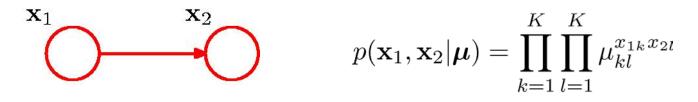
Generative Models

• Causal process for generating images



Discrete Variables (1)

• General joint distribution: K² -1 parameters



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

$$\sum_{k=1}^{\mathbf{x}_{2}} \sum_{k=1}^{\mathbf{x}_{2}} \hat{p}(\mathbf{x}_{1}, \mathbf{x}_{2} | \boldsymbol{\mu}) = \prod_{k=1}^{K} \mu_{1k}^{x_{1k}} \prod_{l=1}^{K} \mu_{2l}^{x_{2l}}$$

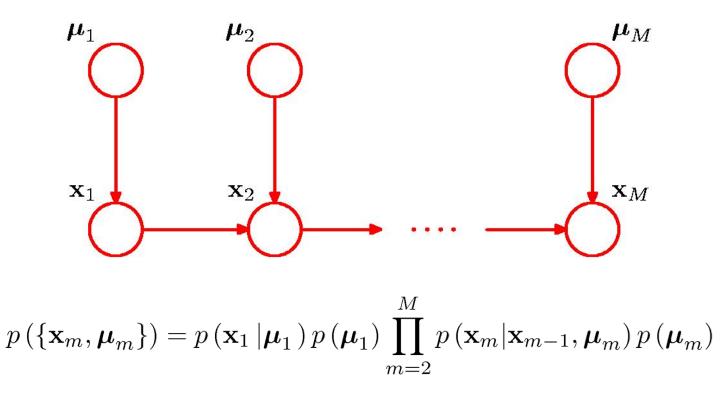
Discrete Variables (2)

General joint distribution over M variables: K^M - 1 parameters

M -node Markov chain: K - I + (M - I) K(K - I) parameters

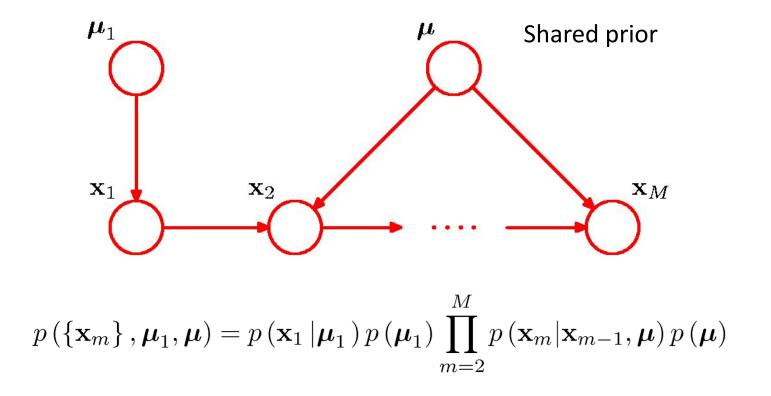


Discrete Variables: Bayesian Parameters (1)

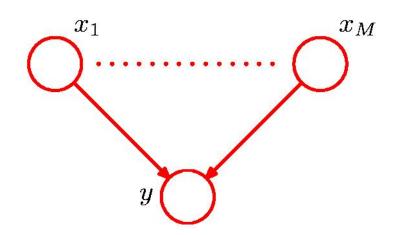


 $p(\boldsymbol{\mu}_m) = \operatorname{Dir}(\boldsymbol{\mu}_m | \boldsymbol{\alpha}_m)$

Discrete Variables: Bayesian Parameters (2)



Parameterized Conditional Distributions



If x_1, \ldots, x_M are discrete, K-state variables, $p(y = 1 | x_1, \ldots, x_M)$ in general has $\square(K^M)$ parameters.

The parameterized form

$$p(y=1|x_1,\ldots,x_M) = \sigma\left(w_0 + \sum_{i=1}^M w_i x_i\right) = \sigma(\mathbf{w}^T \mathbf{x})$$

requires only M + I parameters

Linear-Gaussian Models

• Directed Graph

$$p(x_i | pa_i) = \mathcal{N}\left(x_i \left| \sum_{j \in pa_i} w_{ij} x_j + b_i, v_i \right. \right)$$

Each node is Gaussian, the mean is a linear function of the parents.

Vector-valued Gaussian Nodes

$$p(\mathbf{x}_i | \mathrm{pa}_i) = \mathcal{N}\left(\mathbf{x}_i \left| \sum_{j \in \mathrm{pa}_i} \mathbf{W}_{ij} \mathbf{x}_j + \mathbf{b}_i, \mathbf{\Sigma}_i
ight)$$

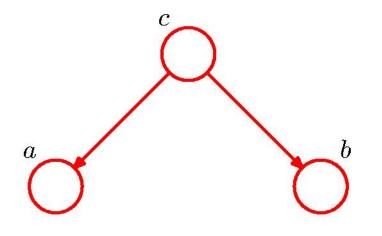
Conditional Independence

• a is independent of b given c

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

• Equivalently p(a,b|c) = p(a|b,c)p(b|c)= p(a|c)p(b|c)

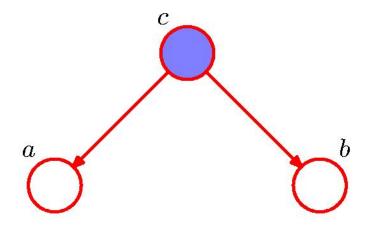
• Notation $a \perp b \mid c$



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

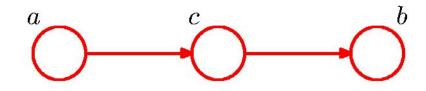
$$p(a,b) = \sum_{c} p(a|c)p(b|c)p(c)$$

 $a \not\perp b \mid \emptyset$



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

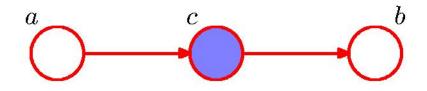
 $a \perp\!\!\!\perp b \mid c$



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

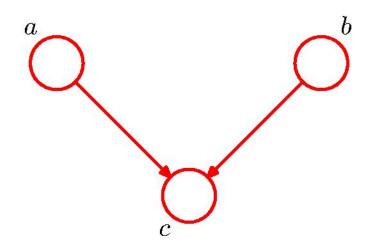
$$p(a,b) = p(a) \sum_{c} p(c|a)p(b|c) = p(a)p(b|a)$$

 $a \not\!\!\perp b \mid \emptyset$



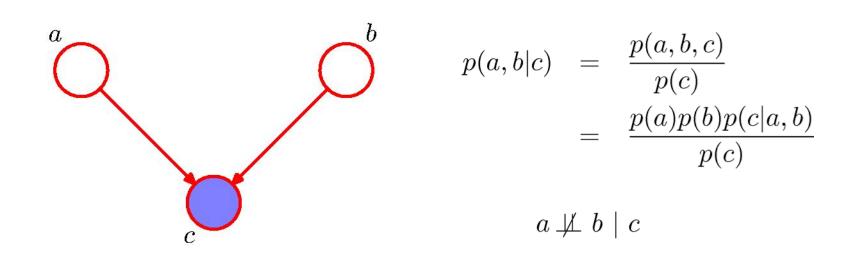
$$p(a,b|c) = \frac{p(a,b,c)}{p(c)}$$
$$= \frac{p(a)p(c|a)p(b|c)}{p(c)}$$
$$= p(a|c)p(b|c)$$

$$a \perp\!\!\!\perp b \mid c$$



p(a, b, c) = p(a)p(b)p(c|a, b)p(a, b) = p(a)p(b) $a \perp\!\!\!\perp b \mid \emptyset$

• Note: this is the opposite of Example 1, with c unobserved.



Note: this is the opposite of Example 1, with c observed.

"Am I out of fuel?"

$$p(G = 1 | B = 1, F = 1) = 0.8$$

$$p(G = 1 | B = 1, F = 0) = 0.2$$

$$p(G = 1 | B = 0, F = 1) = 0.2$$

$$p(G = 1 | B = 0, F = 0) = 0.1$$

$$p(B = 1) = 0.9$$

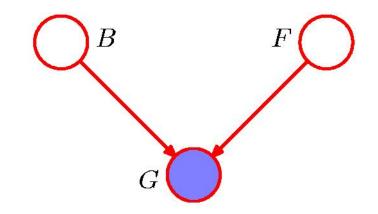
 $p(F = 1) = 0.9$

and hence

$$p(F=0) = 0.1$$

- B = Battery (0=flat, 1=fully charged)
- F = Fuel Tank (0=empty, 1=full)
- G = Fuel Gauge Reading (0=empty, 1=full)

"Am I out of fuel?"

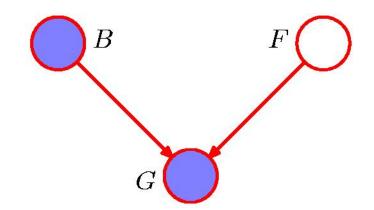


$$p(F = 0|G = 0) = \frac{p(G = 0|F = 0)p(F = 0)}{p(G = 0)}$$

\$\approx 0.257\$

Probability of an empty tank increased by observing G = 0.

"Am I out of fuel?"



$$p(F = 0|G = 0, B = 0) = \frac{p(G = 0|B = 0, F = 0)p(F = 0)}{\sum_{F \in \{0,1\}} p(G = 0|B = 0, F)p(F)}$$

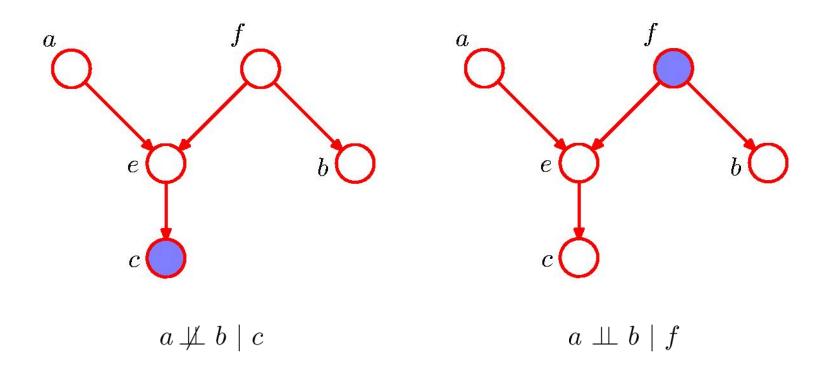
\$\approx 0.111\$

Probability of an empty tank reduced by observing B = D. This referred to as "explaining away".

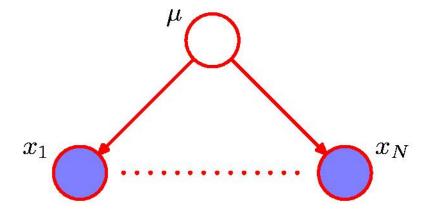
D-separation

- A, B, and C are non-intersecting subsets of nodes in a directed graph.
- A path from A to B is blocked if it contains a node such that either
 - a) the arrows on the path meet either head-to-tail or tailto-tail at the node, and the node is in the set [], or
 - b) the arrows meet head-to-head at the node, and neither the node, nor any of its descendants, are in the set [].
- If all paths from A to B are blocked, A is said to be d-separated from B by C.
- If A is d-separated from B by C, the joint distribution over all variables in the graph satisfies $A \perp \!\!\!\perp B \mid \!\!\! . C$

D-separation: Example



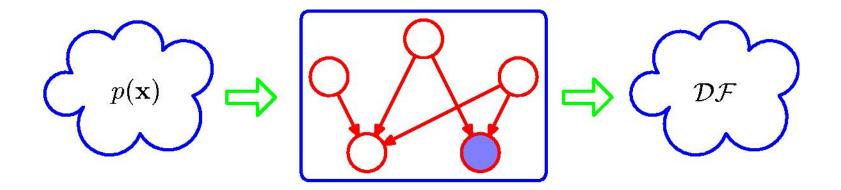
D-separation: I.I.D. Data



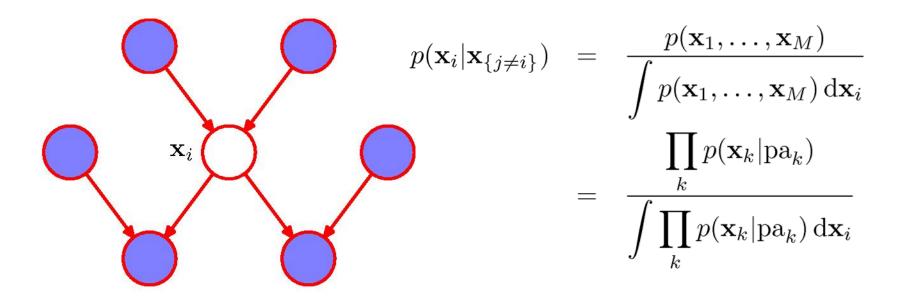
$$p(\mathcal{D}|\mu) = \prod_{n=1}^{N} p(x_n|\mu)$$

$$p(\mathcal{D}) = \int_{-\infty}^{\infty} p(\mathcal{D}|\mu) p(\mu) \,\mathrm{d}\mu \neq \prod_{n=1}^{N} p(x_n)$$

Directed Graphs as Distribution Filters



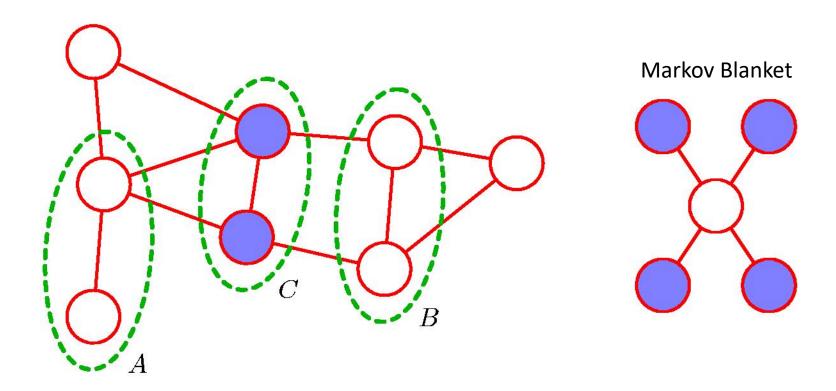
The Markov Blanket



Factors independent of X_i cancel between numerator and denominator.

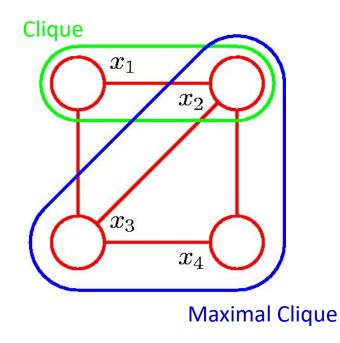
MARKOV RANDOM FIELDS

Markov Random Fields



 $A \bot\!\!\!\!\perp B | C$

Cliques and Maximal Cliques



Joint Distribution

$$p(\mathbf{x}) = \frac{1}{Z} \prod_{C} \psi_C(\mathbf{x}_C)$$

• where $\psi_C(\mathbf{x}_C)$ is the potential over clique \complement and

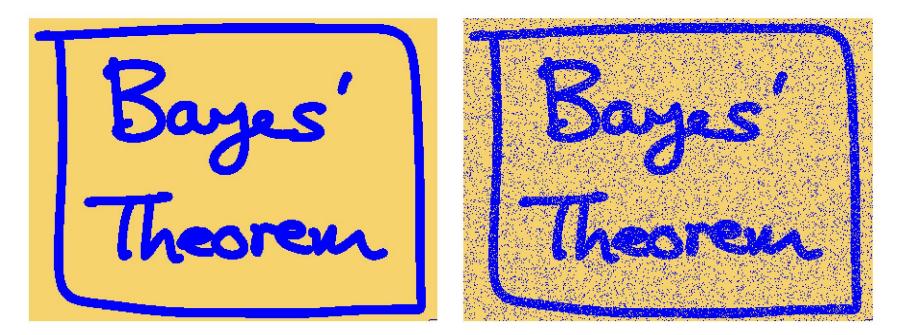
$$Z = \sum_{\mathbf{x}} \prod_{C} \psi_C(\mathbf{x}_C)$$

• is the normalization coefficient; note: M K-state variables $\rightarrow K^{M}$ terms in Z.

• Energies and the Boltzmann distribution

$$\psi_C(\mathbf{x}_C) = \exp\left\{-E(\mathbf{x}_C)\right\}$$

Illustration: Image De-Noising (1)



Original Image

Noisy Image

Illustration: Image De-Noising (2)

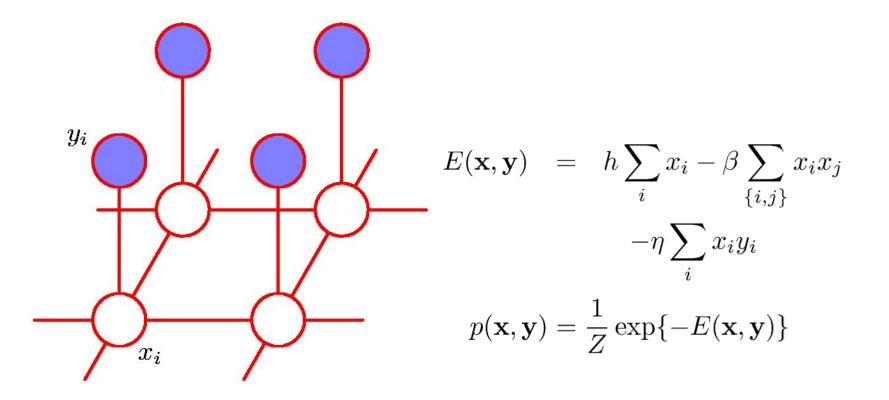
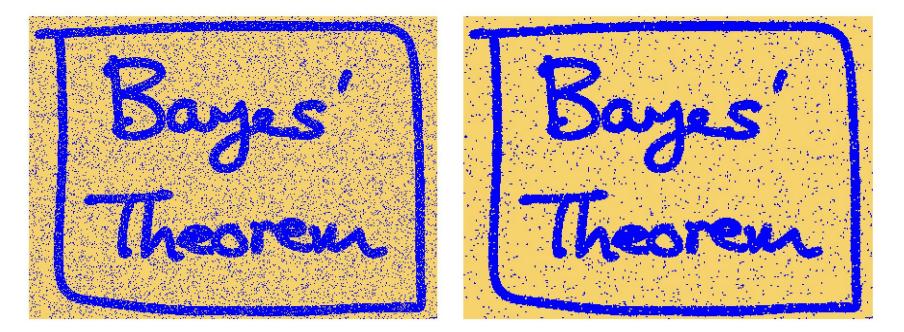


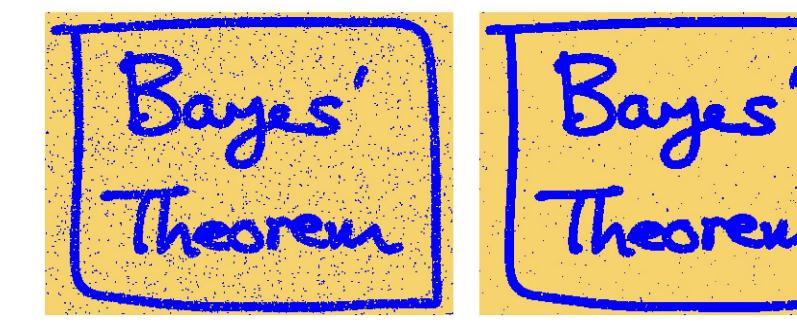
Illustration: Image De-Noising (3)



Noisy Image

Restored Image (ICM)

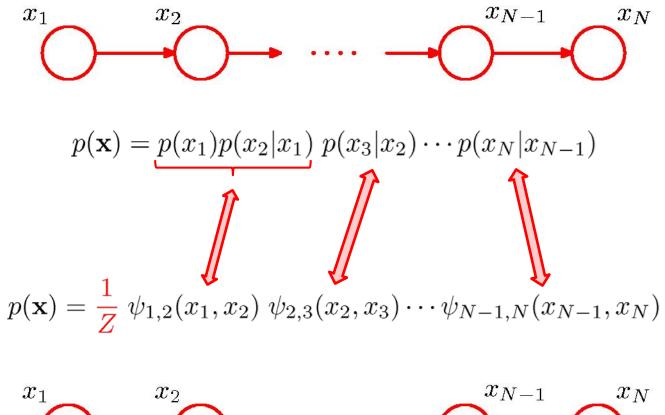
Illustration: Image De-Noising (4)



Restored Image (ICM)

Restored Image (Graph cuts)

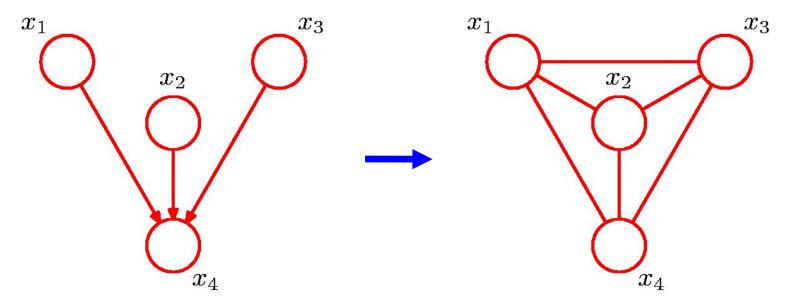
Converting Directed to Undirected Graphs (1)





Converting Directed to Undirected Graphs (2)

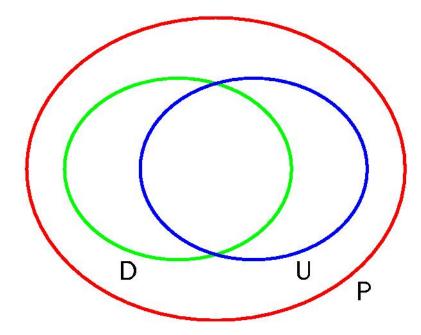
• Additional links



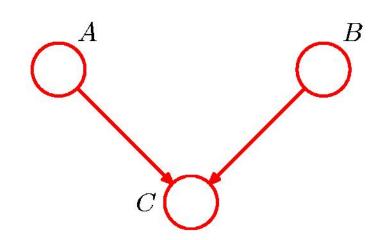
$$p(\mathbf{x}) = p(x_1)p(x_2)p(x_3)p(x_4|x_1, x_2, x_3)$$

= $\frac{1}{Z}\psi_A(x_1, x_2, x_3)\psi_B(x_2, x_3, x_4)\psi_C(x_1, x_2, x_4)$

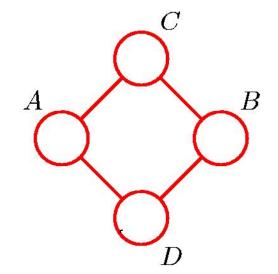
Directed vs. Undirected Graphs (1)



Directed vs. Undirected Graphs (2)



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



 $A \not\!\!\perp B \mid \emptyset$ $A \perp\!\!\perp B \mid C \cup D$ $C \perp\!\!\perp D \mid A \cup B$

INFERENCE IN GRAPHICAL MODELS

Inference Tasks

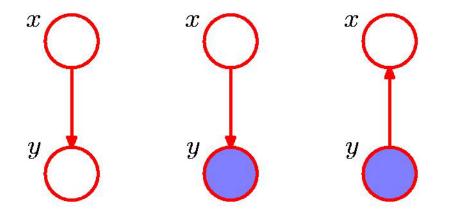
• Marginalization:

$$p(y) = \sum_{x'} p(y|x')p(x')$$

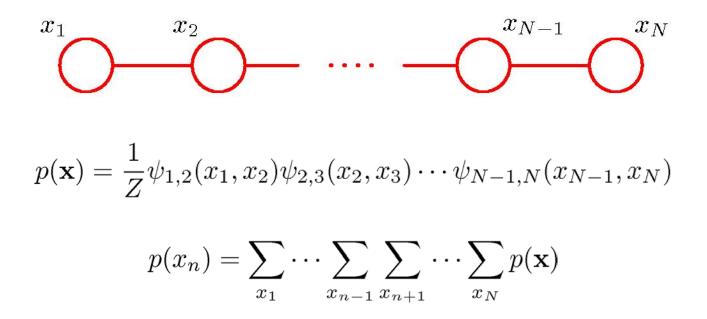
• Maximization:

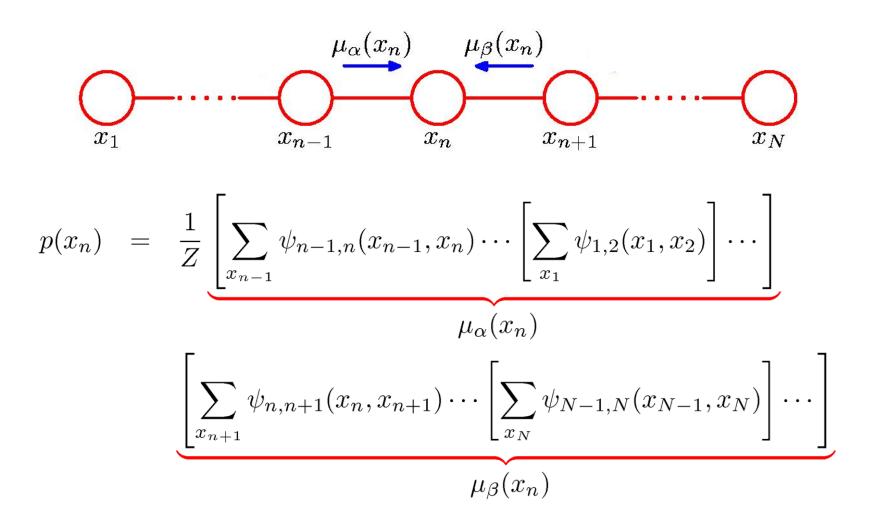
$$\mathbf{x}^{\max} = \operatorname*{arg\,max}_{\mathbf{x}} p(\mathbf{x})$$

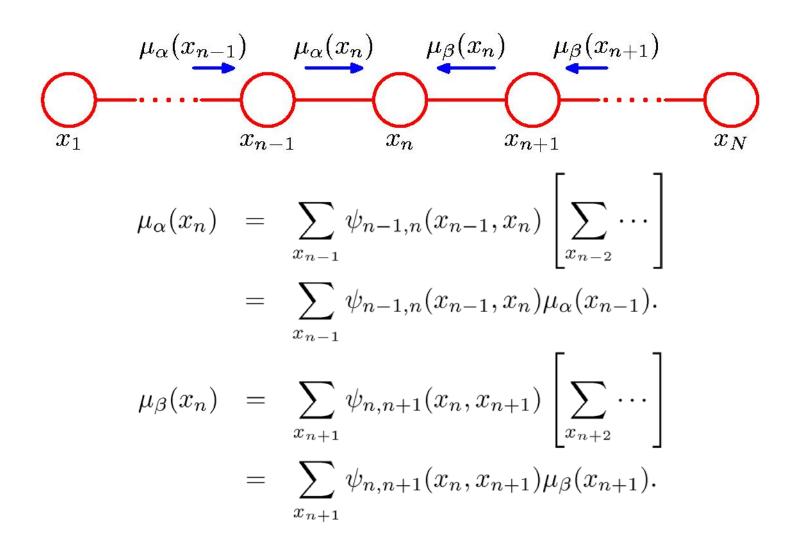
Inference in Graphical Models

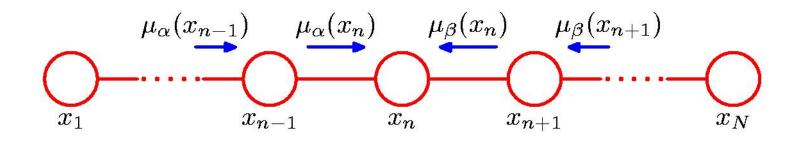


$$p(y) = \sum_{x'} p(y|x')p(x')$$
 $p(x|y) = \frac{p(y|x)p(x)}{p(y)}$









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

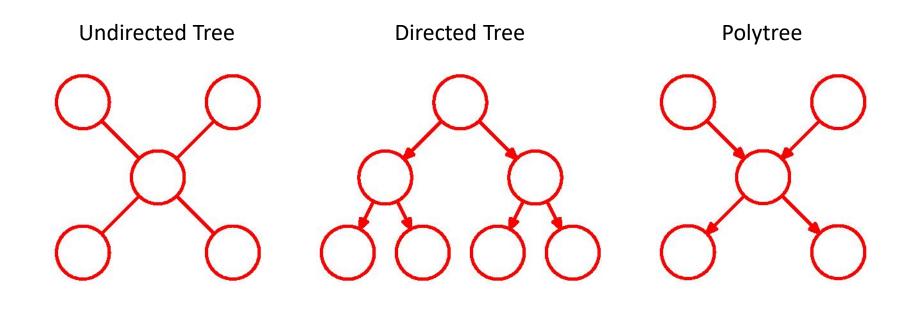
$$Z = \sum_{x_n} \mu_{\alpha}(x_n) \mu_{\beta}(x_n)$$

- 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 at any node X_m
 - Compute

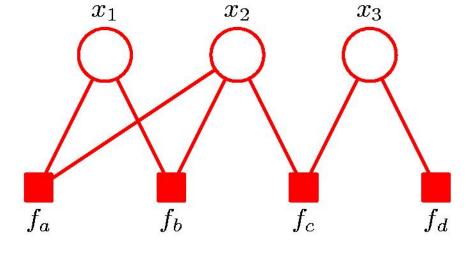
$$p(x_n) = \frac{1}{Z} \mu_{\alpha}(x_n) \mu_{\beta}(x_n)$$

for all variables required.

Trees



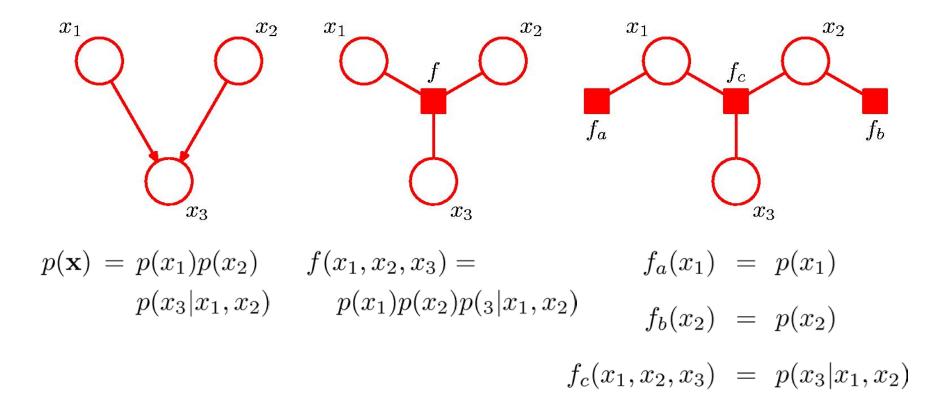
Factor Graphs



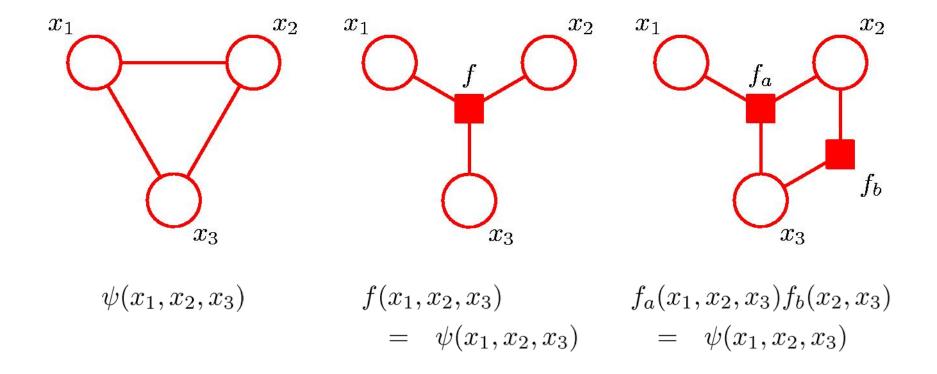
 $p(\mathbf{x}) = f_a(x_1, x_2) f_b(x_1, x_2) f_c(x_2, x_3) f_d(x_3)$

$$p(\mathbf{x}) = \prod_{s} f_s(\mathbf{x}_s)$$

Factor Graphs from Directed Graphs



Factor Graphs from Undirected Graphs

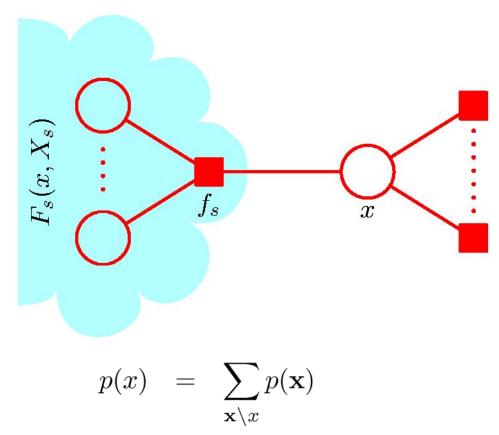


The Sum-Product Algorithm (1)

- Objective:
 - to obtain an efficient, exact inference algorithm for finding marginals;
 - in situations where several marginals are required, to allow computations to be shared efficiently.
- Key idea: Distributive Law

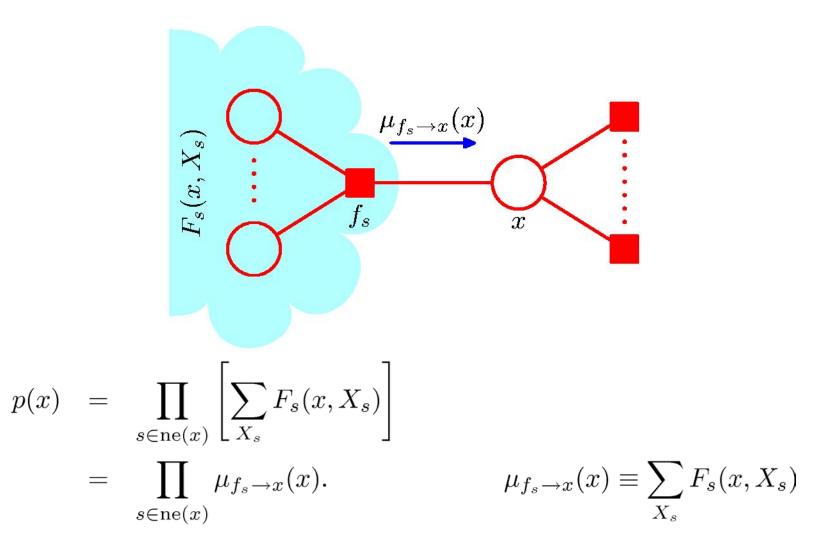
ab + ac = a(b + c)

The Sum-Product Algorithm (2)

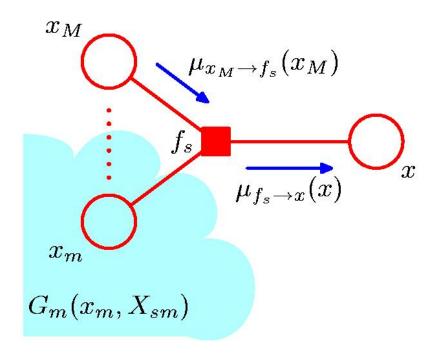


$$p(\mathbf{x}) = \prod_{s \in \operatorname{ne}(x)} F_s(x, X_s)$$

The Sum-Product Algorithm (3)



The Sum-Product Algorithm (4)

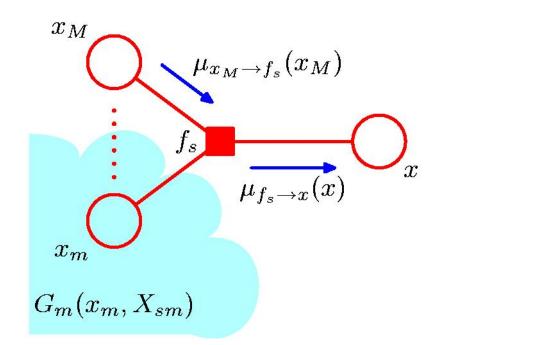


$$F_s(x, X_s) = f_s(x, x_1, \dots, x_M) G_1(x_1, X_{s1}) \dots G_M(x_M, X_{sM})$$

The Sum-Product Algorithm (5)

$$\mu_{f_s \to x}(x) = \sum_{x_1} \dots \sum_{x_M} f_s(x, x_1, \dots, x_M) \prod_{m \in \operatorname{ne}(f_s) \setminus x} \left[\sum_{X_{sm}} G_m(x_m, X_{sm}) \right]$$
$$= \sum_{x_1} \dots \sum_{x_M} f_s(x, x_1, \dots, x_M) \prod_{m \in \operatorname{ne}(f_s) \setminus x} \mu_{x_m \to f_s}(x_m)$$

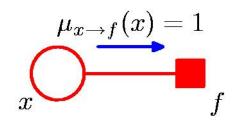
The Sum-Product Algorithm (6)

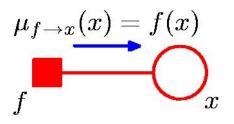


$$\mu_{x_m \to f_s}(x_m) \equiv \sum_{X_{sm}} G_m(x_m, X_{sm}) = \sum_{X_{sm}} \prod_{l \in ne(x_m) \setminus f_s} F_l(x_m, X_{ml})$$
$$= \prod_{l \in ne(x_m) \setminus f_s} \mu_{f_l \to x_m}(x_m)$$

The Sum-Product Algorithm (7)

Initialization

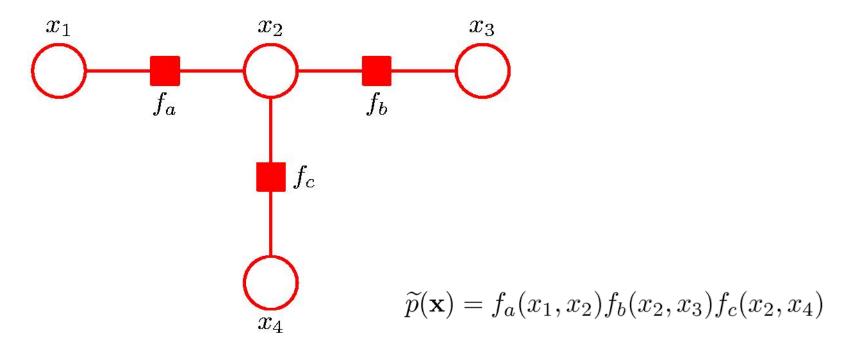




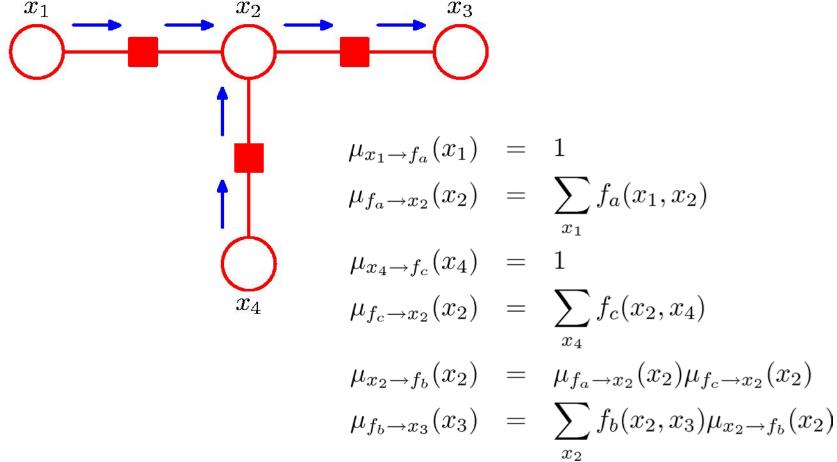
The Sum-Product Algorithm (8)

- To compute local marginals:
 - Pick an arbitrary node as root
 - Compute and propagate messages from the leaf nodes to the root, storing received messages at every node.
 - Compute and propagate messages from the root to the leaf nodes, storing received messages at every node.
 - Compute the product of received messages at each node for which the marginal is required, and normalize if necessary.

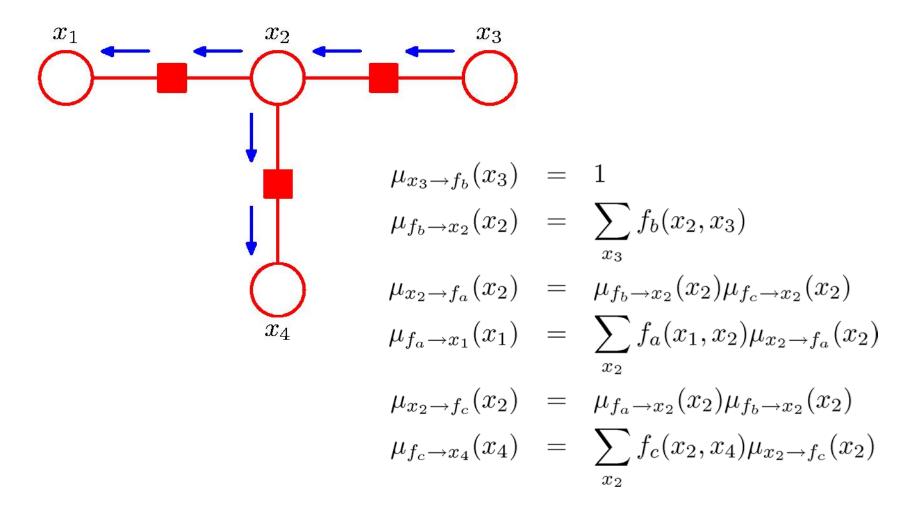
Sum-Product: Example (1)



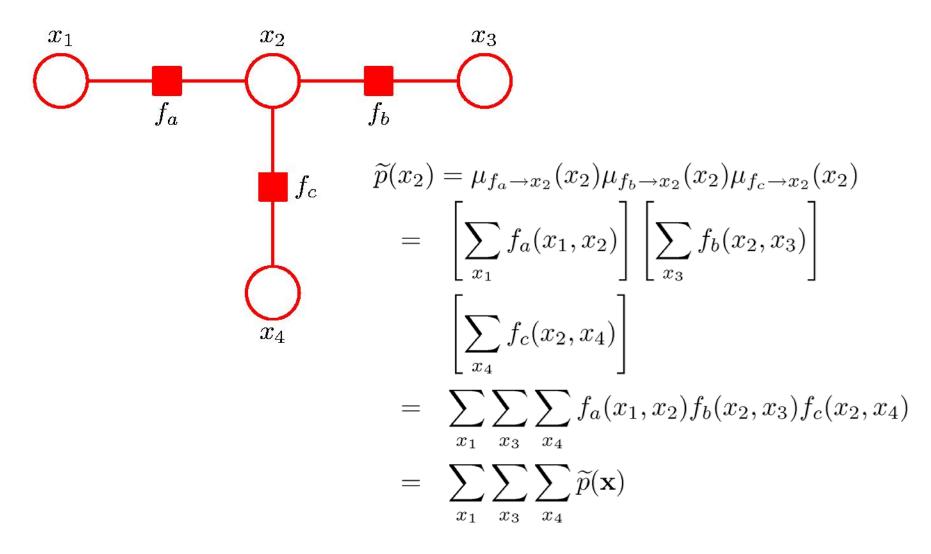
Sum-Product: Example (2)



Sum-Product: Example (3)



Sum-Product: Example (4)



The Max-Sum Algorithm (1)

- Objective: an efficient algorithm for finding
 - i. the value x^{max} that maximises p(x);
 - ii. the value of $p(x^{max})$.
- In general, maximum marginals ≠ joint maximum.

$$\begin{array}{c|ccc} x = 0 & x = 1 \\ \hline y = 0 & 0.3 & 0.4 \\ y = 1 & 0.3 & 0.0 \\ \end{array}$$

$$\arg\max_{x} p(x, y) = 1 \qquad \arg\max_{x} p(x) = 0$$

The Max-Sum Algorithm (2)

Maximizing over a chain (max-product)

$$= \frac{1}{Z} \max_{x_1} \left[\max_{x_2} \left[\psi_{1,2}(x_1, x_2) \left[\cdots \max_{x_N} \psi_{N-1,N}(x_{N-1}, x_N) \right] \cdots \right] \right]$$

The Max-Sum Algorithm (3)

Generalizes to tree-structured factor graph

$$\max_{\mathbf{x}} p(\mathbf{x}) = \max_{x_n} \prod_{f_s \in \operatorname{ne}(x_n)} \max_{X_s} f_s(x_n, X_s)$$

maximizing as close to the leaf nodes as possible

The Max-Sum Algorithm (4)

• Max-Product \rightarrow Max-Sum

- For numerical reasons, use

$$\ln\left(\max_{\mathbf{x}} p(\mathbf{x})\right) = \max_{\mathbf{x}} \ln p(\mathbf{x}).$$

Again, use distributive law

$$\max(a+b, a+c) = a + \max(b, c).$$

The Max-Sum Algorithm (5)

Initialization (leaf nodes)

$$\mu_{x \to f}(x) = 0 \qquad \qquad \mu_{f \to x}(x) = \ln f(x)$$

• Recursion $\mu_{f \to x}(x) = \max_{x_1, \dots, x_M} \left[\ln f(x, x_1, \dots, x_M) + \sum_{m \in \operatorname{ne}(f_s) \setminus x} \mu_{x_m \to f}(x_m) \right]$ $\phi(x) = \arg \max_{x_1, \dots, x_M} \left[\ln f(x, x_1, \dots, x_M) + \sum_{m \in \operatorname{ne}(f_s) \setminus x} \mu_{x_m \to f}(x_m) \right]$ $\mu_{x \to f}(x) = \sum_{l \in \operatorname{ne}(x) \setminus f} \mu_{f_l \to x}(x)$

The Max-Sum Algorithm (6)

• Termination (root node)

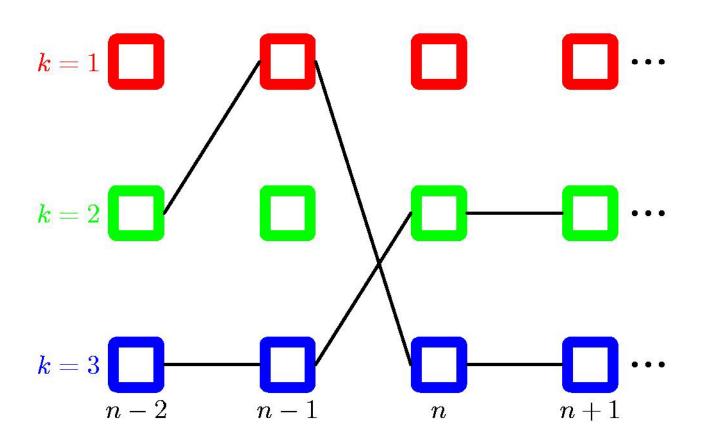
$$p^{\max} = \max_{x} \left[\sum_{s \in ne(x)} \mu_{f_s \to x}(x) \right]$$
$$x^{\max} = \arg \max_{x} \left[\sum_{s \in ne(x)} \mu_{f_s \to x}(x) \right]$$

•Back-track, for all nodes i with | factor nodes to the root (|=[])

$$\mathbf{x}_l^{\max} = \phi(x_{i,l-1}^{\max})$$

The Max-Sum Algorithm (7)

• Example: Markov chain



The Junction Tree Algorithm

- *Exact* inference on general graphs.
- Works by turning the initial graph into a junction tree and then running a sum-productlike algorithm.
- *Intractable* on graphs with large cliques.

Loopy Belief Propagation

- Sum-Product on general graphs.
- Initial unit messages passed across all links, after which messages are passed around until convergence (not guaranteed!).
- Approximate but tractable for large graphs.
- Sometime works well, sometimes not at all.