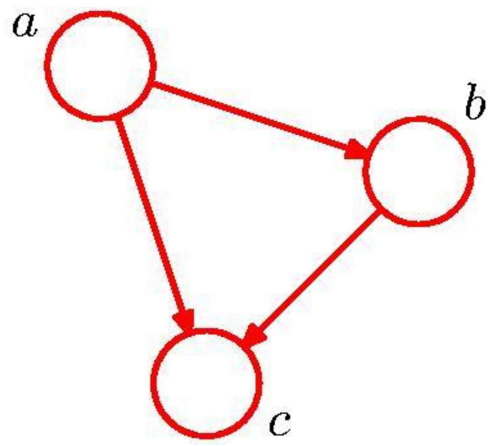
PATTERN RECOGNITION AND MACHINE LEARNING

CHAPTER 8: GRAPHICAL MODELS

Bayesian Networks

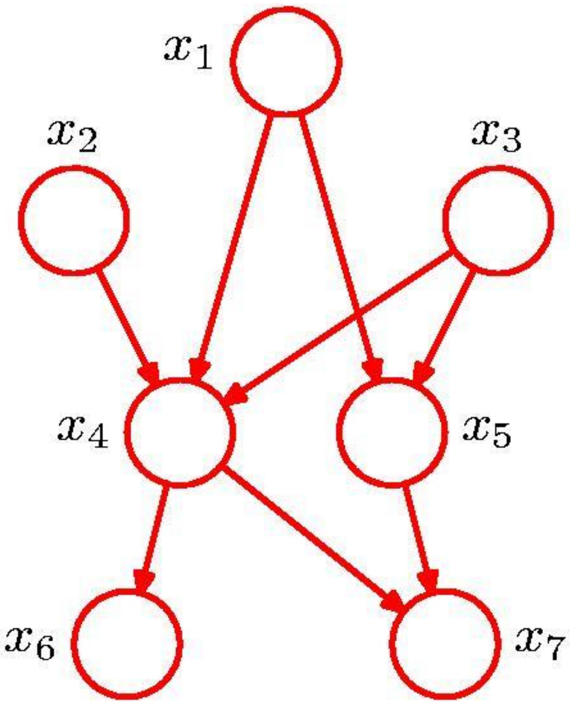
Directed Acyclic Graph (DAG)



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

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

Bayesian Networks

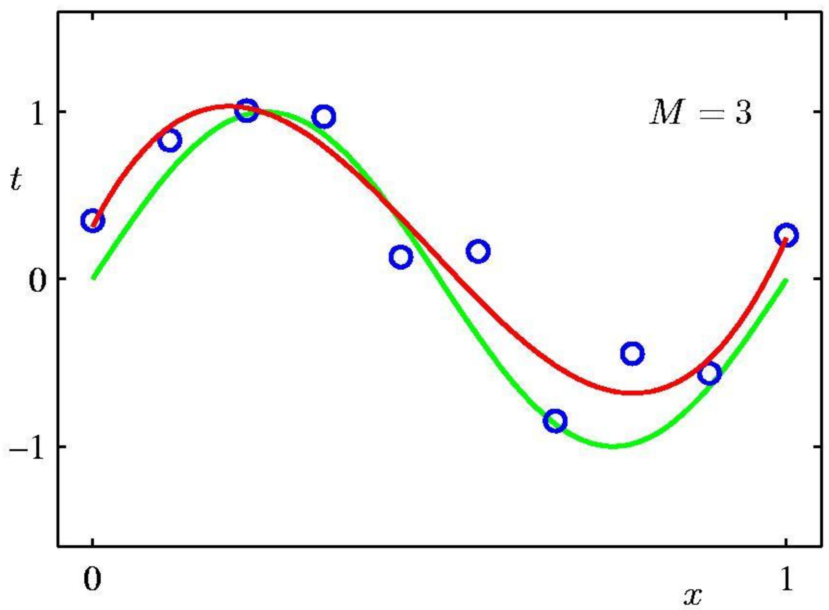


$$p(x_1, \ldots, x_7) = p(x_1)p(x_2)p(x_3)p(x_4|x_1, x_2, x_3) \\ p(x_5|x_1, x_3)p(x_6|x_4)p(x_7|x_4, x_5)$$

General Factorization

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

Bayesian Curve Fitting (1)



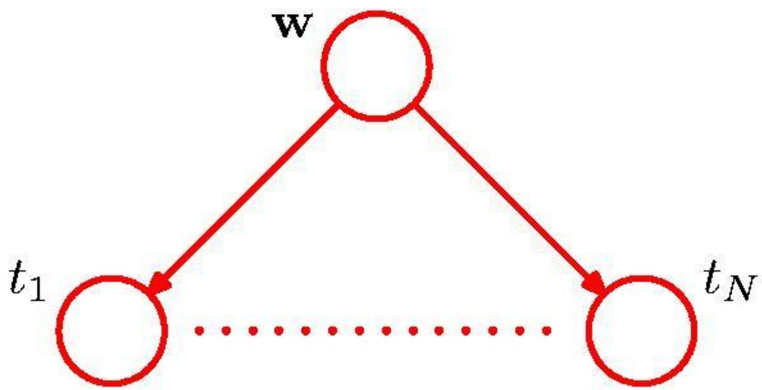
Polynomial

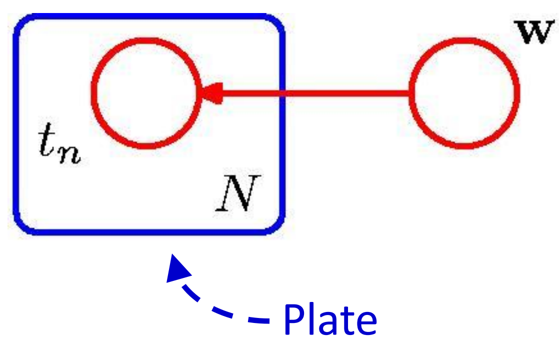
$$y(x, \mathbf{w}) = \sum_{j=0}^{M} w_j x^j$$

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

Bayesian Curve Fitting (2)

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

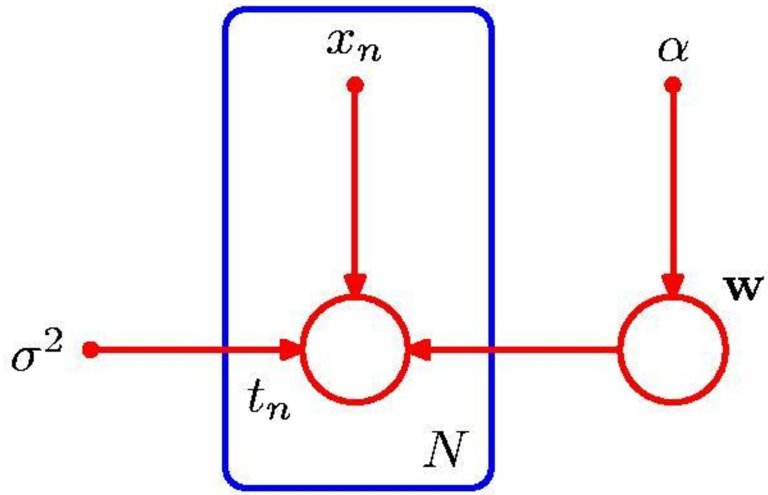




Bayesian Curve Fitting (3)

Input variables and explicit hyperparameters

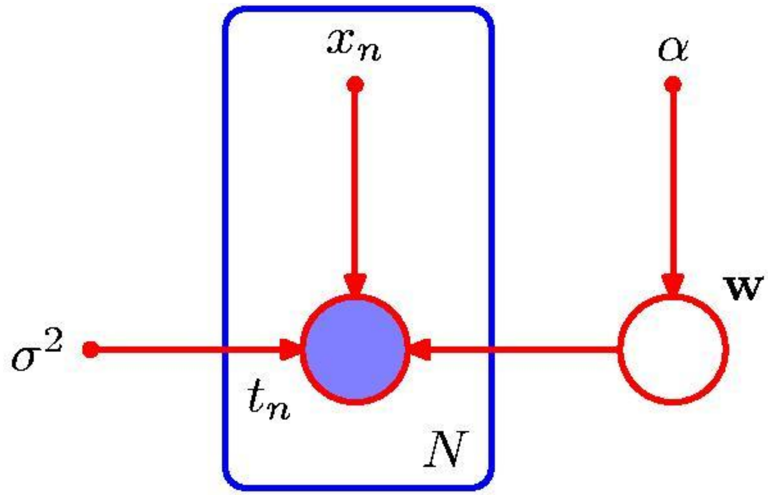
$$p(\mathbf{t}, \mathbf{w}|\mathbf{x}, \alpha, \sigma^2) = p(\mathbf{w}|\alpha) \prod_{n=1}^{N} p(t_n|\mathbf{w}, x_n, \sigma^2).$$



Bayesian Curve Fitting—Learning

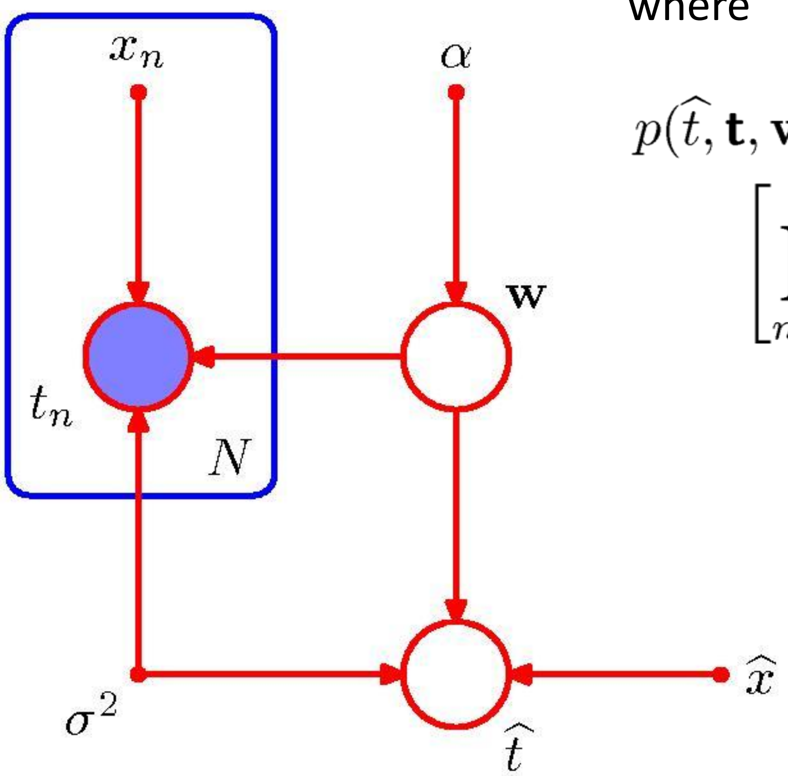
Condition on data

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



Bayesian Curve Fitting—Prediction

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

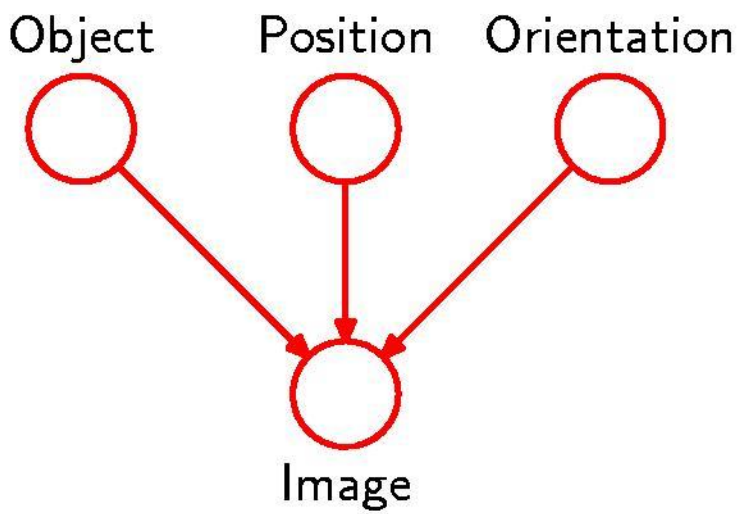


where

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

Generative Models

Causal process for generating images



Discrete Variables (1)

General joint distribution: $K^2 - 1$ parameters

$$p(\mathbf{x}_1, \mathbf{x}_2 | \boldsymbol{\mu}) = \prod_{k=1}^{K} \prod_{l=1}^{K} \mu_{kl}^{x_{1k} x_{2l}}$$

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

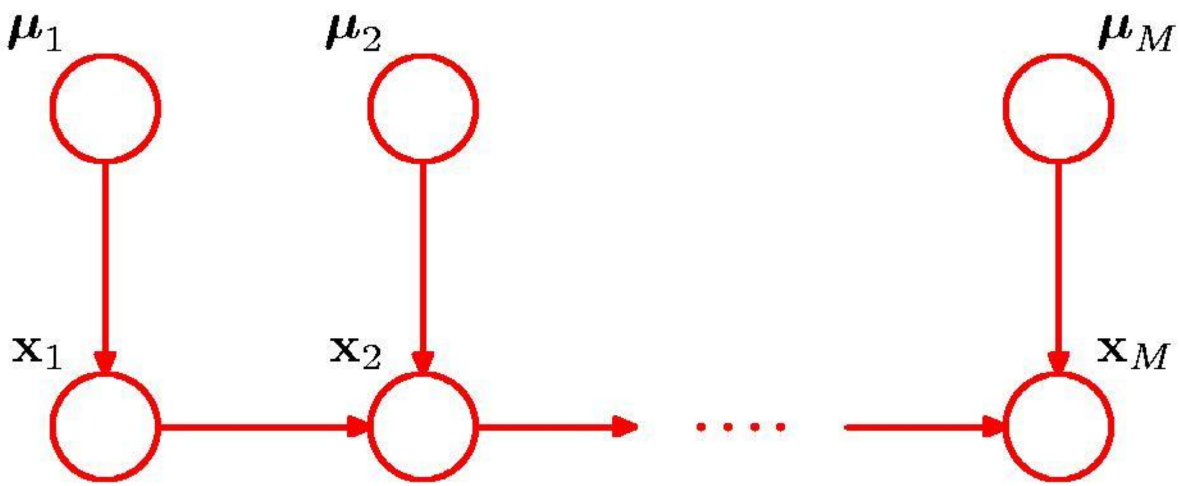
$$\hat{p}(\mathbf{x}_1, \mathbf{x}_2 | \boldsymbol{\mu}) = \prod_{k=1}^{K} \mu_{1k}^{x_{1k}} \prod_{l=1}^{K} \mu_{2l}^{x_{2l}}$$

Discrete Variables (2)

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

M-node Markov chain: $K - 1 + (M - 1)K(K - 1)$ parameters

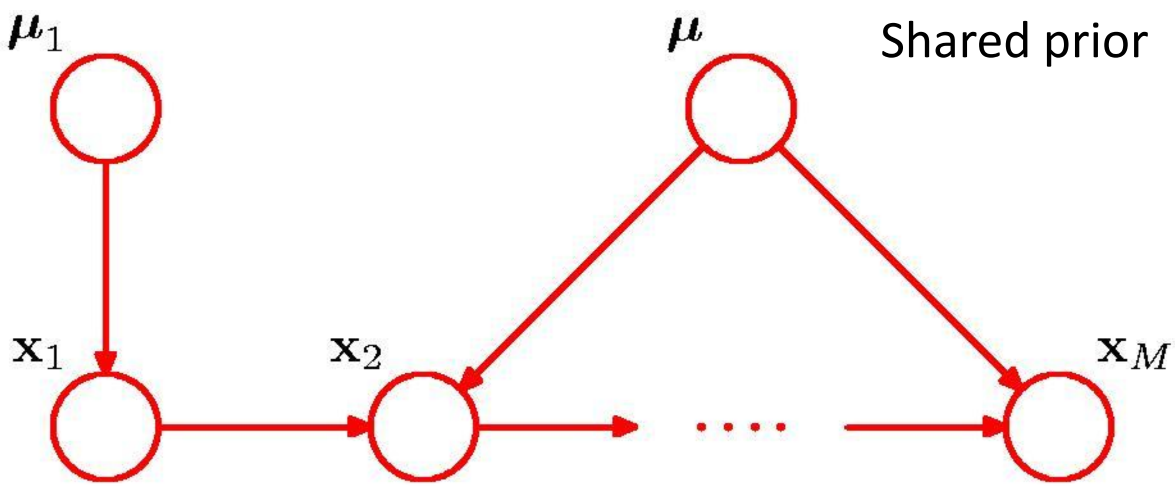
Discrete Variables: Bayesian Parameters (1)



$$p(\{\mathbf{x}_m, \boldsymbol{\mu}_m\}) = p(\mathbf{x}_1 | \boldsymbol{\mu}_1) p(\boldsymbol{\mu}_1) \prod_{m=2}^{M} p(\mathbf{x}_m | \mathbf{x}_{m-1}, \boldsymbol{\mu}_m) p(\boldsymbol{\mu}_m)$$

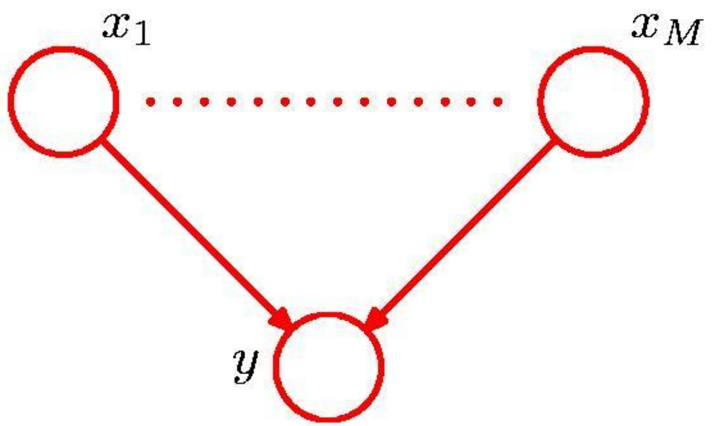
$$p(\boldsymbol{\mu}_m) = \mathrm{Dir}(\boldsymbol{\mu}_m | \boldsymbol{\alpha}_m)$$

Discrete Variables: Bayesian Parameters (2)



$$p\left(\{\mathbf{x}_m\}, \boldsymbol{\mu}_1, \boldsymbol{\mu}\right) = p\left(\mathbf{x}_1 | \boldsymbol{\mu}_1\right) p\left(\boldsymbol{\mu}_1\right) \prod_{m=2}^{M} p\left(\mathbf{x}_m | \mathbf{x}_{m-1}, \boldsymbol{\mu}\right) p\left(\boldsymbol{\mu}\right)$$

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 $O(K^M)$ parameters.

The parameterized form

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

requires only $M + 1$ parameters

Linear-Gaussian Models

Directed Graph

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

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

Vector-valued Gaussian Nodes

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

Conditional Independence

a is independent of b given c

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

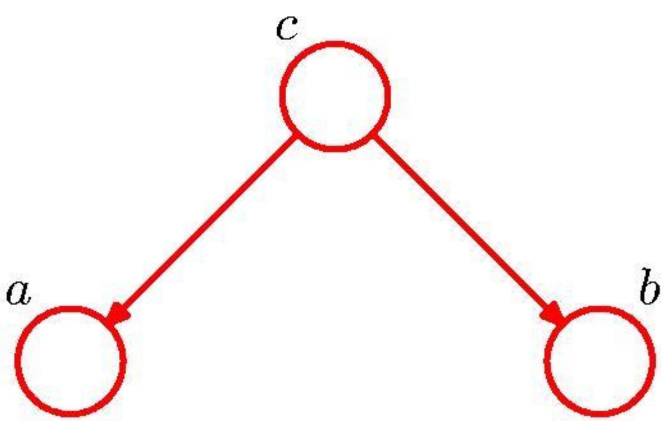
Equivalently

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

Notation

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

Conditional Independence: Example 1

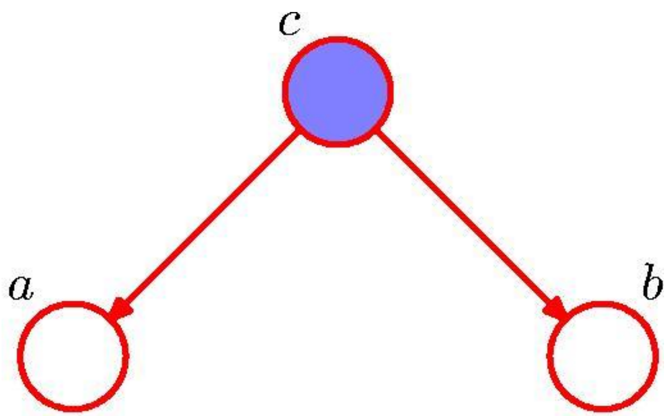


$$p(a, b, c) = p(a|c)p(b|c)p(c)$$

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

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

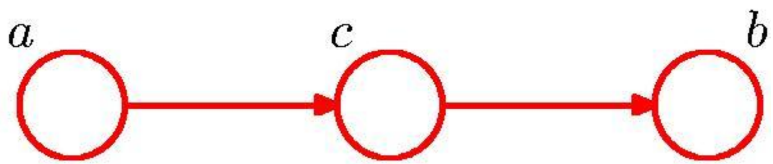
Conditional Independence: Example 1



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

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

Conditional Independence: Example 2

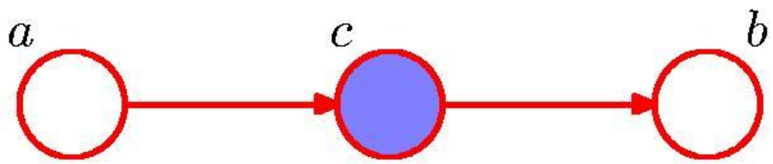


$$p(a, b, c) = p(a)p(c|a)p(b|c)$$

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

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

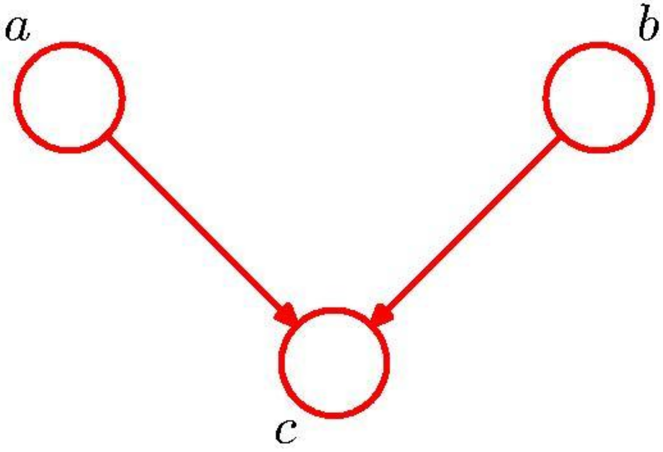
Conditional Independence: Example 2



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

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

Conditional Independence: Example 3



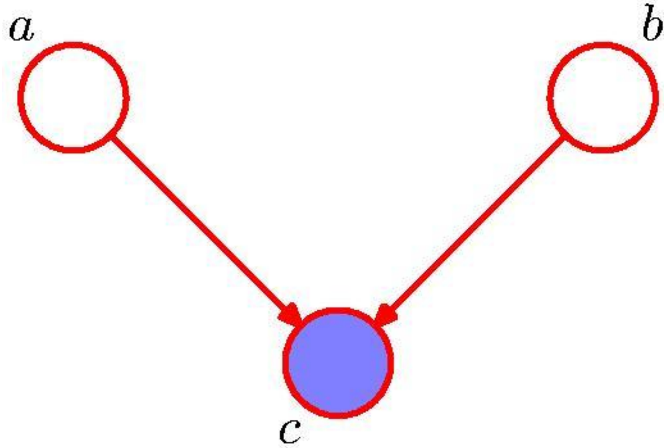
$$p(a, b, c) = p(a)p(b)p(c|a, b)$$

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

$$a \perp\!\!\!\perp b \mid \emptyset$$

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

Conditional Independence: Example 3



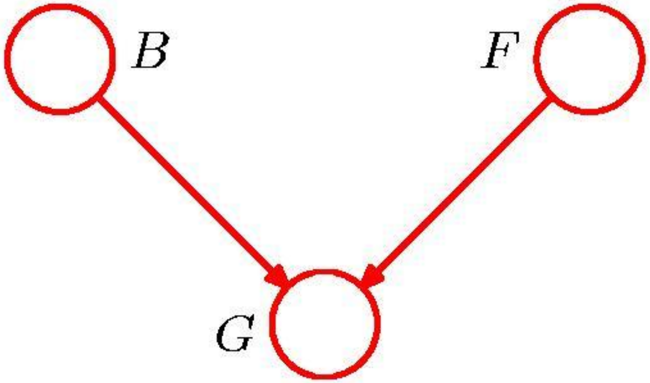
$$p(a, b|c) = \frac{p(a, b, c)}{p(c)}$$
$$= \frac{p(a)p(b)p(c|a, b)}{p(c)}$$

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

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

“Am I out of fuel?”

$$
\begin{aligned}
p(G=1|B=1,F=1) &= 0.8 \\
p(G=1|B=1,F=0) &= 0.2 \\
p(G=1|B=0,F=1) &= 0.2 \\
p(G=1|B=0,F=0) &= 0.1
\end{aligned}
$$



$$
\begin{aligned}
p(B=1) &= 0.9 \\
p(F=1) &= 0.9
\end{aligned}
$$

and hence

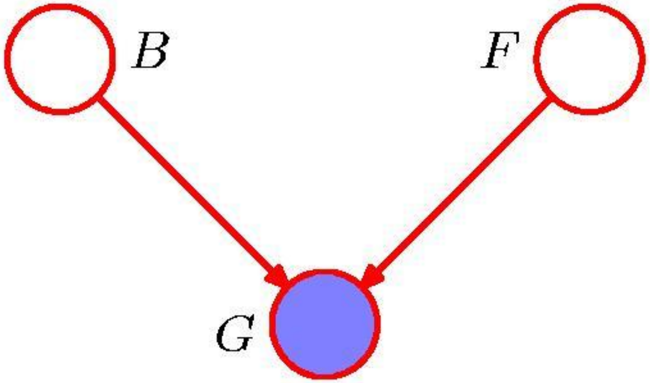
$$
p(F=0) = 0.1
$$

B = Battery (0=flat, 1=fully charged)

F = Fuel Tank (0=empty, 1=full)

G = Fuel Gauge Reading (0=empty, 1=full)

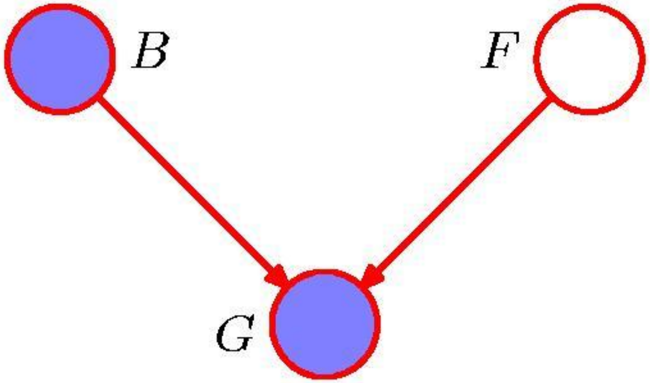
“Am I out of fuel?”



$$p(F=0|G=0) = \frac{p(G=0|F=0)p(F=0)}{p(G=0)} \simeq 0.257$$

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

“Am I out of fuel?”



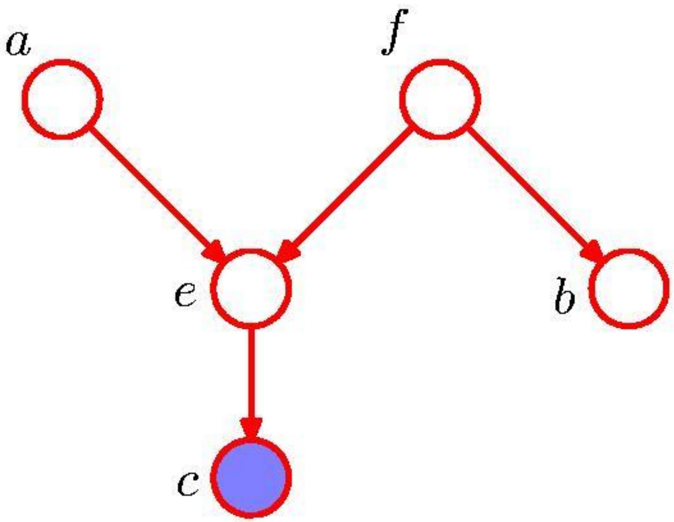
$$p(F=0|G=0,B=0) = \frac{p(G=0|B=0,F=0)p(F=0)}{\sum_{F\in\{0,1\}} p(G=0|B=0,F)p(F)} \simeq 0.111$$

Probability of an empty tank reduced by observing $B=0$.
This referred to as “explaining away”.

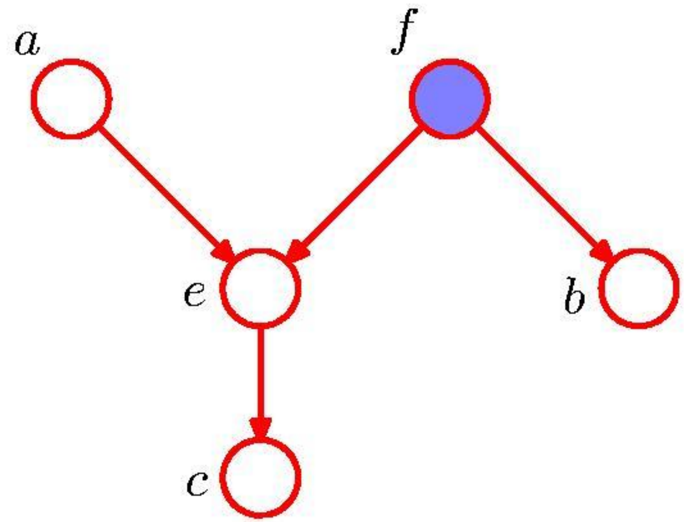
D-separation

- 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 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.
- 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

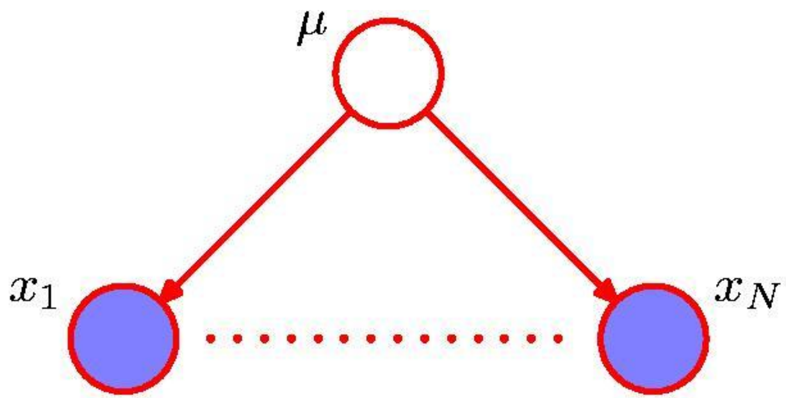


$a \not\perp\!\!\!\perp b \mid c$



$a \perp\!\!\!\perp b \mid f$

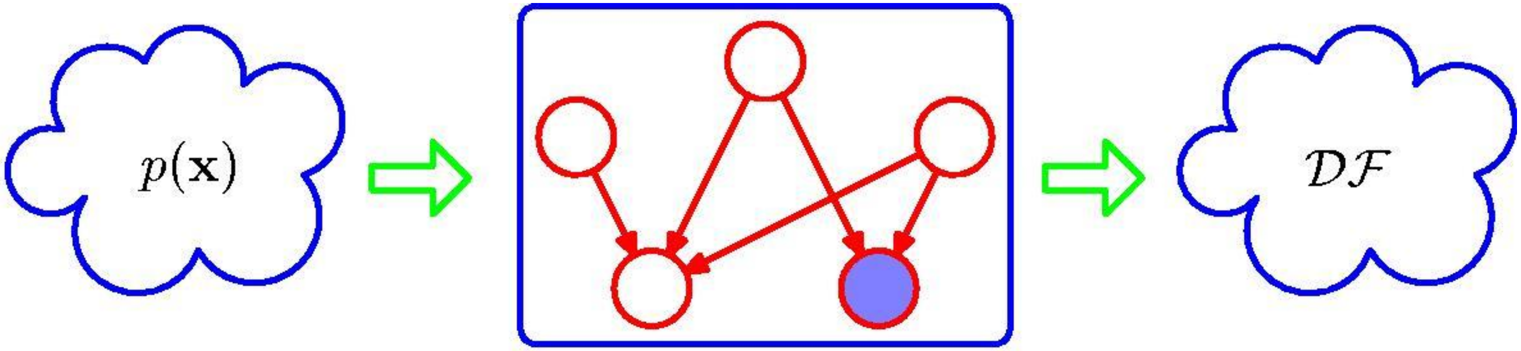
D-separation: I.I.D. Data



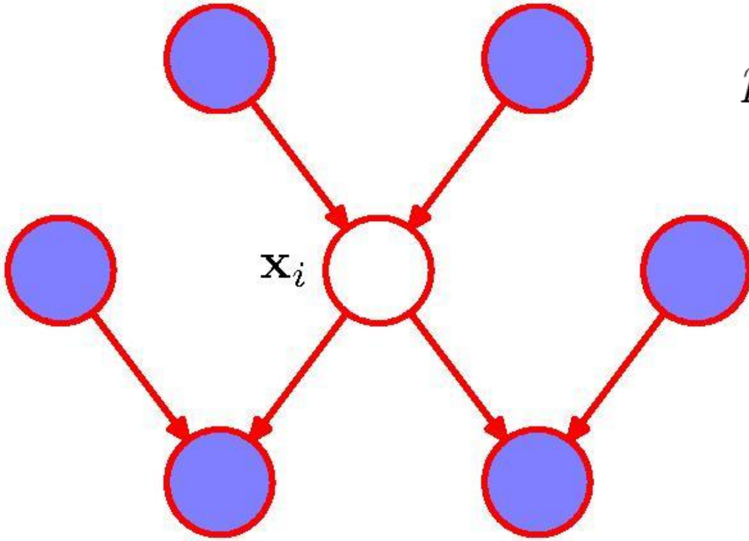
$$p(\mathcal{D}|\mu) = \prod_{n=1}^{N} p(x_n|\mu)$$

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

Directed Graphs as Distribution Filters



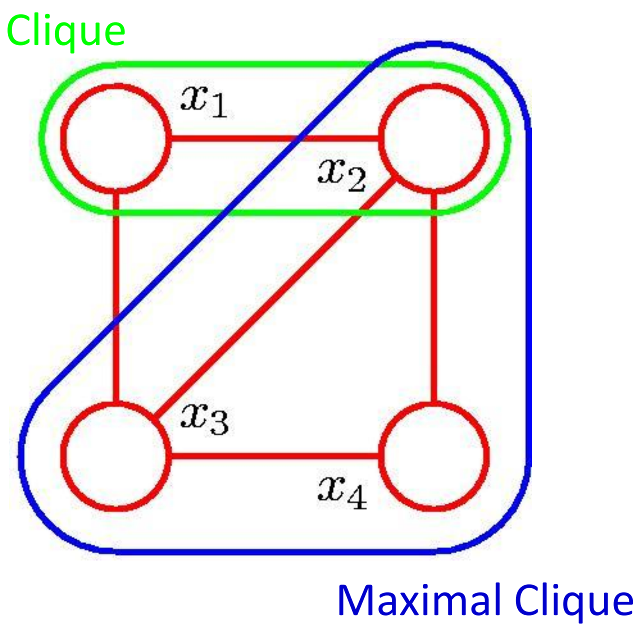
The Markov Blanket



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

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

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 C and

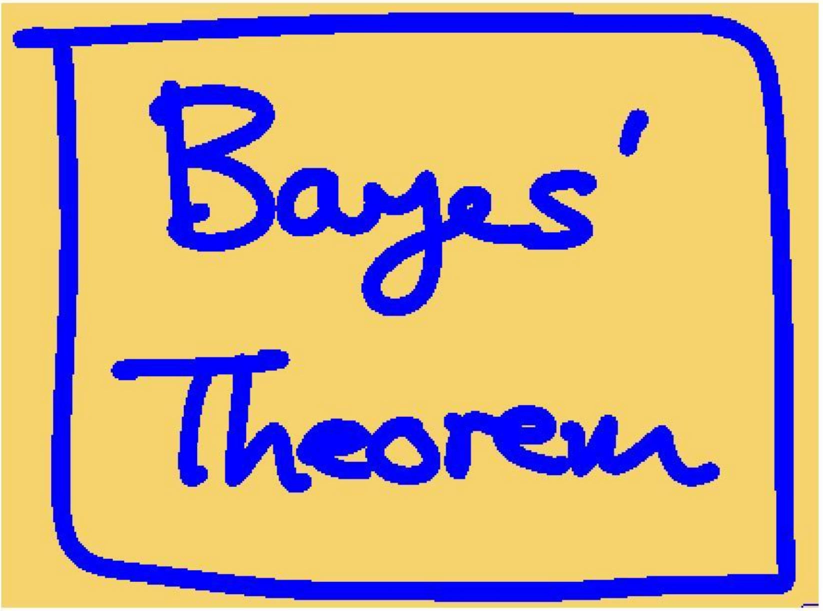
$$Z = \sum_{\mathbf{x}} \prod_C \psi_C(\mathbf{x}_C)$$

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

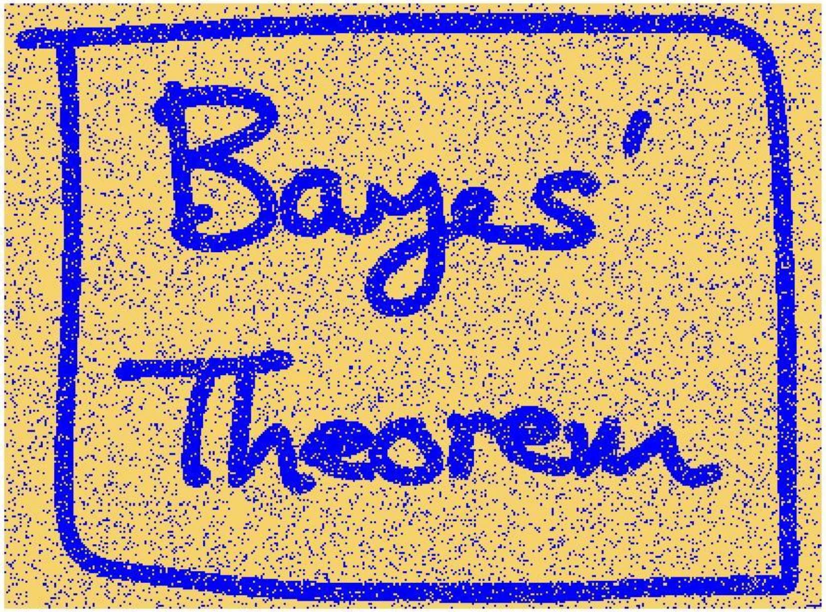
Energies and the Boltzmann distribution

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

Illustration: Image De-Noising (1)

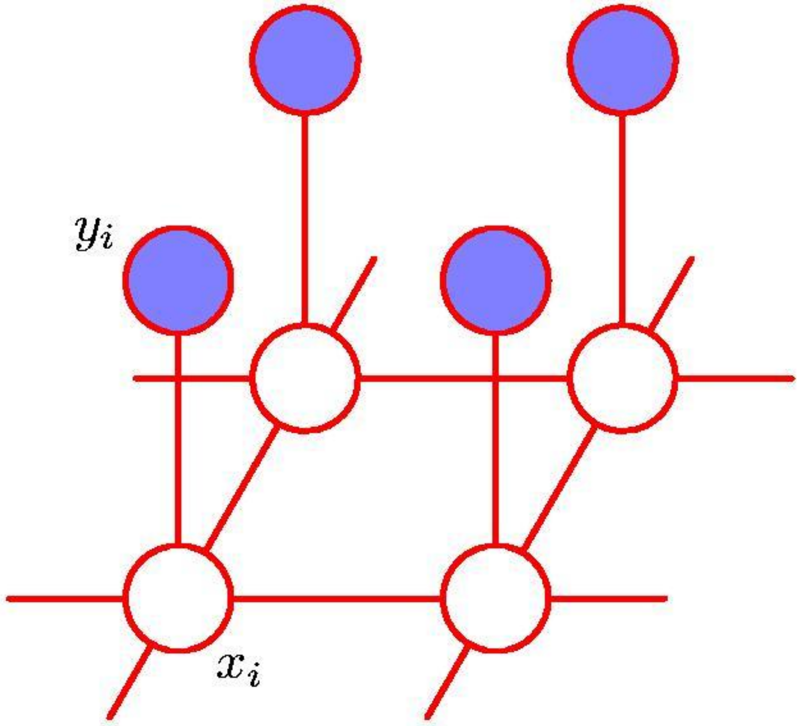


Original Image



Noisy Image

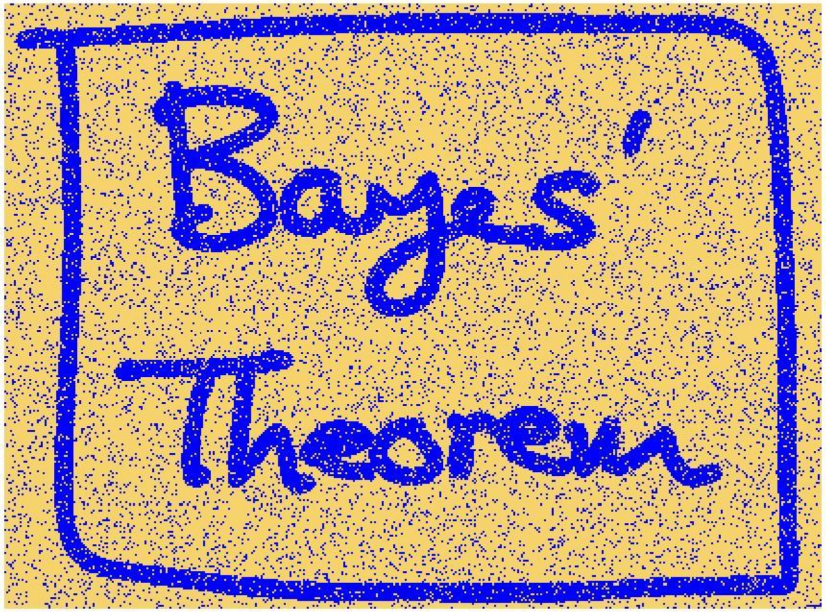
Illustration: Image De-Noising (2)



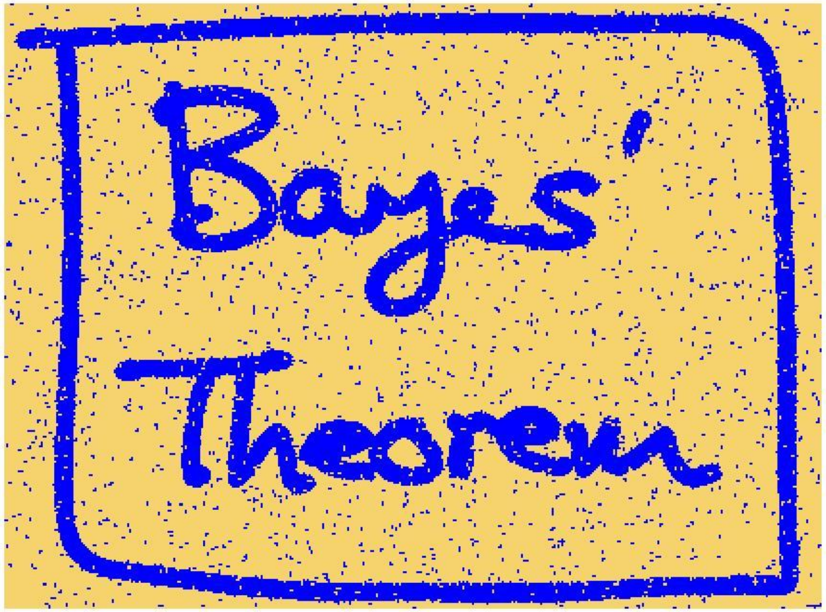
$$E(\mathbf{x}, \mathbf{y}) = h\sum_i x_i - \beta \sum_{\{i,j\}} x_i x_j - \eta \sum_i x_i y_i$$

$$p(\mathbf{x}, \mathbf{y}) = \frac{1}{Z} \exp\{-E(\mathbf{x}, \mathbf{y})\}$$

Illustration: Image De-Noising (3)

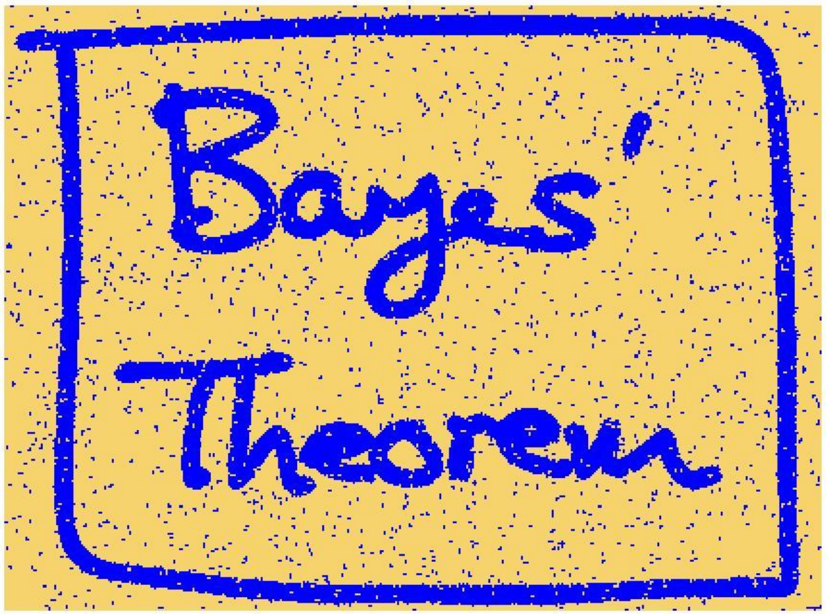


Noisy Image

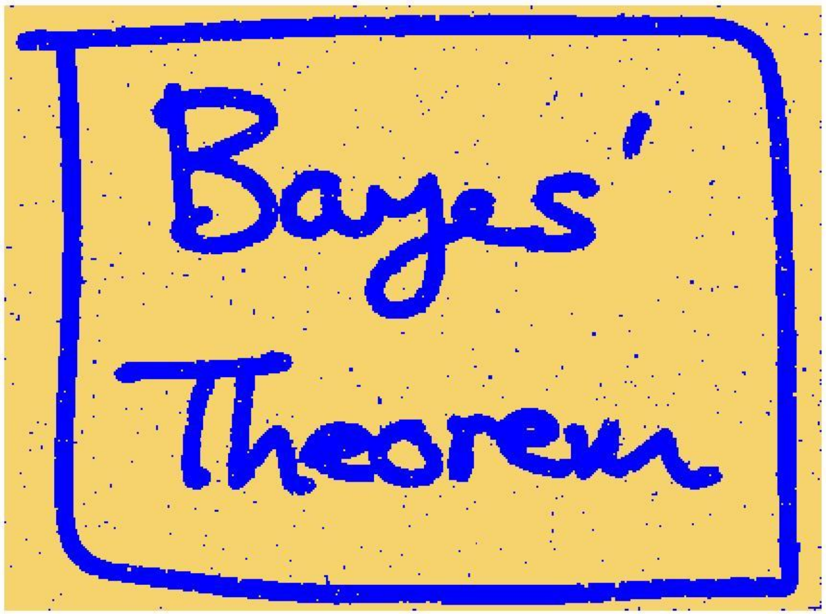


Restored Image (ICM)

Illustration: Image De-Noising (4)

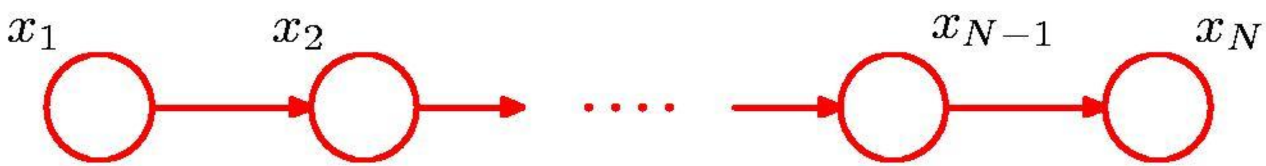


Restored Image (ICM)



Restored Image (Graph cuts)

Converting Directed to Undirected Graphs (1)

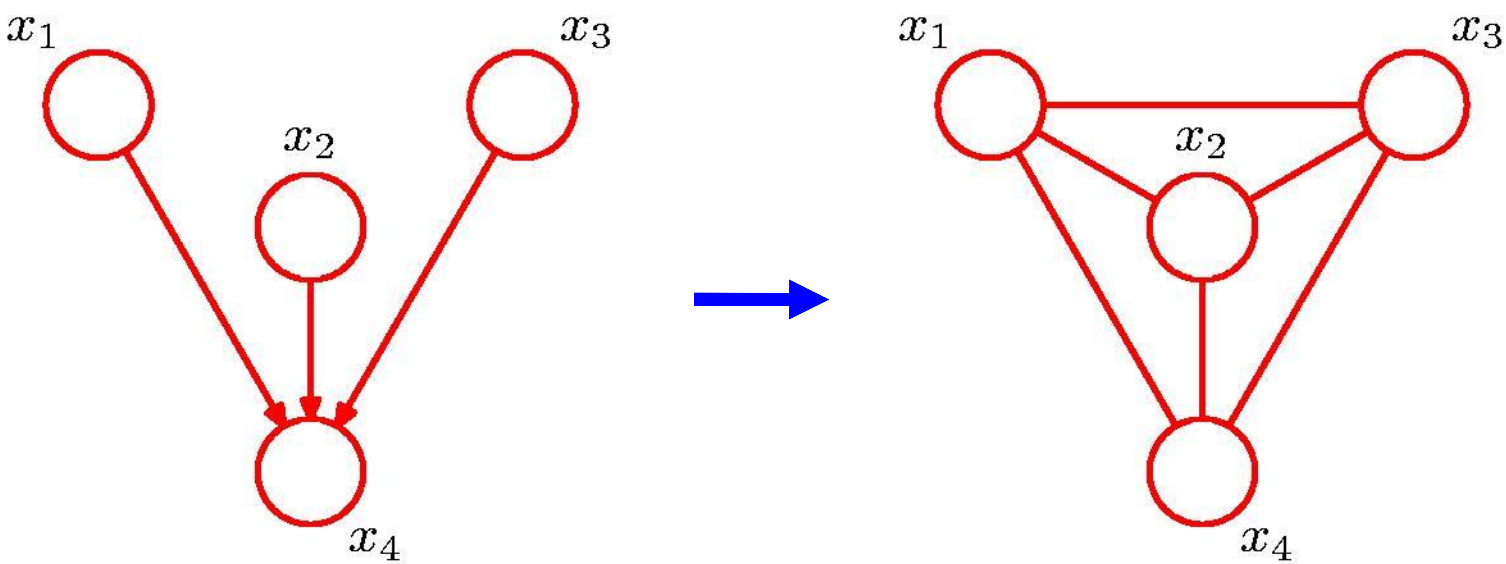


$$p(\mathbf{x}) = \underbrace{p(x_1)p(x_2|x_1)}\, p(x_3|x_2) \cdots p(x_N|x_{N-1})$$

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

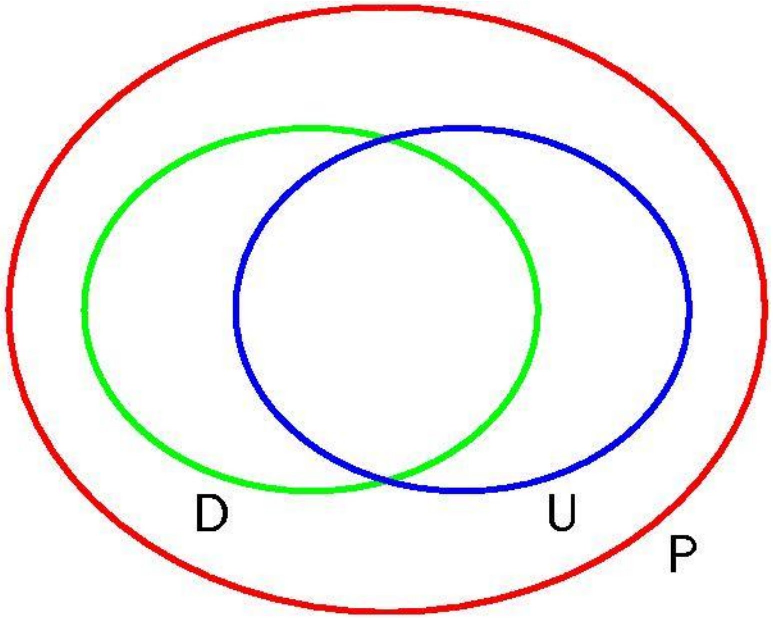
Converting Directed to Undirected Graphs (2)

Additional links

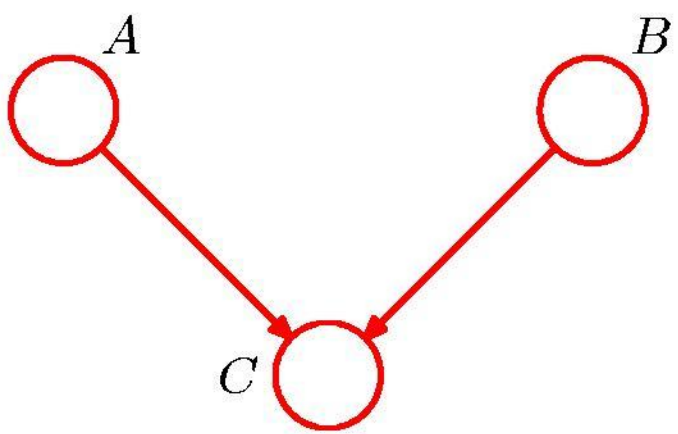


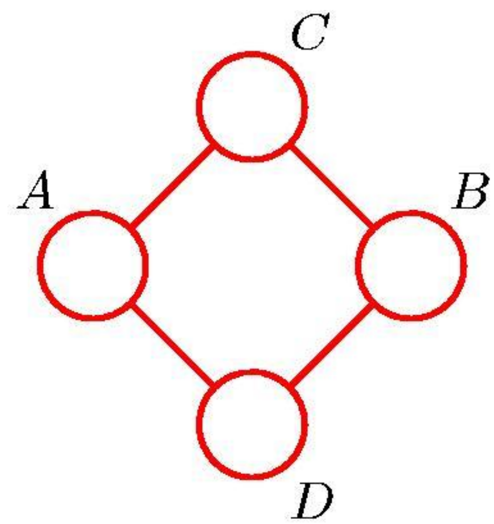
$$
\begin{aligned}
p(\mathbf{x}) &= p(x_1)p(x_2)p(x_3)p(x_4|x_1, x_2, x_3) \\
&= \frac{1}{Z}\psi_A(x_1, x_2, x_3)\psi_B(x_2, x_3, x_4)\psi_C(x_1, x_2, x_4)
\end{aligned}
$$

Directed vs. Undirected Graphs (1)



Directed vs. Undirected Graphs (2)





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

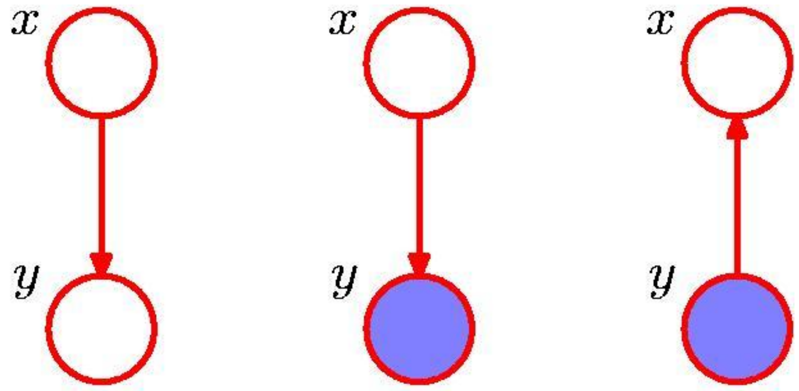
$$A \not\perp\!\!\!\perp B \mid C$$

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

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

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

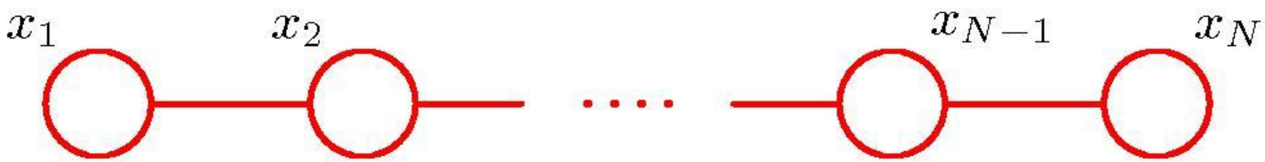
Inference in Graphical Models



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

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

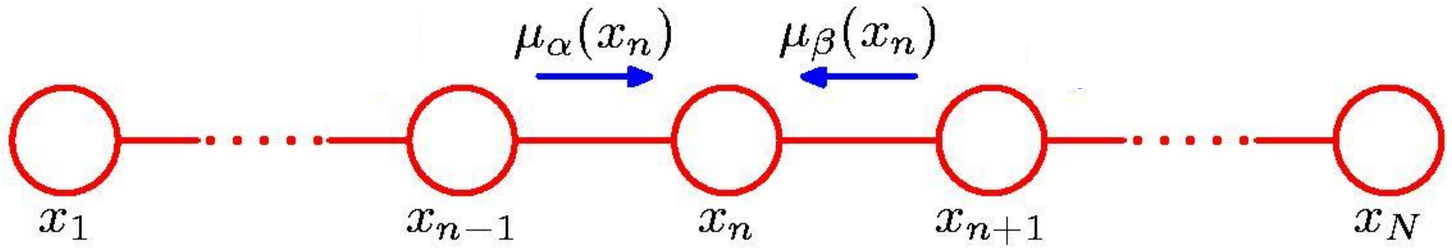
Inference on a Chain



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

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

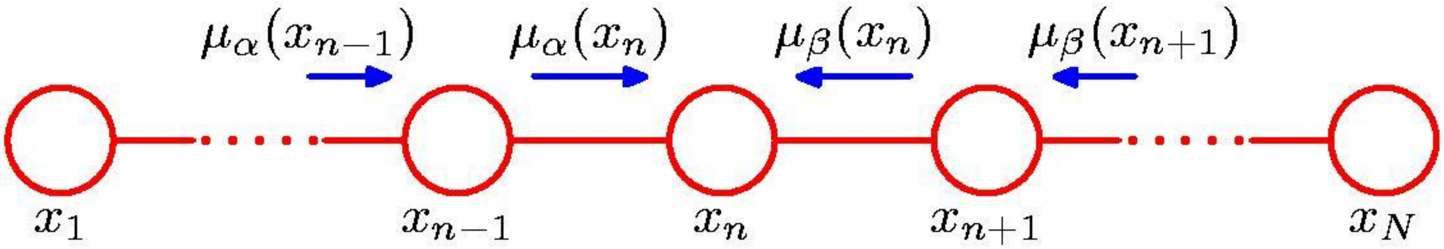
Inference on a Chain



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

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

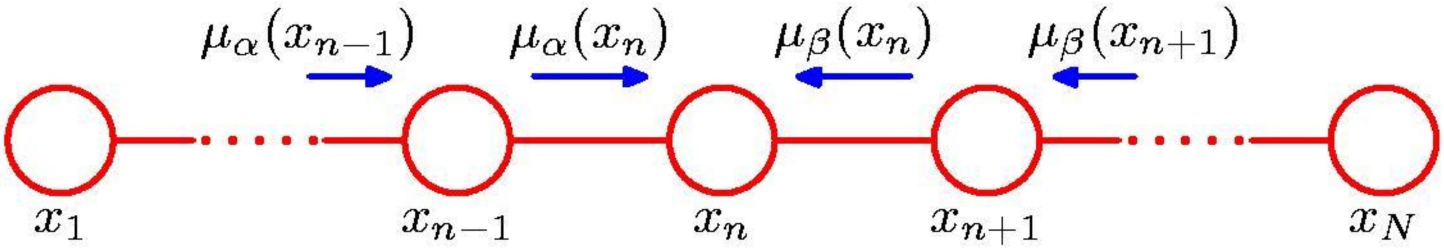
Inference on a Chain



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

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

Inference on a Chain



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

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

Inference on a Chain

To compute local marginals:

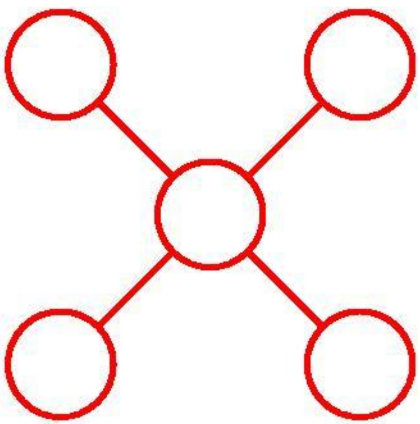
- Compute and store all forward messages, $\mu_\alpha(x_n)$.
- Compute and store all backward messages, $\mu_\beta(x_n)$.
- Compute Z at any node x_m
- Compute

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

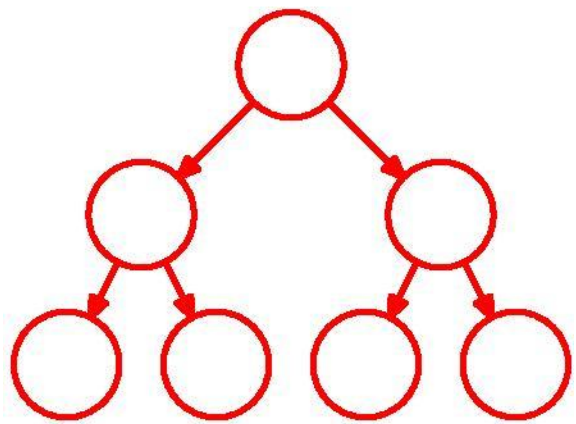
for all variables required.

Trees

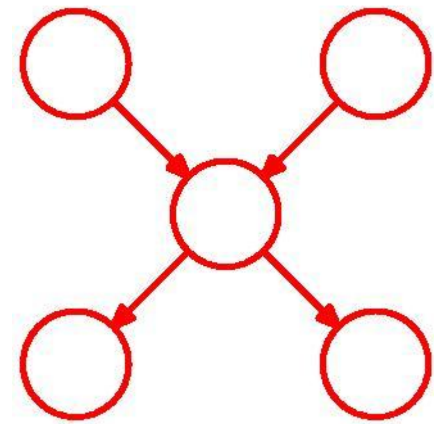
Undirected Tree



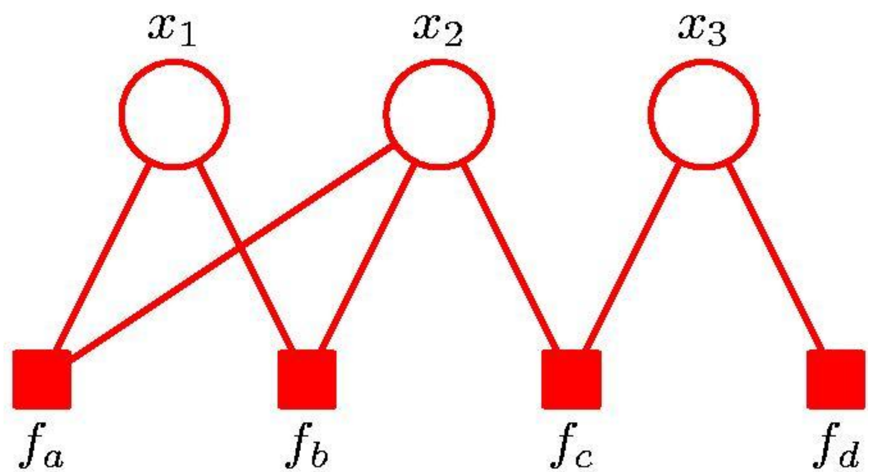
Directed Tree



Polytree



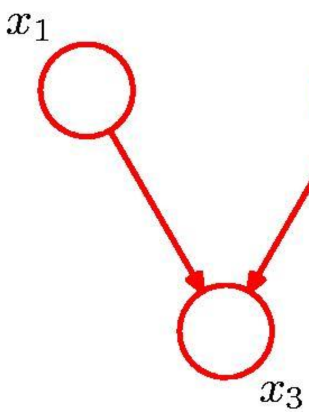
Factor Graphs

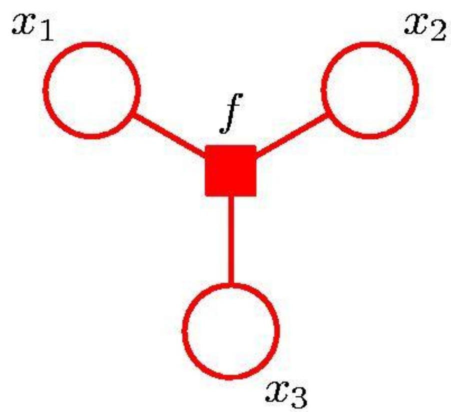


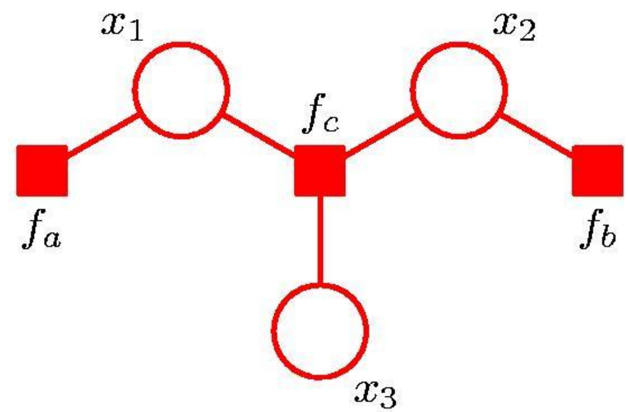
$$p(\mathbf{x}) = f_a(x_1, x_2) f_b(x_1, x_2) f_c(x_2, x_3) f_d(x_3)$$

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

Factor Graphs from Directed Graphs







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

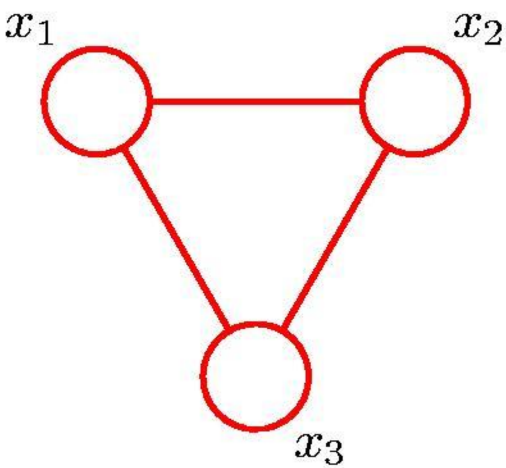
$$f(x_1, x_2, x_3) = p(x_1)p(x_2)p({}_3|x_1, x_2)$$

$$f_a(x_1) = p(x_1)$$

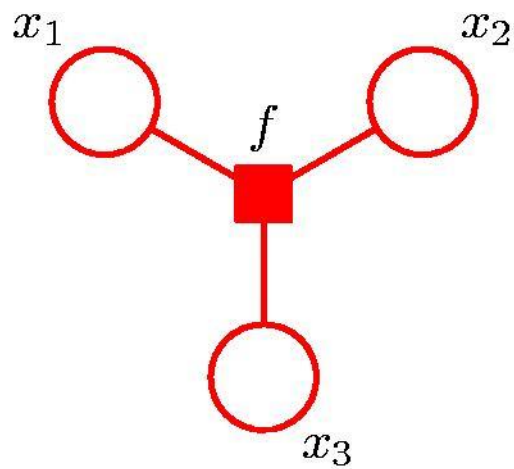
$$f_b(x_2) = p(x_2)$$

$$f_c(x_1, x_2, x_3) = p(x_3|x_1, x_2)$$

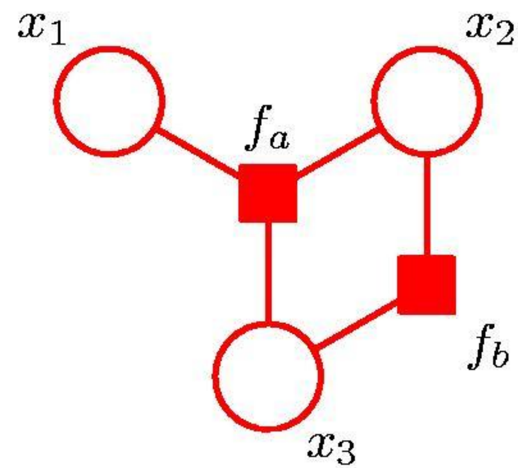
Factor Graphs from Undirected Graphs



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



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



$$f_a(x_1, x_2, x_3) f_b(x_2, x_3) = \psi(x_1, x_2, x_3)$$

The Sum-Product Algorithm (1)

Objective:

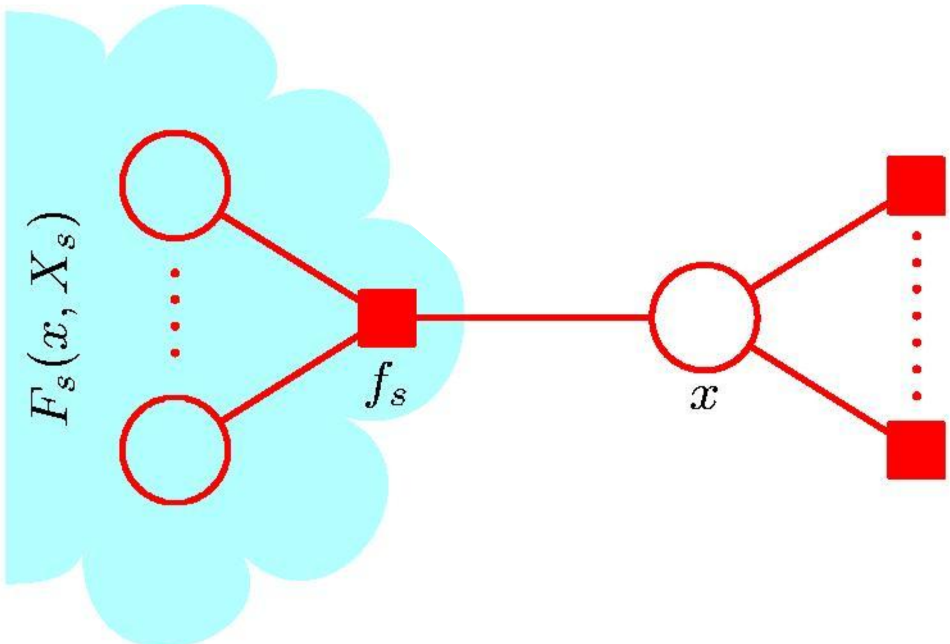
i. to obtain an efficient, exact inference algorithm for finding marginals;

ii. in situations where several marginals are required, to allow computations to be shared efficiently.

Key idea: Distributive Law

$$ab + ac = a(b + c)$$

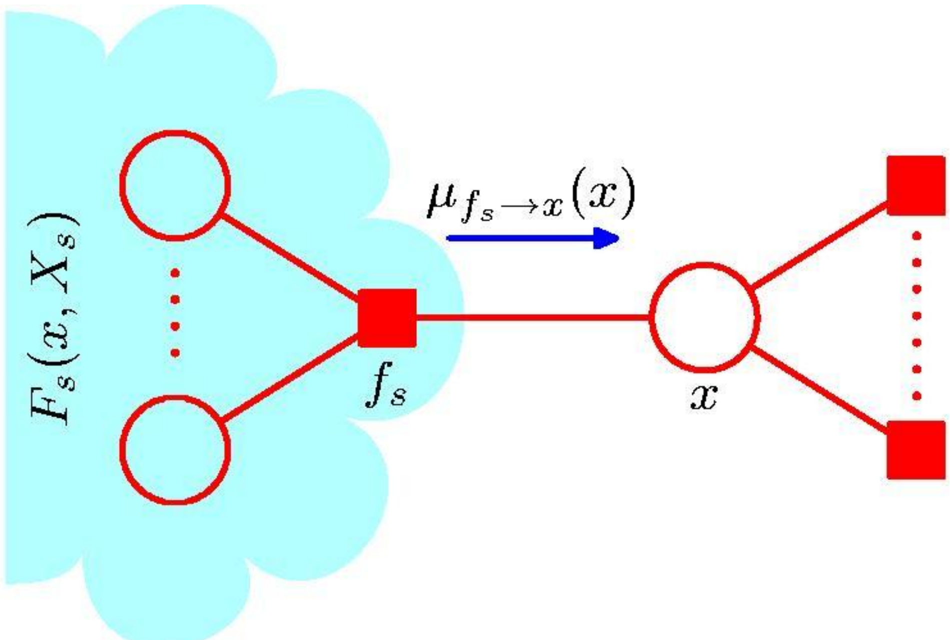
The Sum-Product Algorithm (2)



$$p(x) = \sum_{\mathbf{x} \setminus x} p(\mathbf{x})$$

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

The Sum-Product Algorithm (3)

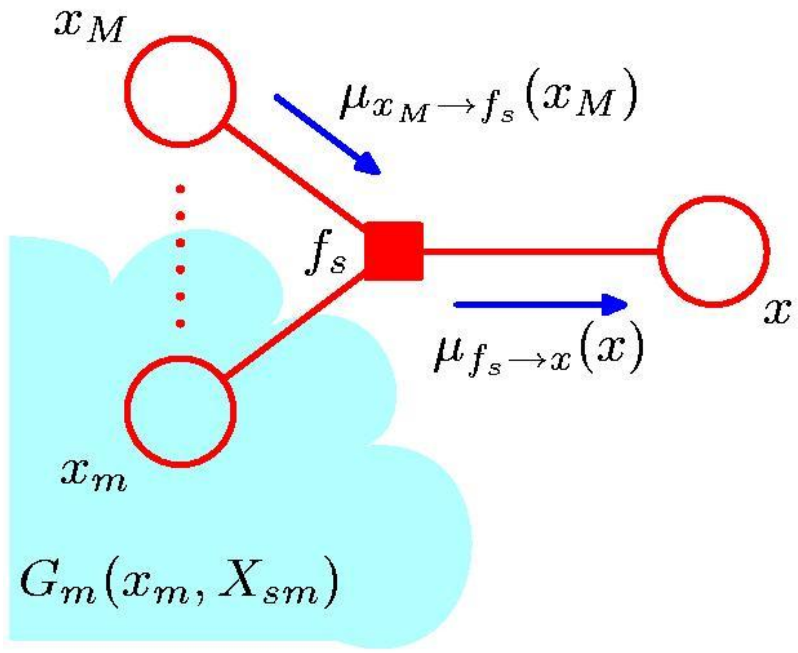


$$p(x) = \prod_{s \in \mathrm{ne}(x)} \left[\sum_{X_s} F_s(x, X_s) \right]$$

$$= \prod_{s \in \mathrm{ne}(x)} \mu_{f_s \to x}(x).$$

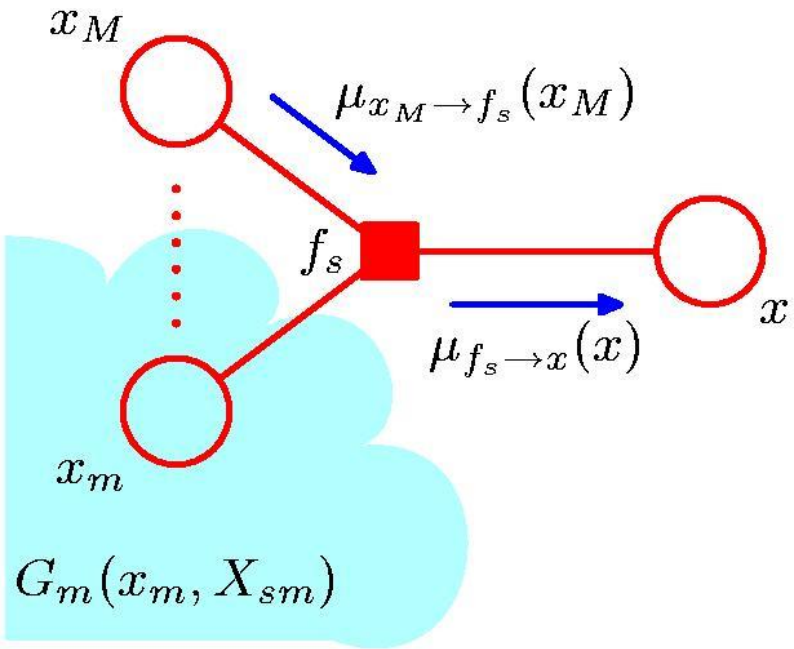
$$\mu_{f_s \to x}(x) \equiv \sum_{X_s} F_s(x, X_s)$$

The Sum-Product Algorithm (4)



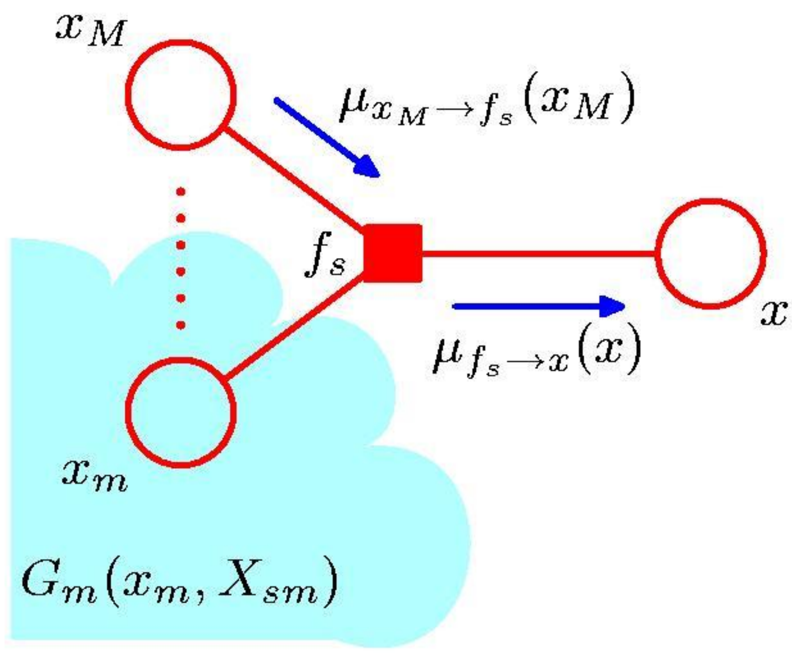
$$F_s(x, X_s) = f_s(x, x_1, \ldots, x_M) G_1(x_1, X_{s1}) \ldots G_M(x_M, X_{sM})$$

The Sum-Product Algorithm (5)



$$
\begin{aligned}
\mu_{f_s \to x}(x) &= \sum_{x_1} \cdots \sum_{x_M} f_s(x, x_1, \ldots, x_M) \prod_{m \in \mathrm{ne}(f_s) \setminus x} \left[\sum_{X_{sm}} G_m(x_m, X_{sm}) \right] \\
&= \sum_{x_1} \cdots \sum_{x_M} f_s(x, x_1, \ldots, x_M) \prod_{m \in \mathrm{ne}(f_s) \setminus x} \mu_{x_m \to f_s}(x_m)
\end{aligned}
$$

The Sum-Product Algorithm (6)

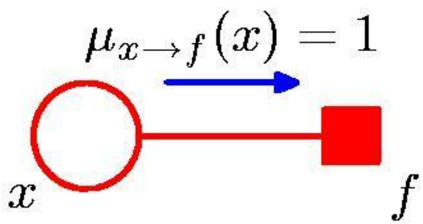


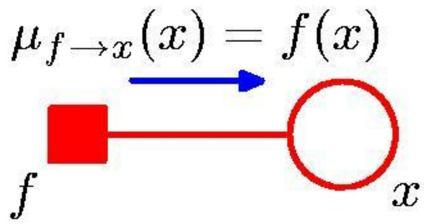
$$\mu_{x_m \to f_s}(x_m) \equiv \sum_{X_{sm}} G_m(x_m, X_{sm}) = \sum_{X_{sm}} \prod_{l \in \mathrm{ne}(x_m) \setminus f_s} F_l(x_m, X_{ml})$$

$$= \prod_{l \in \mathrm{ne}(x_m) \setminus f_s} \mu_{f_l \to x_m}(x_m)$$

The Sum-Product Algorithm (7)

Initialization



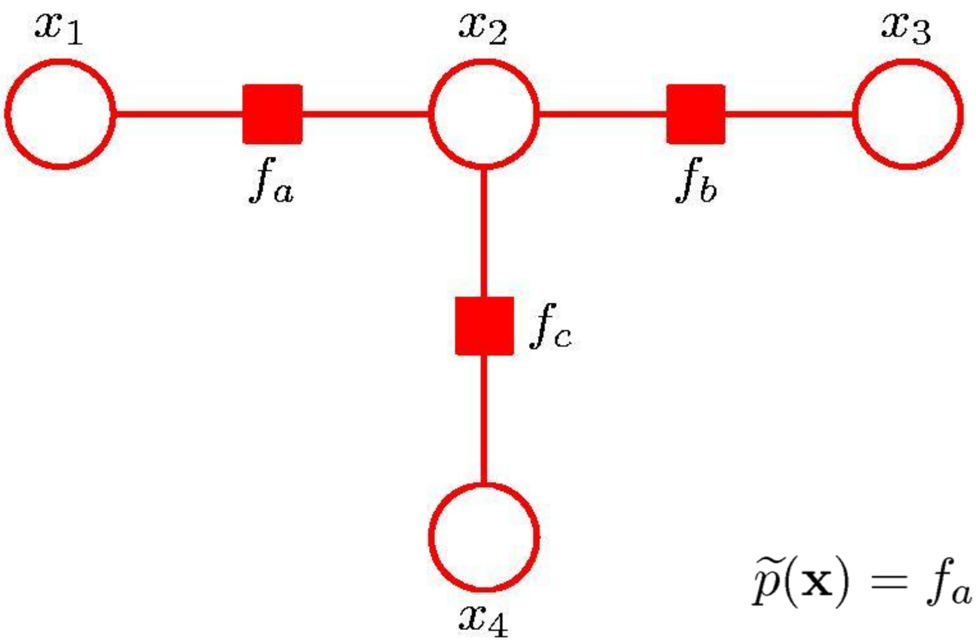


The Sum-Product Algorithm (8)

To compute local marginals:

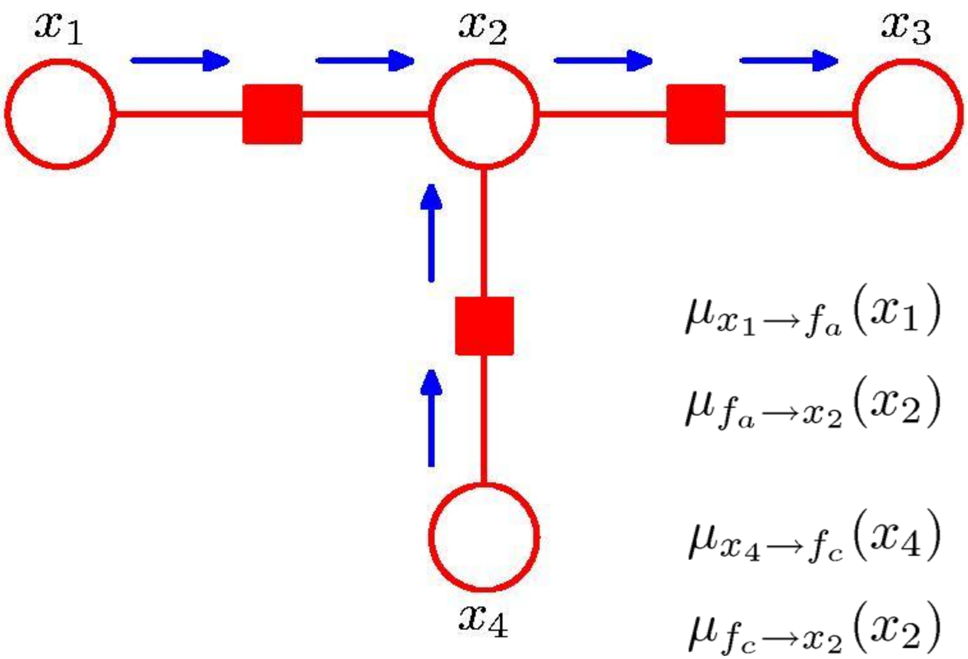
- Pick an arbitrary node as root
- Compute and propagate messages from the leaf nodes to the root, storing received messages at every node.
- Compute and propagate messages from the root to the leaf nodes, storing received messages at every node.
- Compute the product of received messages at each node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

Sum-Product: Example (1)



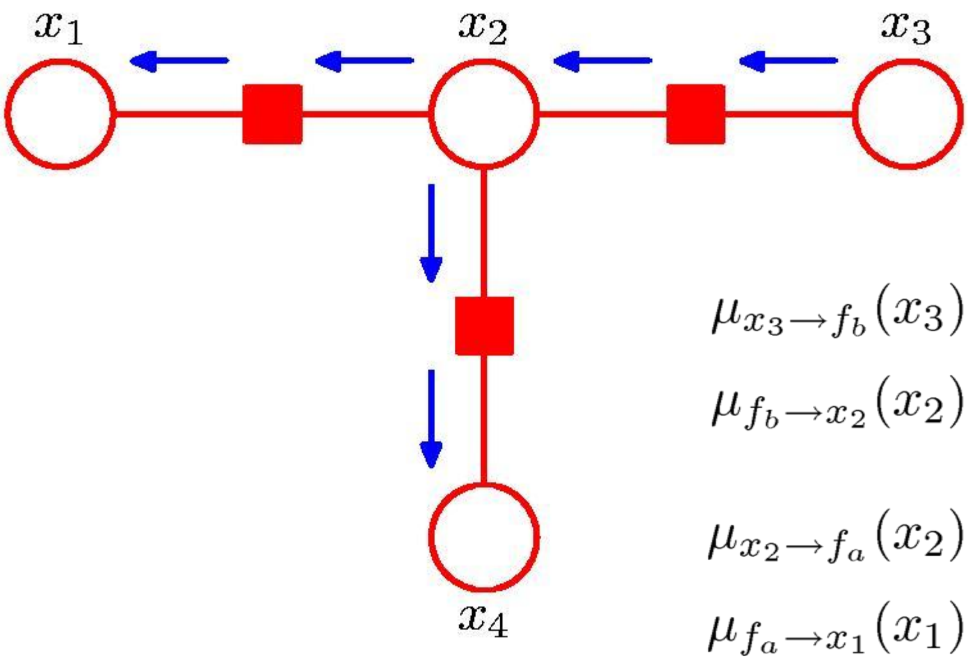
$$\widetilde{p}(\mathbf{x}) = f_a(x_1, x_2) f_b(x_2, x_3) f_c(x_2, x_4)$$

Sum-Product: Example (2)



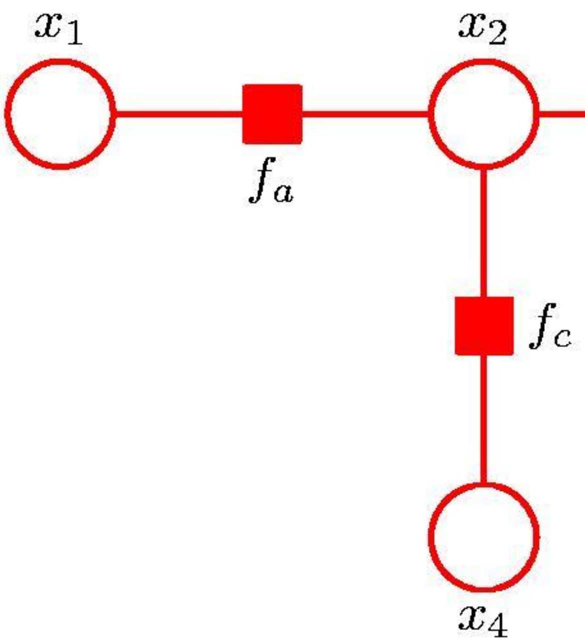
$$
\begin{aligned}
\mu_{x_1 \to f_a}(x_1) &= 1 \\
\mu_{f_a \to x_2}(x_2) &= \sum_{x_1} f_a(x_1, x_2) \\
\mu_{x_4 \to f_c}(x_4) &= 1 \\
\mu_{f_c \to x_2}(x_2) &= \sum_{x_4} f_c(x_2, x_4) \\
\mu_{x_2 \to f_b}(x_2) &= \mu_{f_a \to x_2}(x_2)\mu_{f_c \to x_2}(x_2) \\
\mu_{f_b \to x_3}(x_3) &= \sum_{x_2} f_b(x_2, x_3)\mu_{x_2 \to f_b}(x_2)
\end{aligned}
$$

Sum-Product: Example (3)



$$
\begin{aligned}
\mu_{x_3 \to f_b}(x_3) &= 1 \\
\mu_{f_b \to x_2}(x_2) &= \sum_{x_3} f_b(x_2, x_3) \\
\mu_{x_2 \to f_a}(x_2) &= \mu_{f_b \to x_2}(x_2)\mu_{f_c \to x_2}(x_2) \\
\mu_{f_a \to x_1}(x_1) &= \sum_{x_2} f_a(x_1, x_2)\mu_{x_2 \to f_a}(x_2) \\
\mu_{x_2 \to f_c}(x_2) &= \mu_{f_a \to x_2}(x_2)\mu_{f_b \to x_2}(x_2) \\
\mu_{f_c \to x_4}(x_4) &= \sum_{x_2} f_c(x_2, x_4)\mu_{x_2 \to f_c}(x_2)
\end{aligned}
$$

Sum-Product: Example (4)



$$\widetilde{p}(x_2) = \mu_{f_a \to x_2}(x_2)\mu_{f_b \to x_2}(x_2)\mu_{f_c \to x_2}(x_2)$$

$$= \left[\sum_{x_1} f_a(x_1, x_2)\right]\left[\sum_{x_3} f_b(x_2, x_3)\right]$$

$$\left[\sum_{x_4} f_c(x_2, x_4)\right]$$

$$= \sum_{x_1}\sum_{x_3}\sum_{x_4} f_a(x_1, x_2) f_b(x_2, x_3) f_c(x_2, x_4)$$

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

The Max-Sum Algorithm (1)

Objective: an efficient algorithm for finding

i. the value $\mathbf{x}^{\max}$ that maximises $p(\mathbf{x})$;

ii. the value of $p(\mathbf{x}^{\max})$.

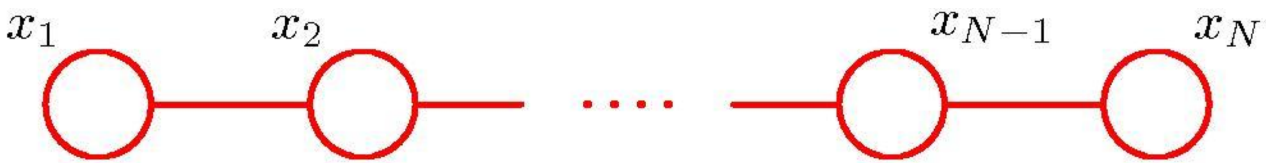
In general, maximum marginals $\neq$ joint maximum.

	$x = 0$	$x = 1$
$y = 0$	0.3	0.4
$y = 1$	0.3	0.0

$$\arg\max_x p(x, y) = 1 \qquad \arg\max_x p(x) = 0$$

The Max-Sum Algorithm (2)

Maximizing over a chain (max-product)



$$p(\mathbf{x}^{\max}) = \max_{\mathbf{x}} p(\mathbf{x}) = \max_{x_1} \ldots \max_{x_M} p(\mathbf{x})$$

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

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

The Max-Sum Algorithm (3)

Generalizes to tree-structured factor graph

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

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)

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

Recursion

$$\mu_{f\to x}(x) = \max_{x_1,\ldots,x_M}\left[\ln f(x, x_1, \ldots, x_M) + \sum_{m\in \mathrm{ne}(f_s)\setminus x} \mu_{x_m\to f}(x_m)\right]$$

$$\phi(x) = \arg\max_{x_1,\ldots,x_M}\left[\ln f(x, x_1, \ldots, x_M) + \sum_{m\in \mathrm{ne}(f_s)\setminus x} \mu_{x_m\to f}(x_m)\right]$$

$$\mu_{x\to f}(x) = \sum_{l\in \mathrm{ne}(x)\setminus f} \mu_{f_l\to x}(x)$$

The Max-Sum Algorithm (6)

Termination (root node)

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

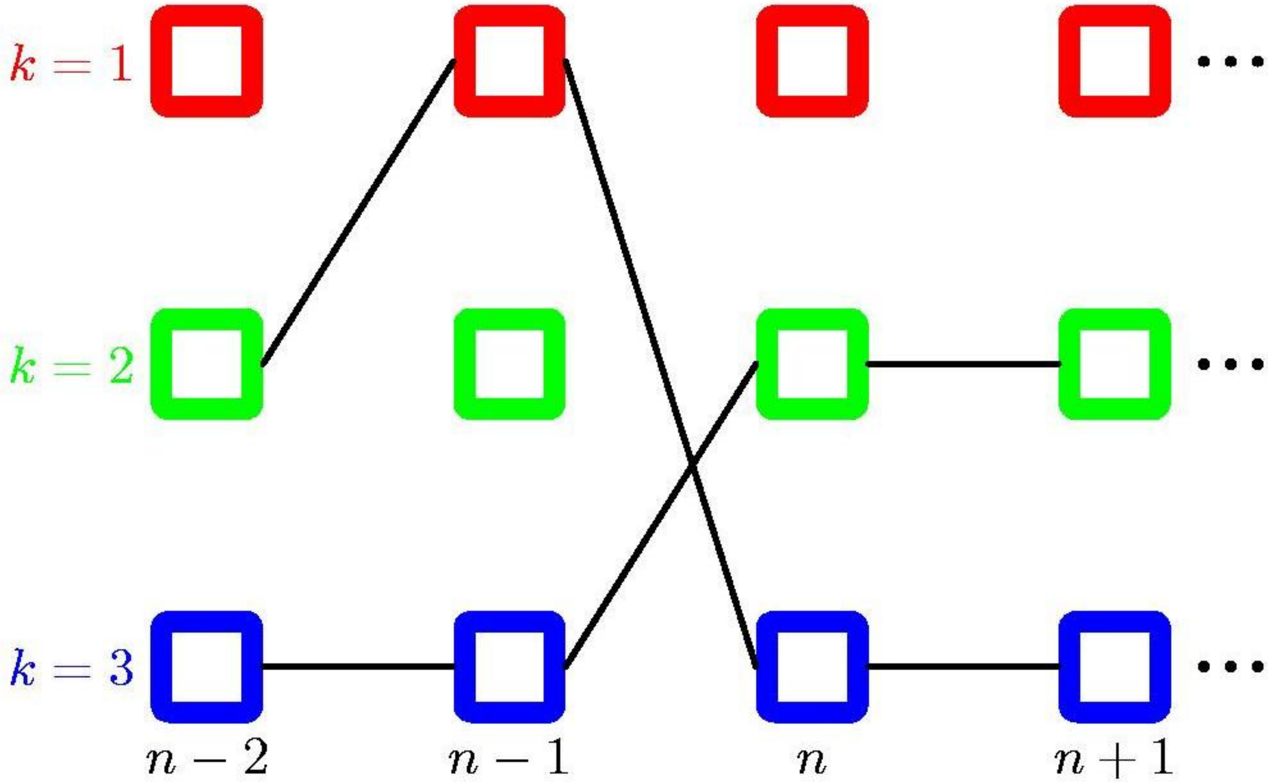
$$x^{\max} = \arg\max_x \left[\sum_{s \in \mathrm{ne}(x)} \mu_{f_s \to x}(x) \right]$$

Back-track, for all nodes i with l factor nodes to the root ($l=0$)

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

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-product-like 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.