PATTERN RECOGNITION AND MACHINE LEARNING

CHAPTER 8: GRAPHICAL MODELS

Learning Objectives

1、What are Bayesian Networks (BNs)?

2、How to use BNs to represent curve fitting, HMM, linear Gaussian models?

3、What is conditional independence?

4、What are Markov random fields?

5、What are directed, undirected and factor graphs?

6、How to perform sum-product algorithms within factor graphs?

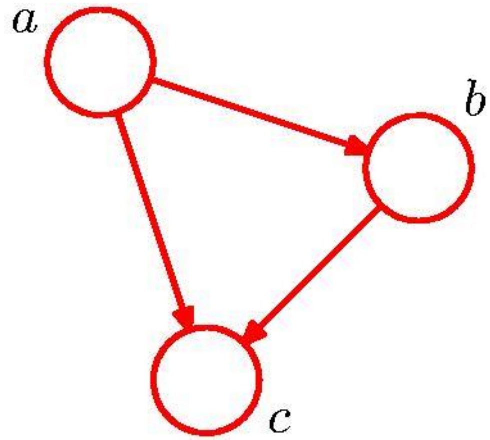
7、How to perform max-product algorithms within factor graphs?

Outlines

- Bayesian Networks
- Bayesian Curve Fitting
- Discrete Variables and Linear Gaussian Models
- Conditional Independence
- Markov Random Fields
- Inference in Graphical Models

Bayesian Networks

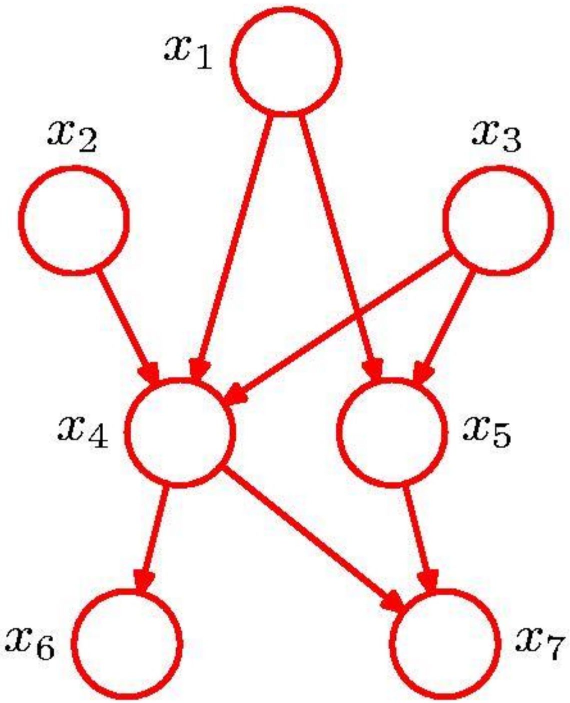
Directed Acyclic Graph (DAG)



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

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

Bayesian Networks



$$
\begin{aligned}
p(x_1, \ldots, x_7) \quad &= \quad p(x_1)p(x_2)p(x_3)p(x_4|x_1, x_2, x_3) \\
&\quad\quad p(x_5|x_1, x_3)p(x_6|x_4)p(x_7|x_4, x_5)
\end{aligned}
$$

General Factorization

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

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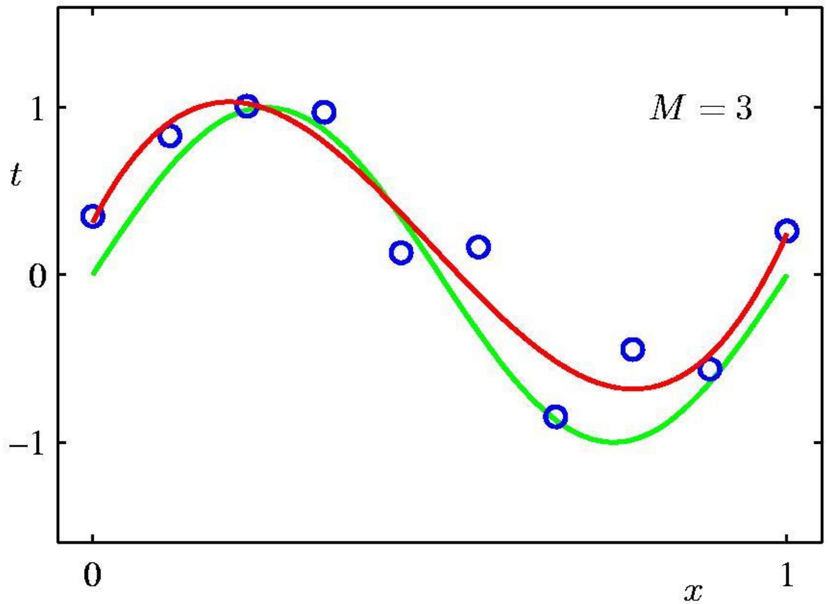
Bayesian Curve Fitting (1)



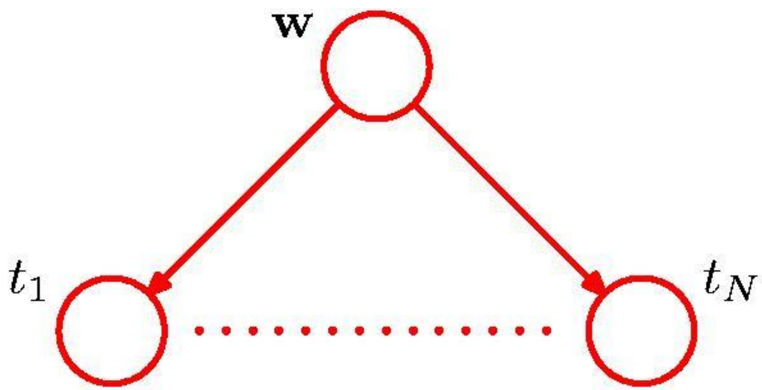
Polynomial

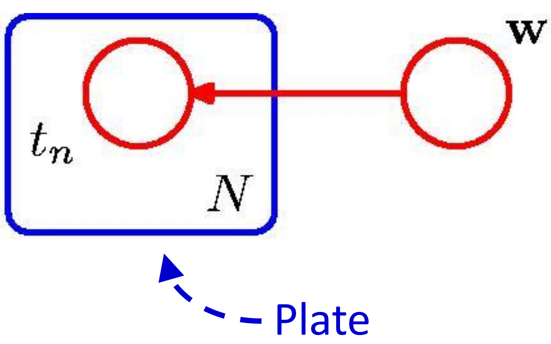
$$y(x, \mathbf{w}) = \sum_{j=0}^{M} w_j x^j$$

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

Bayesian Curve Fitting (2)

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

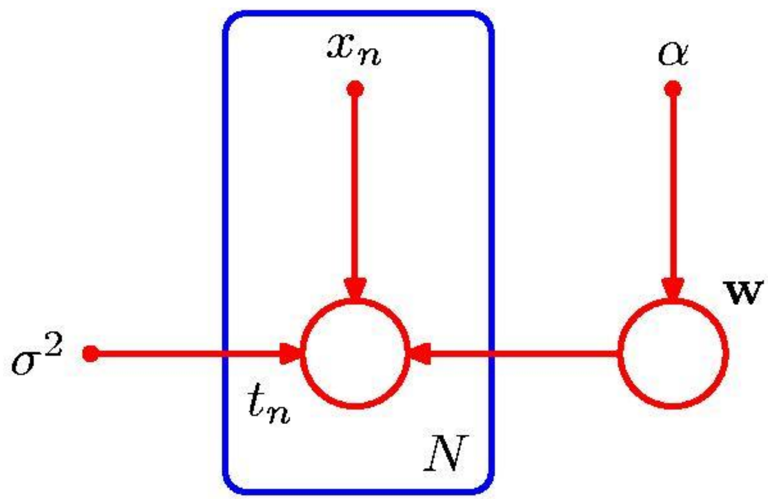




Bayesian Curve Fitting (3)

Input variables and explicit hyperparameters

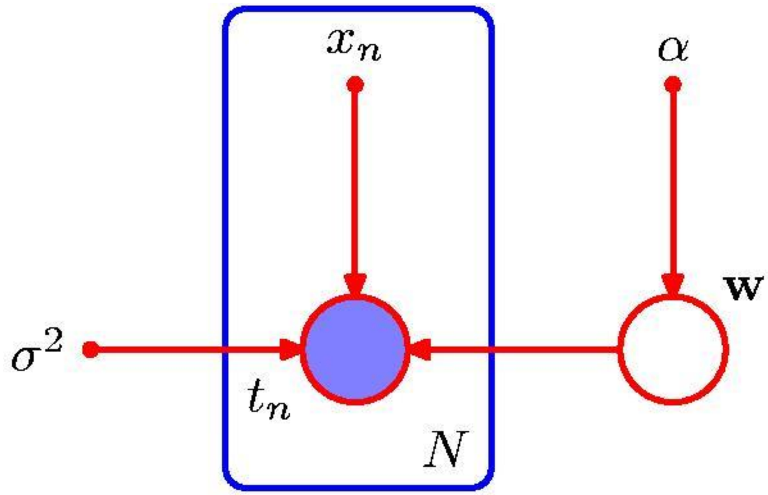
$$p(\mathbf{t}, \mathbf{w}|\mathbf{x}, \alpha, \sigma^2) = p(\mathbf{w}|\alpha) \prod_{n=1}^{N} p(t_n|\mathbf{w}, x_n, \sigma^2).$$



Bayesian Curve Fitting—Learning

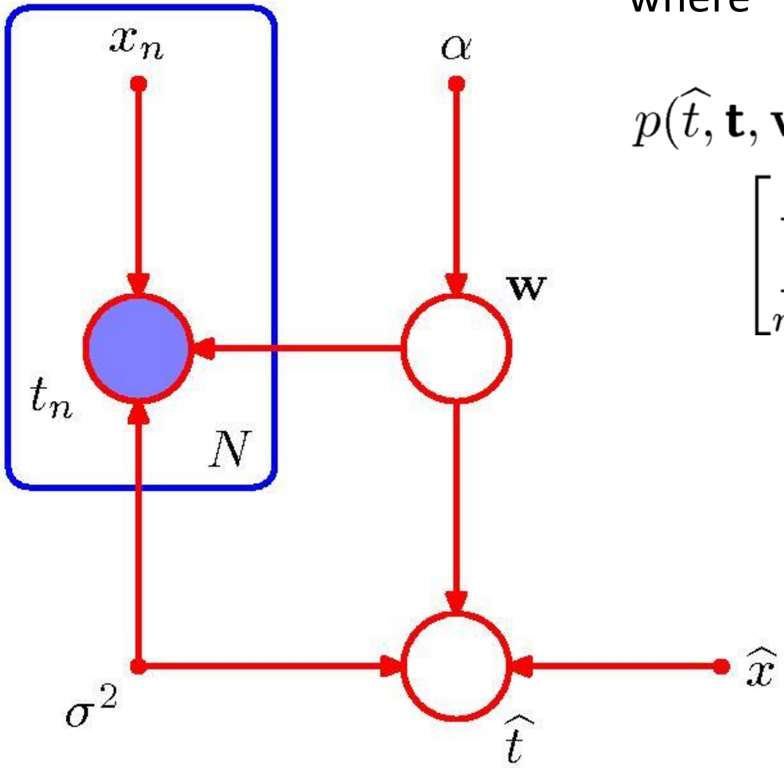
Condition on data

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



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

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

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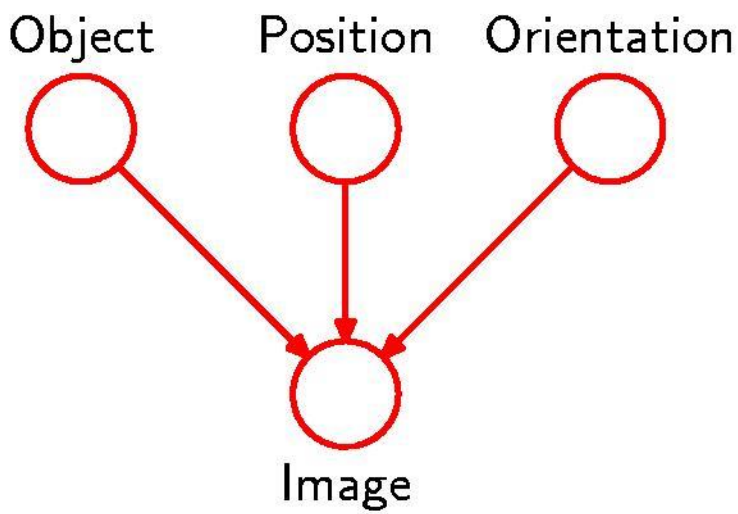
Generative Models

- Causal process for generating images



Discrete Variables (1)

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

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

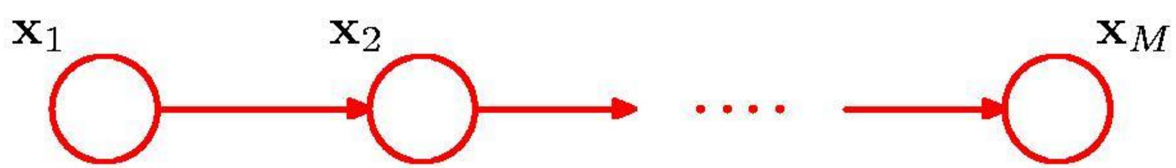
- Independent joint distribution: $2(K-1)$ parameters

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

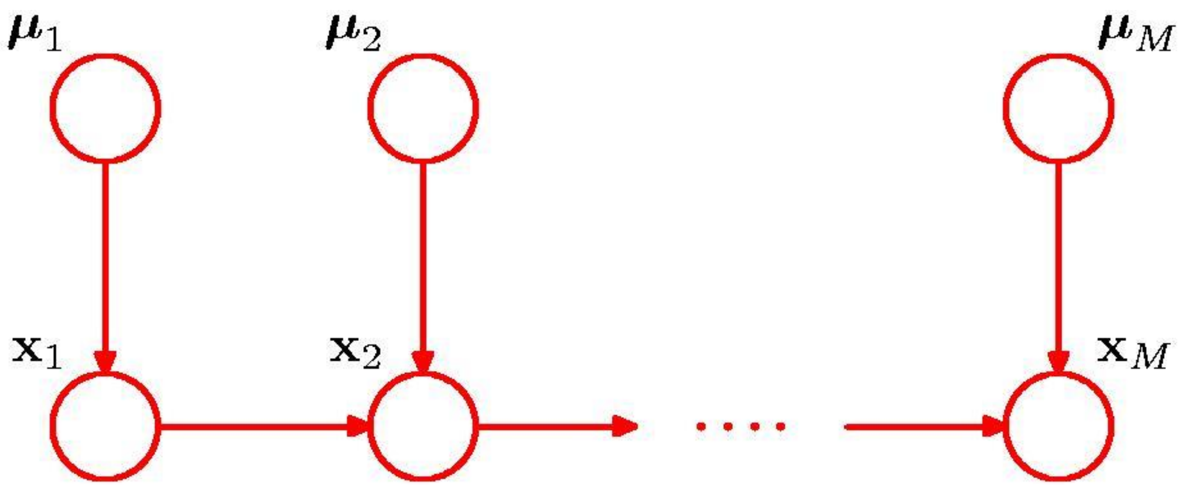
Discrete Variables (2)

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

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



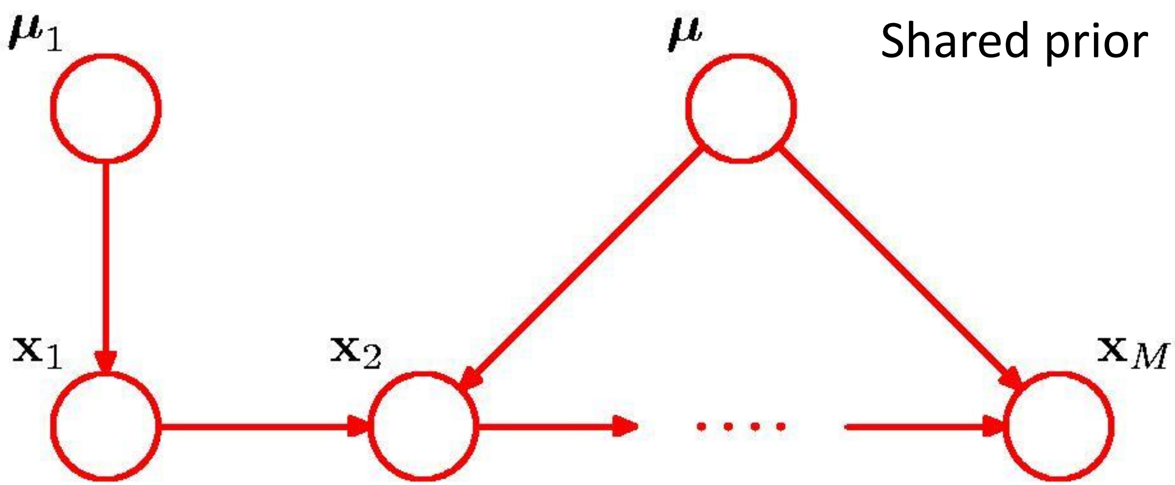
Discrete Variables: Bayesian Parameters (1)



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

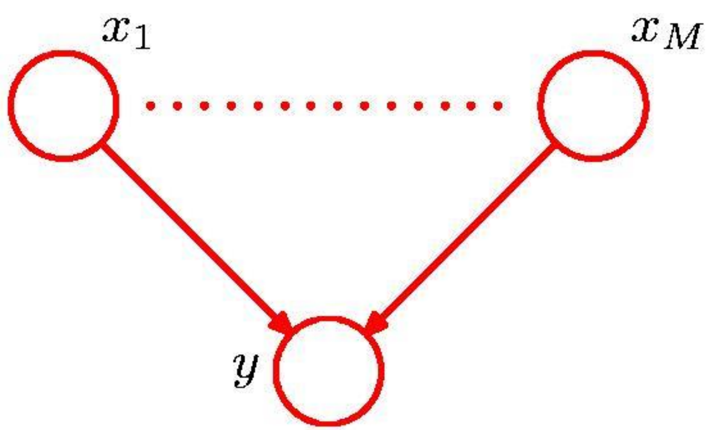
$$p(\boldsymbol{\mu}_m) = \mathrm{Dir}(\boldsymbol{\mu}_m | \boldsymbol{\alpha}_m)$$

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.

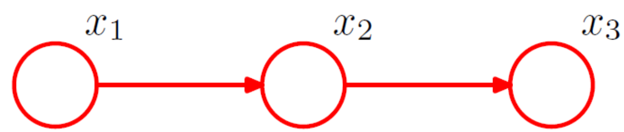
The parameterized form

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

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

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

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Conditional Independence

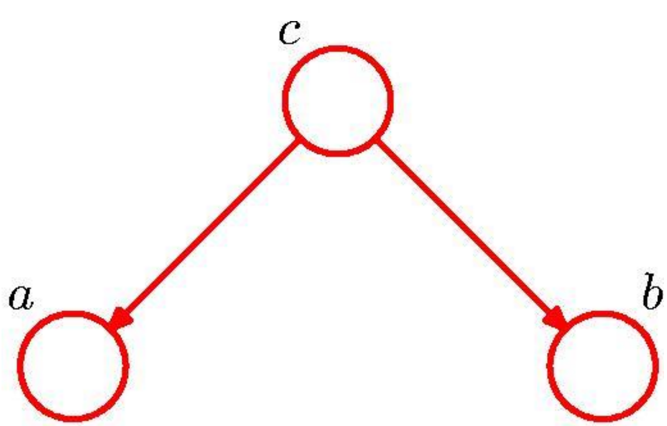
a is independent of b given c

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

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

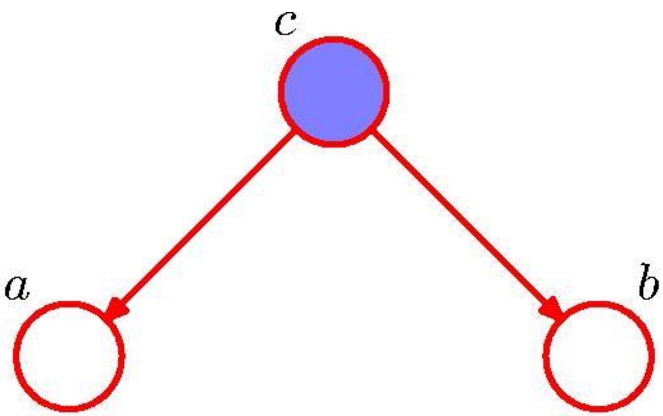


$$p(a, b, c) = p(a|c)p(b|c)p(c)$$

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

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

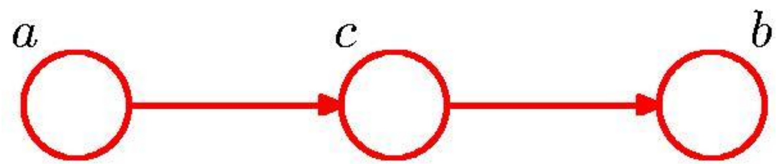
Conditional Independence: Example 1



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

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

Conditional Independence: Example 2

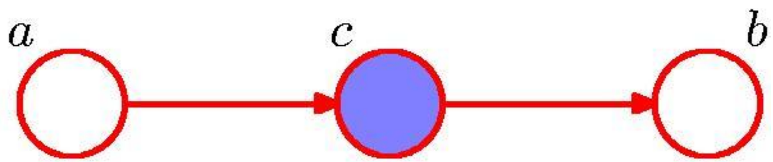


$$p(a, b, c) = p(a)p(c|a)p(b|c)$$

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

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

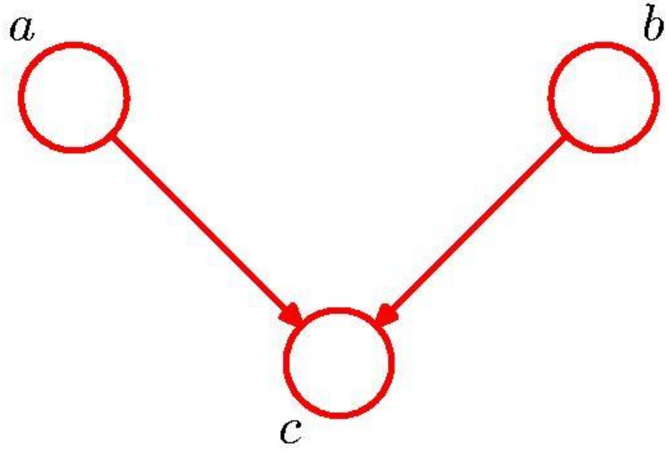
Conditional Independence: Example 2



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

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

Conditional Independence: Example 3



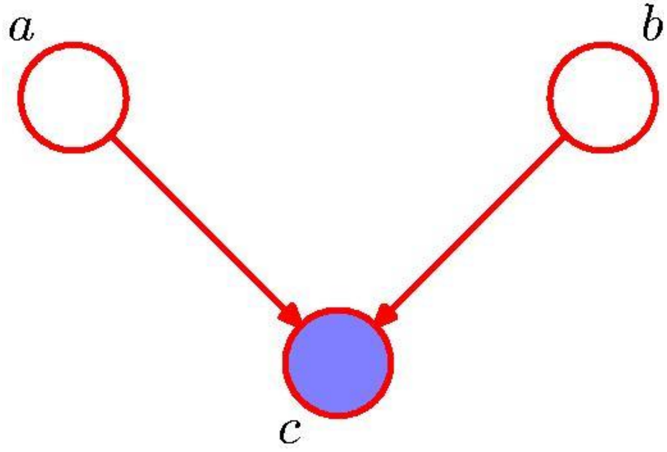
$$p(a, b, c) = p(a)p(b)p(c|a, b)$$

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

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

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

Conditional Independence: Example 3



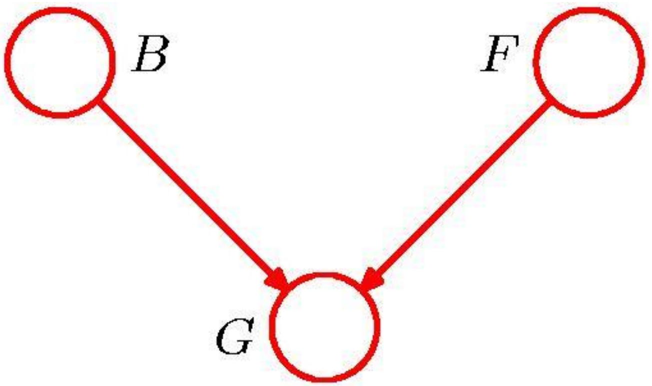
$$
\begin{aligned}
p(a, b|c) &= \frac{p(a, b, c)}{p(c)} \\
&= \frac{p(a)p(b)p(c|a, b)}{p(c)}
\end{aligned}
$$

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

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

“Am I out of fuel?”

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



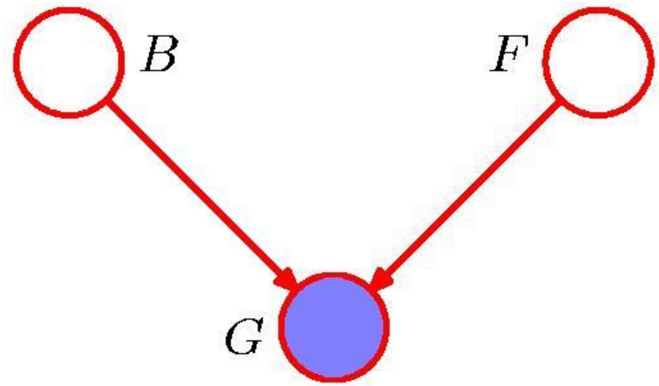
$$
\begin{aligned}
p(B=1) &= 0.9 \\
p(F=1) &= 0.9
\end{aligned}
$$

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)

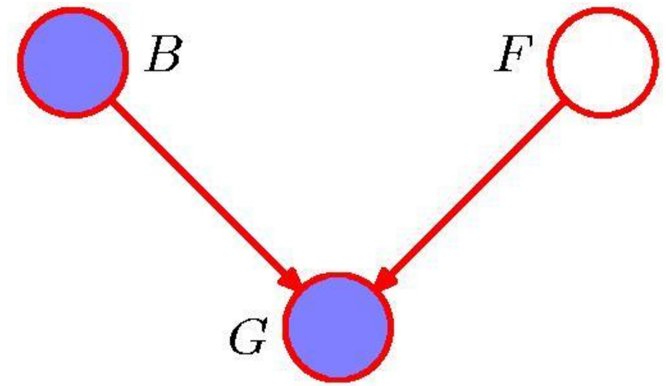
“Am I out of fuel?”



$$
\begin{aligned}
p(F=0|G=0) &= \frac{p(G=0|F=0)p(F=0)}{p(G=0)} \\
&\simeq 0.257
\end{aligned}
$$

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

“Am I out of fuel?”



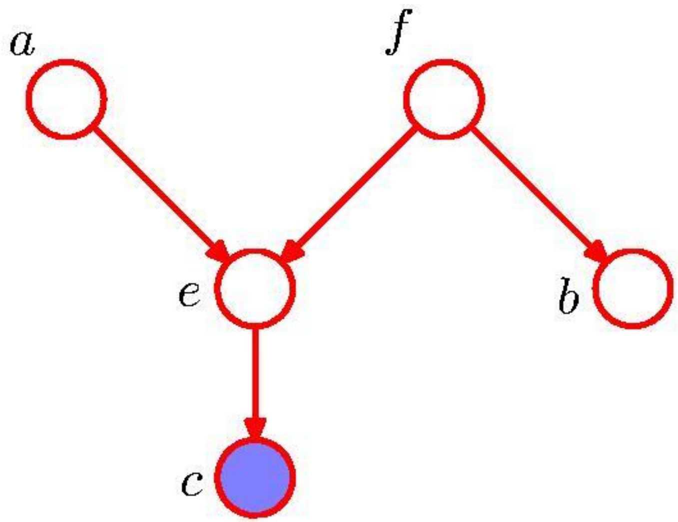
$$
\begin{aligned}
p(F=0|G=0,B=0) &= \frac{p(G=0|B=0,F=0)p(F=0)}{\sum_{F\in\{0,1\}} p(G=0|B=0,F)p(F)} \\
&\simeq 0.111
\end{aligned}
$$

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

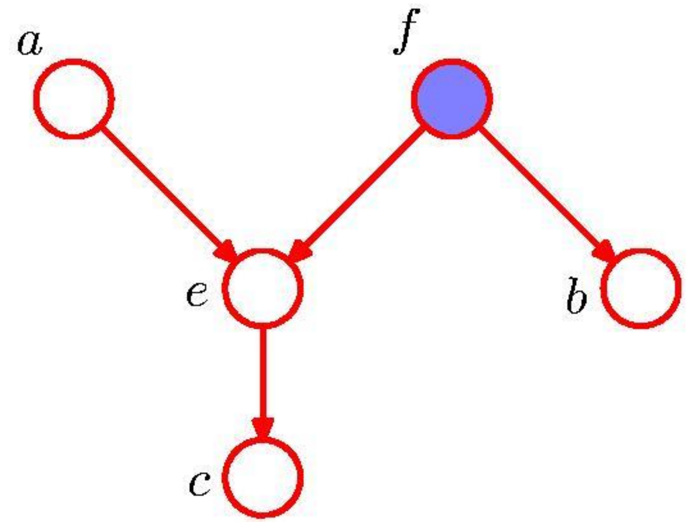
D-separation

- 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
  - ✓ 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
  - ✓ 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

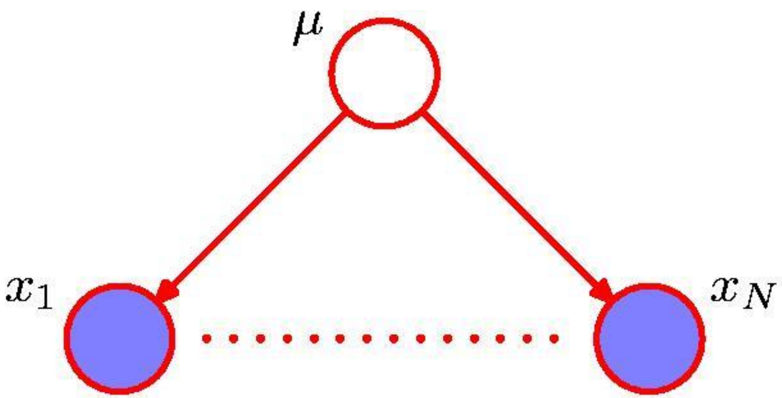


$a \not\perp\!\!\!\perp b \mid c$



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

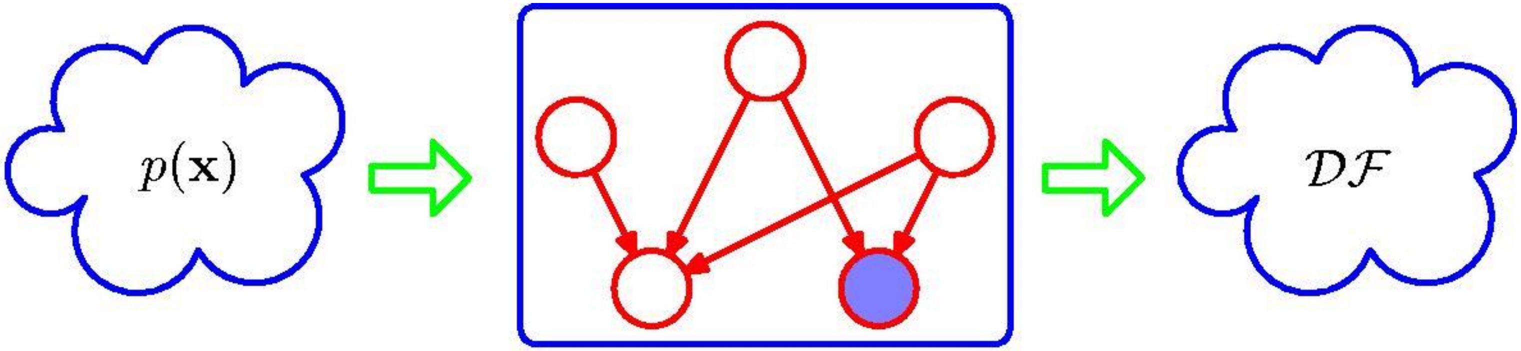
D-separation: I.I.D. Data



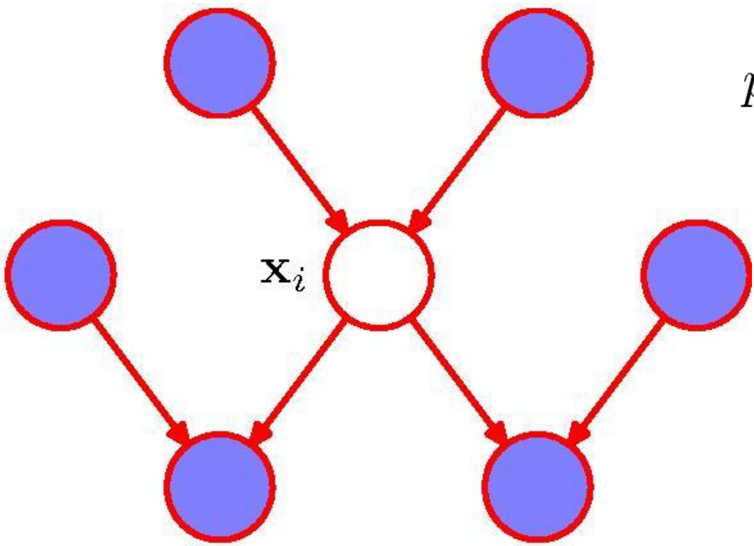
$$p(\mathcal{D}|\mu) = \prod_{n=1}^{N} p(x_n|\mu)$$

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

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.

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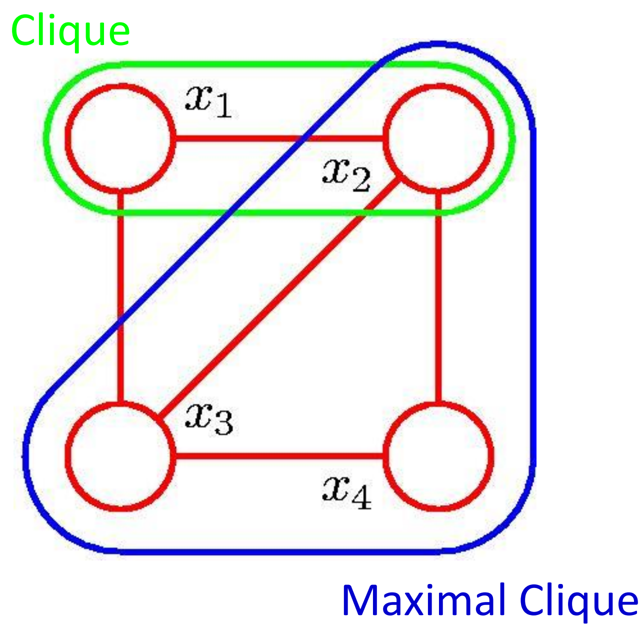
Cliques and Maximal Cliques



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

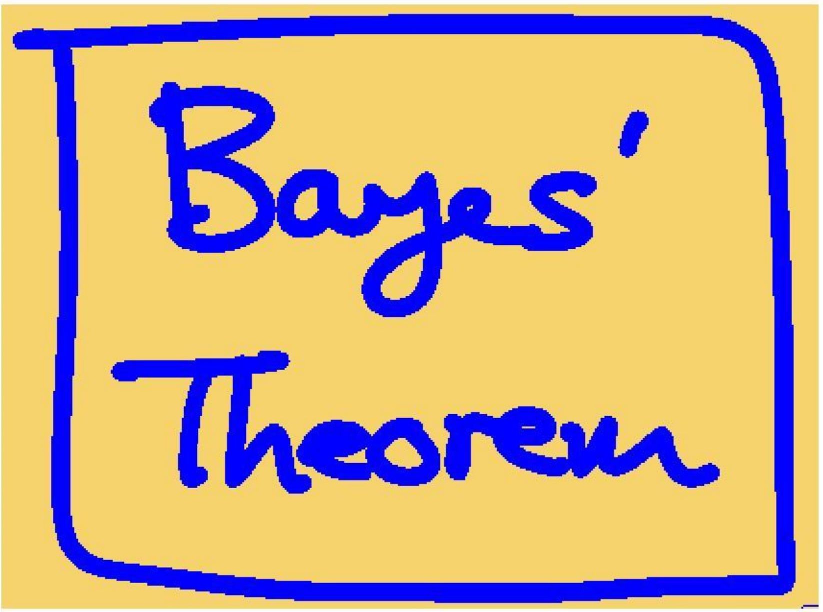
$$Z = \sum_{\mathbf{x}} \prod_C \psi_C(\mathbf{x}_C)$$

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

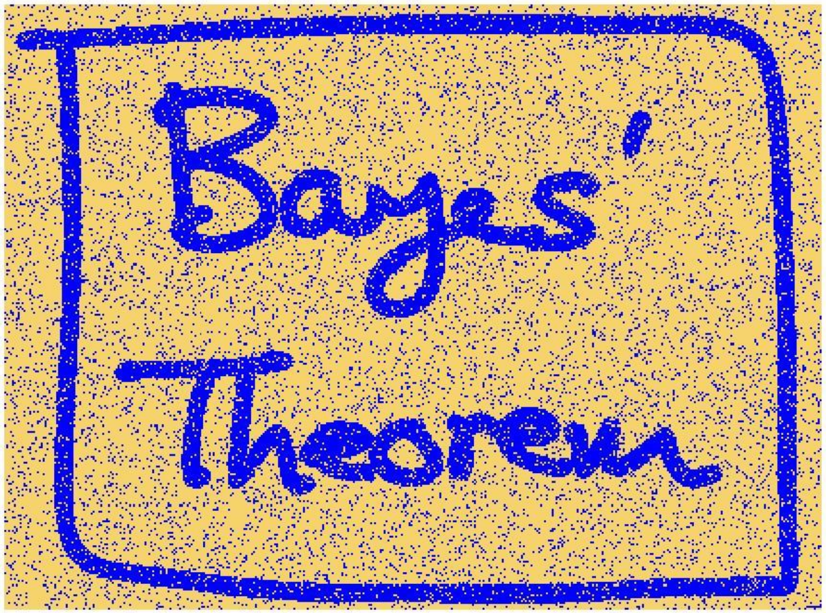
Energies and the Boltzmann distribution

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

Illustration: Image De-Noising (1)

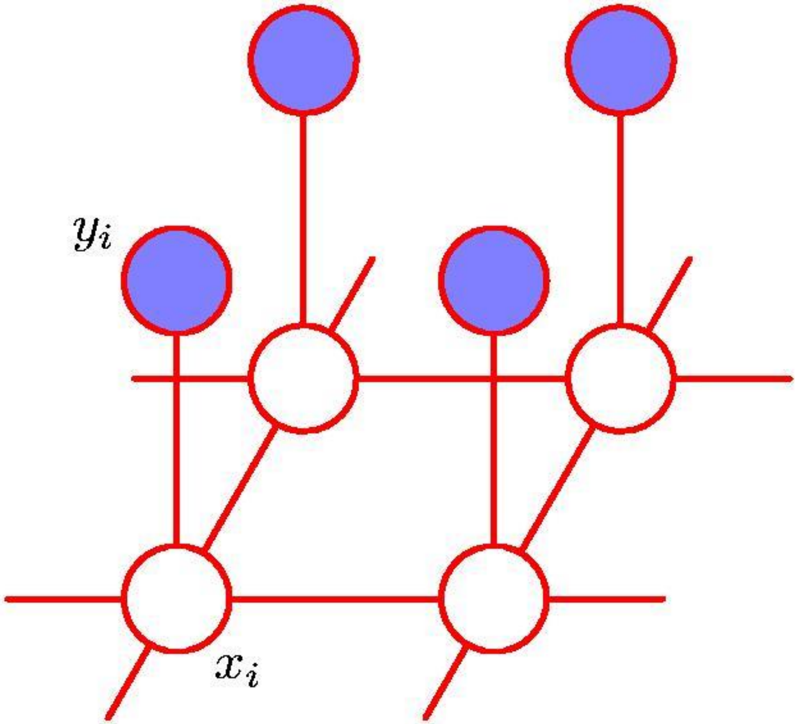


Original Image



Noisy Image

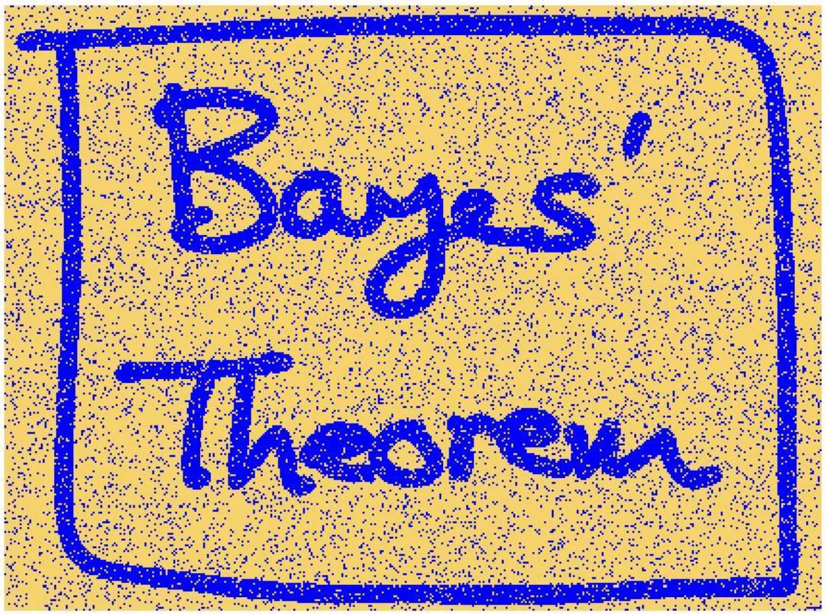
Illustration: Image De-Noising (2)



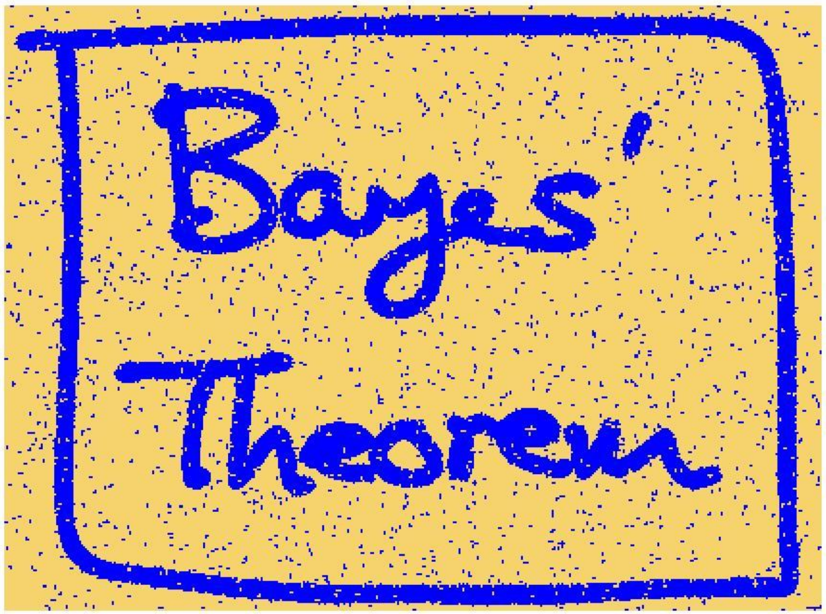
$$E(\mathbf{x},\mathbf{y}) = h\sum_i x_i - \beta\sum_{\{i,j\}} x_i x_j - \eta\sum_i x_i y_i$$

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

Illustration: Image De-Noising (3)

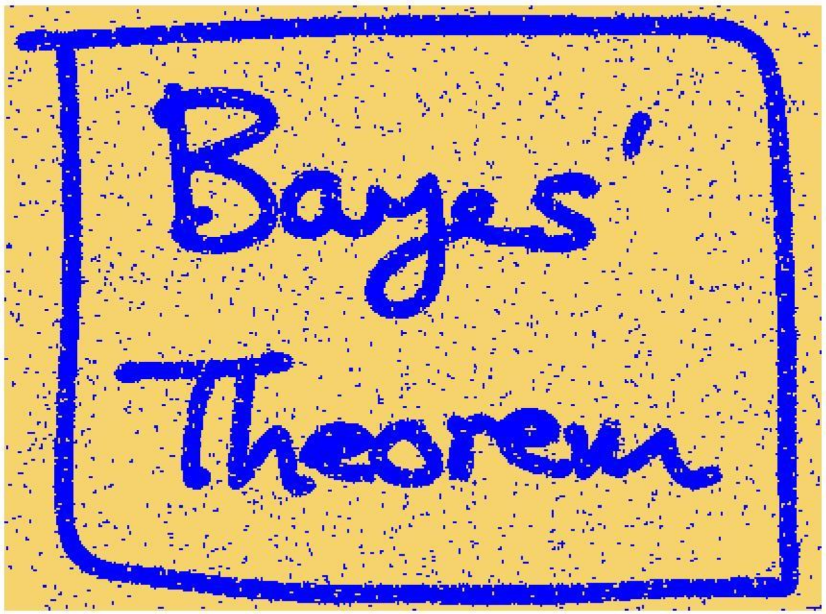


Noisy Image

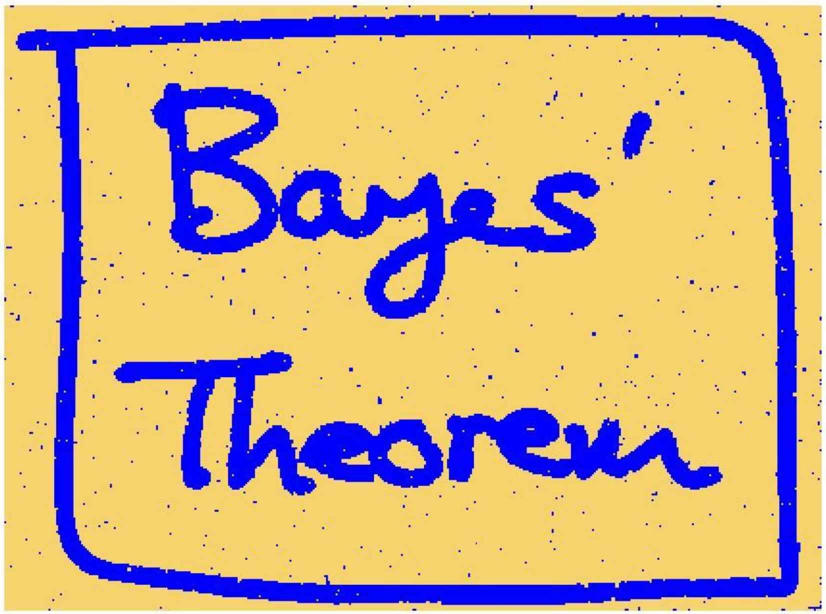


Restored Image (ICM)

Illustration: Image De-Noising (4)

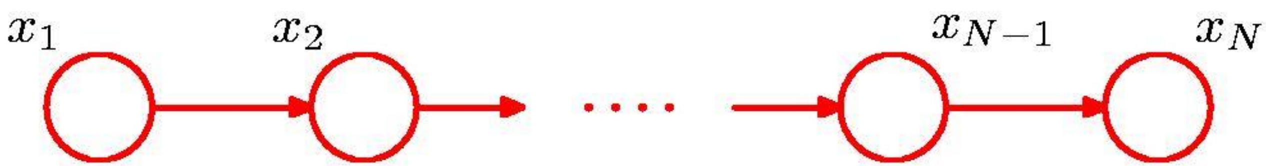


Restored Image (ICM)



Restored Image (Graph cuts)

Converting Directed to Undirected Graphs (1)

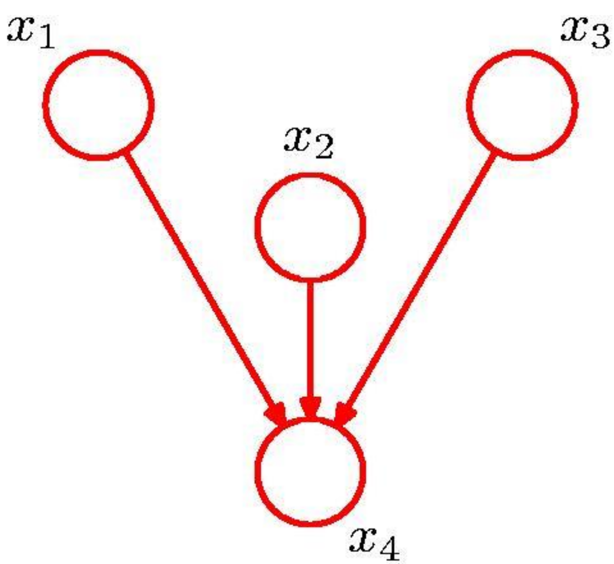


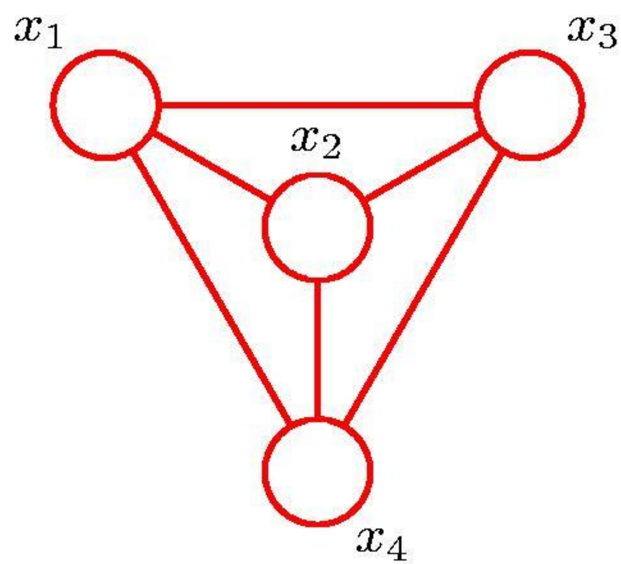
$$p(\mathbf{x}) = \underbrace{p(x_1)p(x_2|x_1)}\, p(x_3|x_2) \cdots p(x_N|x_{N-1})$$

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

Converting Directed to Undirected Graphs (2)

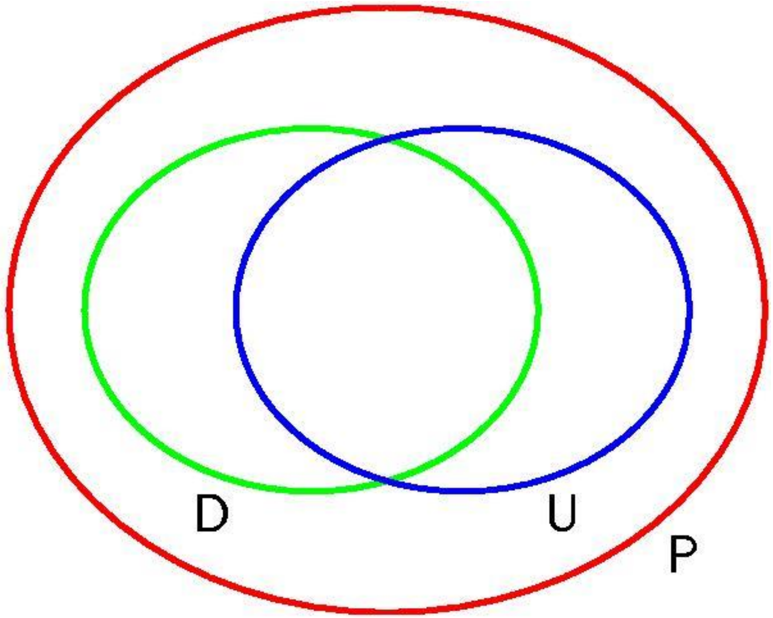
Additional links



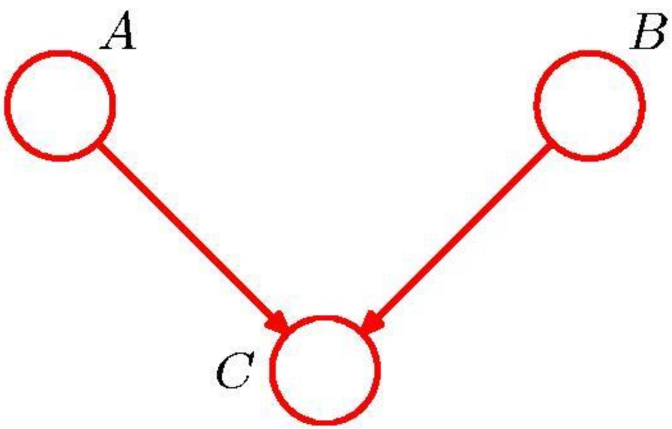


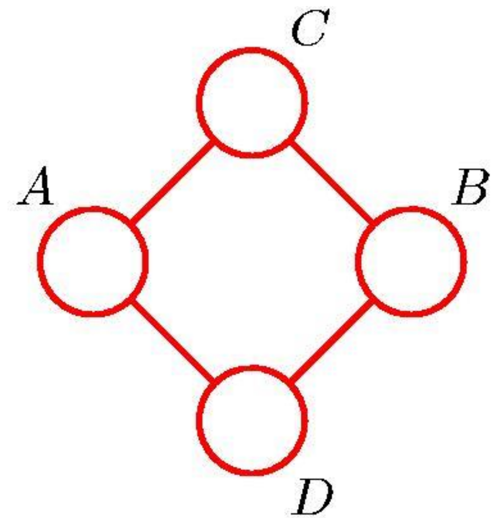
$$
\begin{aligned}
p(\mathbf{x}) &= p(x_1)p(x_2)p(x_3)p(x_4|x_1, x_2, x_3) \\
&= \frac{1}{Z}\psi_A(x_1, x_2, x_3)\psi_B(x_2, x_3, x_4)\psi_C(x_1, x_2, x_4)
\end{aligned}
$$

Directed vs. Undirected Graphs (1)



Directed vs. Undirected Graphs (2)





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

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

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

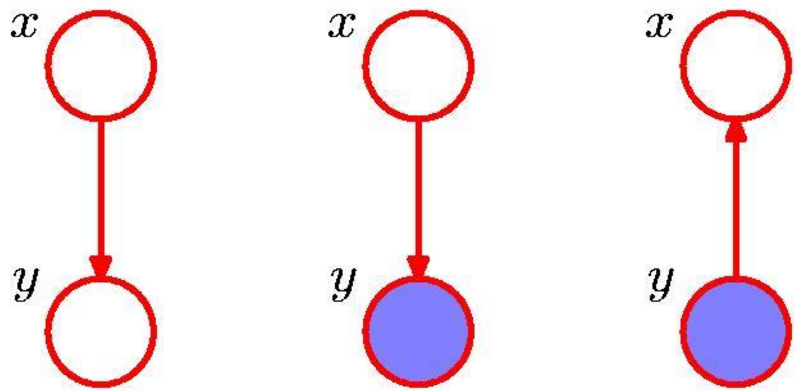
$$A \perp\!\!\!\perp B \mid C \cup D$$

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

Outlines

- Bayesian Networks
- Bayesian Curve Fitting
- Discrete Variables and Linear Gaussian Models
- Conditional Independence
- Markov Random Fields
- Inference in Graphical Models

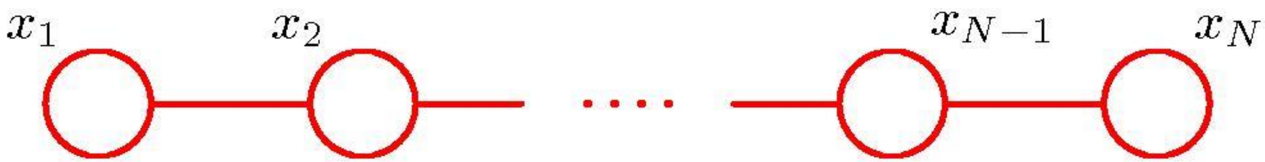
Inference in Graphical Models



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

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

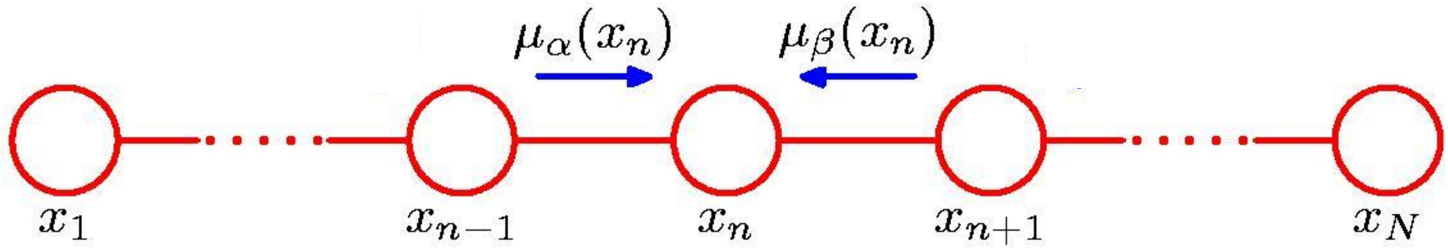
Inference on a Chain



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

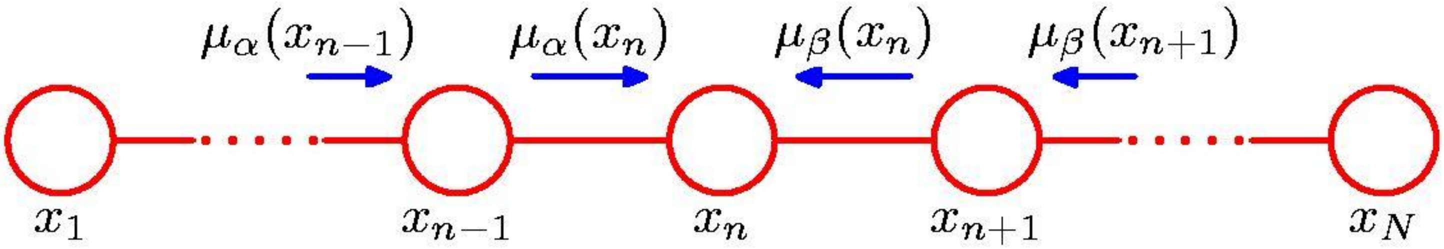
$$p(x_n) = \sum_{x_1}\cdots\sum_{x_{n-1}}\sum_{x_{n+1}}\cdots\sum_{x_N} p(\mathbf{x})$$

Inference on a Chain



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

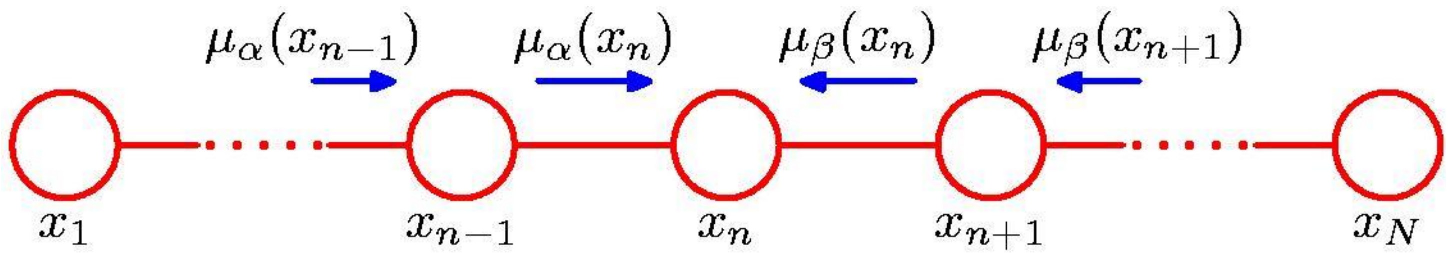
Inference on a Chain



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

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

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

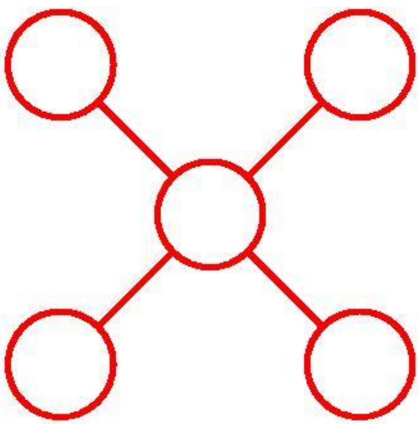
- To compute local marginals:
  - ✓ Compute and store all forward messages, $\mu_\alpha(x_n)$
  - ✓ Compute and store all backward messages, $\mu_\beta(x_n)$
  - ✓ Compute Z at any node x_m
  - ✓ Compute

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

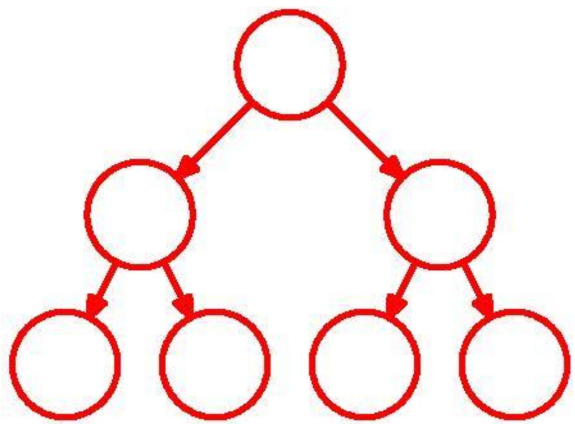
for all variables required.

Trees

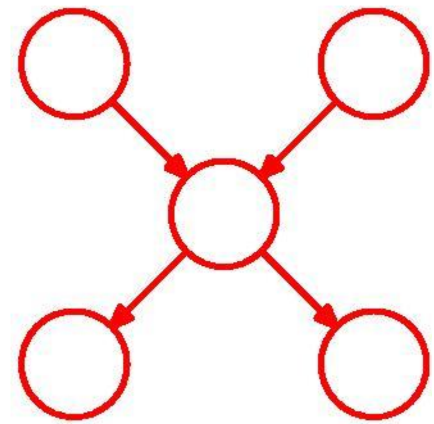
Undirected Tree



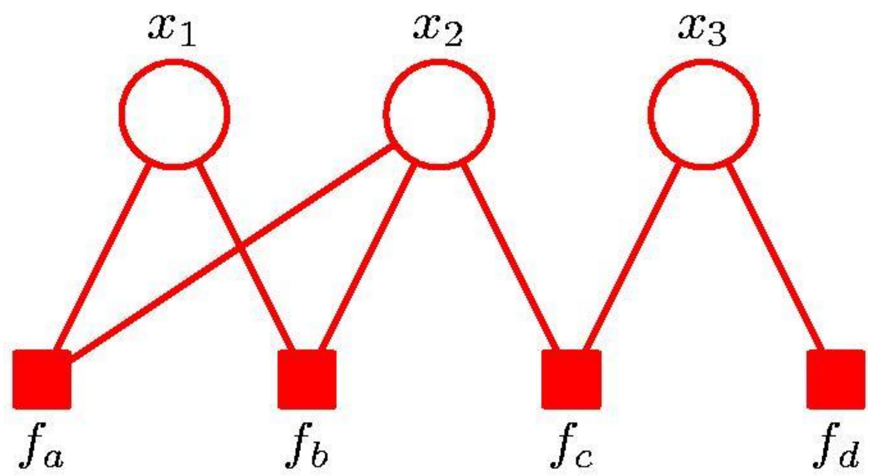
Directed Tree



Polytree



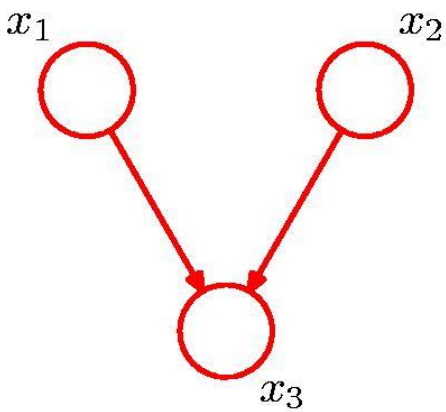
Factor Graphs

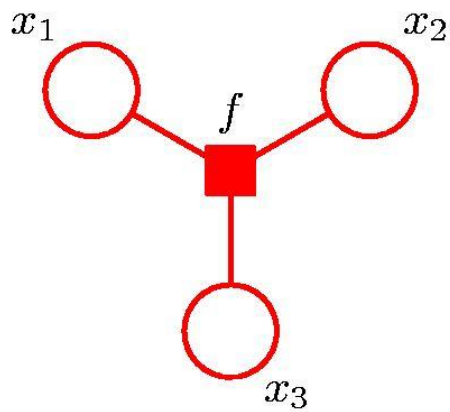


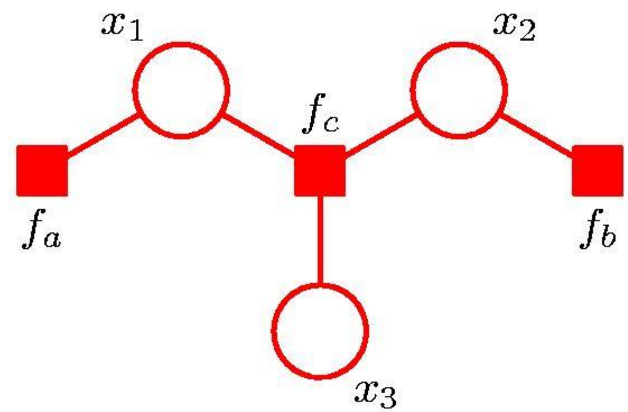
$$p(\mathbf{x}) = f_a(x_1, x_2) f_b(x_1, x_2) f_c(x_2, x_3) f_d(x_3)$$

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

Factor Graphs from Directed Graphs





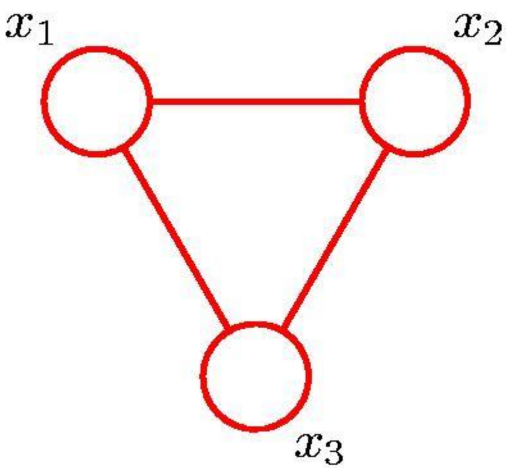


$$p(\mathbf{x}) = p(x_1)p(x_2) \, p(x_3|x_1, x_2)$$

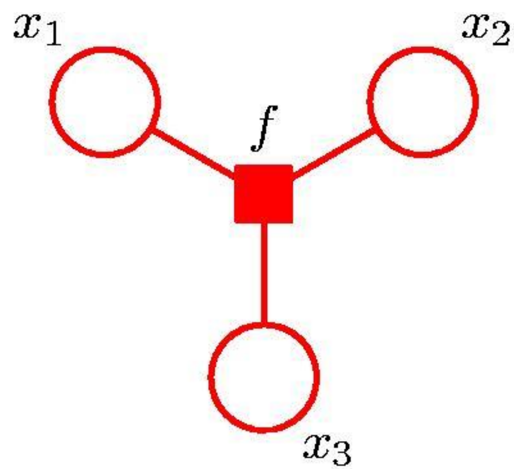
$$f(x_1, x_2, x_3) = p(x_1)p(x_2)p(_3|x_1, x_2)$$

$$\begin{aligned} f_a(x_1) &= p(x_1) \\ f_b(x_2) &= p(x_2) \\ f_c(x_1, x_2, x_3) &= p(x_3|x_1, x_2) \end{aligned}$$

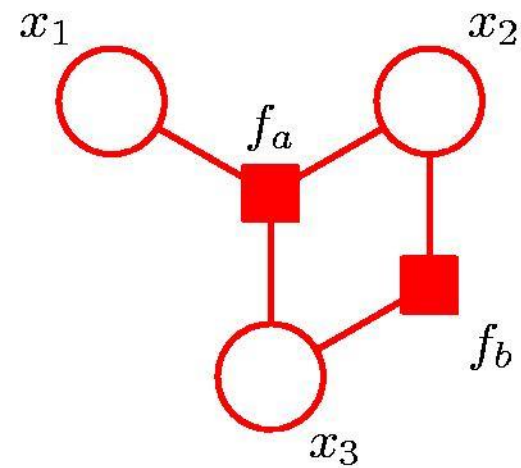
Factor Graphs from Undirected Graphs



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

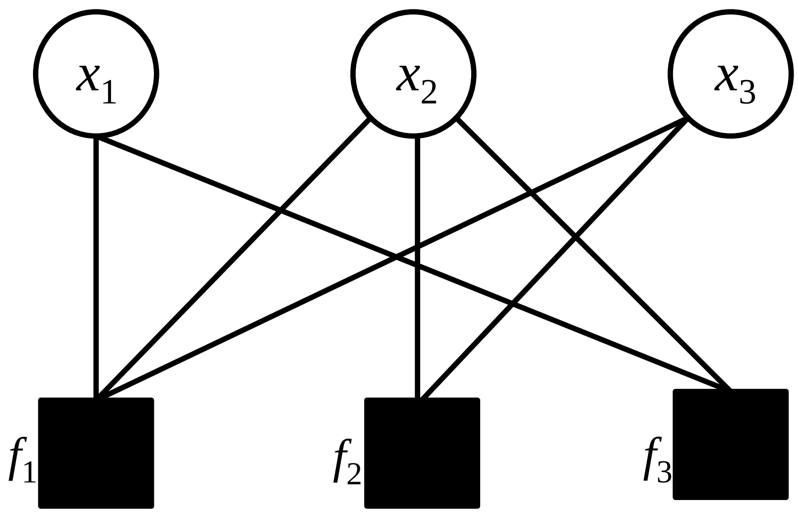


$$\begin{aligned} & f(x_1, x_2, x_3) \\ = \quad & \psi(x_1, x_2, x_3) \end{aligned}$$



$$\begin{aligned} & f_a(x_1, x_2, x_3) f_b(x_2, x_3) \\ = \quad & \psi(x_1, x_2, x_3) \end{aligned}$$

Factor Graph for Solving Equations



$x_1 + 2x_2 + x_3 = 4$ $\quad$ $x_2 + 2x_3 = 3$ $\quad$ $x_1 + x_2 = 2$

(1) $x_1 = 1 \quad x_2 = 1 \quad x_3 = 0$

(2) $f_1 \to x_1$: $x_1 = 4 - 2x_2 - x_3 = 2$

$f_1 \to x_2$: $x_2 = (4 - x_1 - x_3)/2 = 1.5$

$f_1 \to x_3$: $x_3 = 4 - 2x_2 - x_1 = 1$

$f_2 \to x_2$: $x_2 = 3 - 2x_3 = 3$

$f_2 \to x_3$: $x_3 = 3 - 2x_2 = 1$

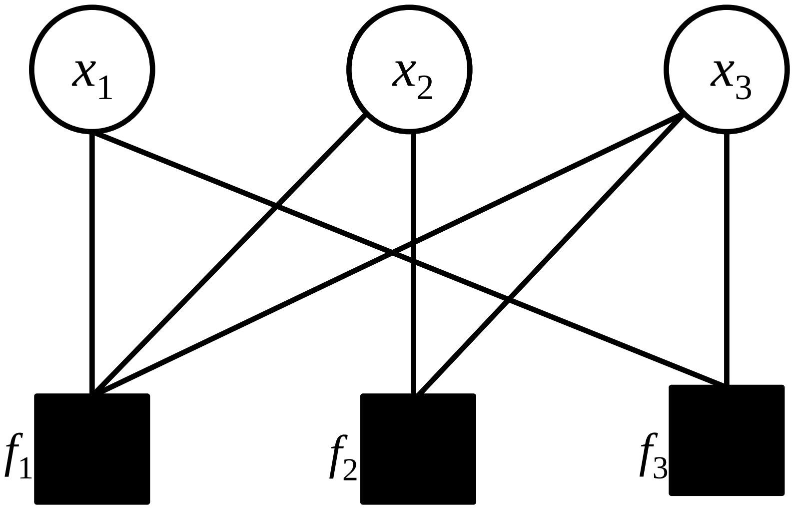
$f_3 \to x_1$: $x_1 = 2 - x_2 = 1$

$f_3 \to x_2$: $x_2 = 2 - x_1 = 1$

(3) $x_1 = (1+2+1)/3 = 4/3 \quad x_2 = (1+1.5+3+1)/4 = 6.5/4 \quad x_3 = (0+1+1)/3 = 2/3$

Factor Graph for Computing Means

$S_i = x_i N_\mathrm{i}$ (1) $S_1 = 11$ $N_1 = 10$ $S_2 = 10$ $N_2 = 10$ $S_3 = 18$ $N_3 = 20$



$\mathrm{x}_1 = x_2 = x_3$ $x_2 = x_3$ $x_1 = x_3$

(2) $f_1 \to x_1$: $S_1 = 28$ $N_1 = 30$

$f_1 \to x_2$: $S_2 = 29$ $N_2 = 30$

$f_1 \to x_3$: $S_3 = 21$ $N_3 = 20$

$f_2 \to x_2$: $S_2 = 18$ $N_2 = 20$

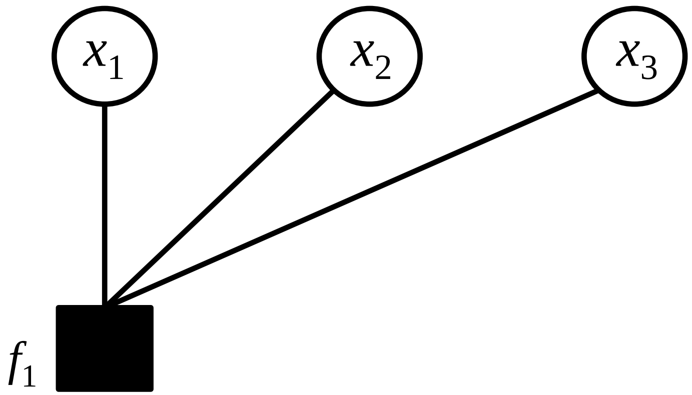
$f_2 \to x_3$: $S_3 = 10$ $N_3 = 10$

$f_3 \to x_1$: $\mathrm{S}_1 = 18$ $N_1 = 20$

$f_3 \to x_3$: $\mathrm{S}_3 = 11$ $N_3 = 10$

(3) $S_1 = 57$ $N_1 = 60$ $S_2 = 57$ $N_2 = 60$ $S_3 = 60$ $N_3 = 60$

Factor Graph for Belief Aggregation



$x_1 = x_2 = x_3$

(1) $x_1 \sim \mathcal{N}(m_1, \Sigma_1)$ $\quad x_2 \sim \mathcal{N}(m_2, \Sigma_2)$

$x_3 \sim \mathcal{N}(m_3, \Sigma_3)$

(2) $f_1 \rightarrow x_1$:

$$\hat{\Sigma}_1^{-1} = \Sigma_2^{-1} + \Sigma_3^{-1} \quad \hat{\Sigma}_1^{-1}\hat{m}_1 = \Sigma_2^{-1}m_2 + \Sigma_3^{-1}m_3$$

$f_1 \rightarrow x_2$:

$$\hat{\Sigma}_2^{-1} = \Sigma_1^{-1} + \Sigma_3^{-1} \quad \hat{\Sigma}_2^{-1}\hat{m}_2 = \Sigma_1^{-1}m_1 + \Sigma_3^{-1}m_3$$

$f_1 \rightarrow x_3$:

$$\hat{\Sigma}_3^{-1} = \Sigma_1^{-1} + \Sigma_3^{-1} \quad \hat{\Sigma}_2^{-1}\hat{m}_2 = \Sigma_1^{-1}m_1 + \Sigma_3^{-1}m_3$$

(3)

$$\bar{\Sigma}_1^{-1} = \Sigma_1^{-1} + \hat{\Sigma}_1^{-1} \quad \bar{\Sigma}_1^{-1}\bar{m}_1 = \Sigma_1^{-1}m_1 + \hat{\Sigma}_1^{-1}\hat{m}_1$$

$$\bar{\Sigma}_2^{-1} = \Sigma_2^{-1} + \hat{\Sigma}_2^{-1} \quad \bar{\Sigma}_2^{-1}\bar{m}_2 = \Sigma_2^{-1}m_2 + \hat{\Sigma}_2^{-1}\hat{m}_2$$

$$\bar{\Sigma}_3^{-1} = \Sigma_3^{-1} + \hat{\Sigma}_3^{-1} \quad \bar{\Sigma}_3^{-1}\bar{m}_3 = \Sigma_3^{-1}m_3 + \hat{\Sigma}_3^{-1}\hat{m}_3$$

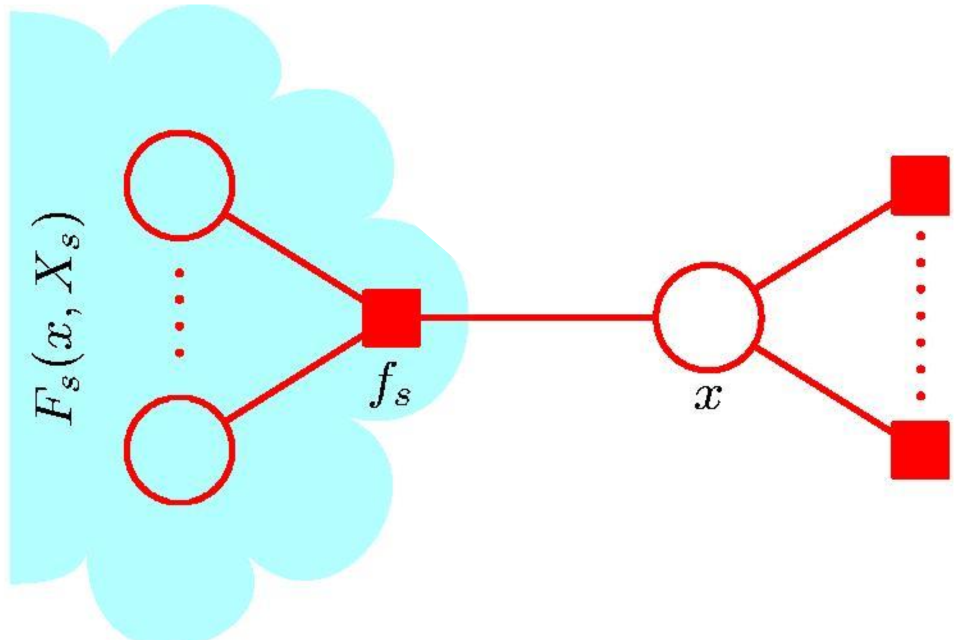
The Sum-Product Algorithm (1)

- 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

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

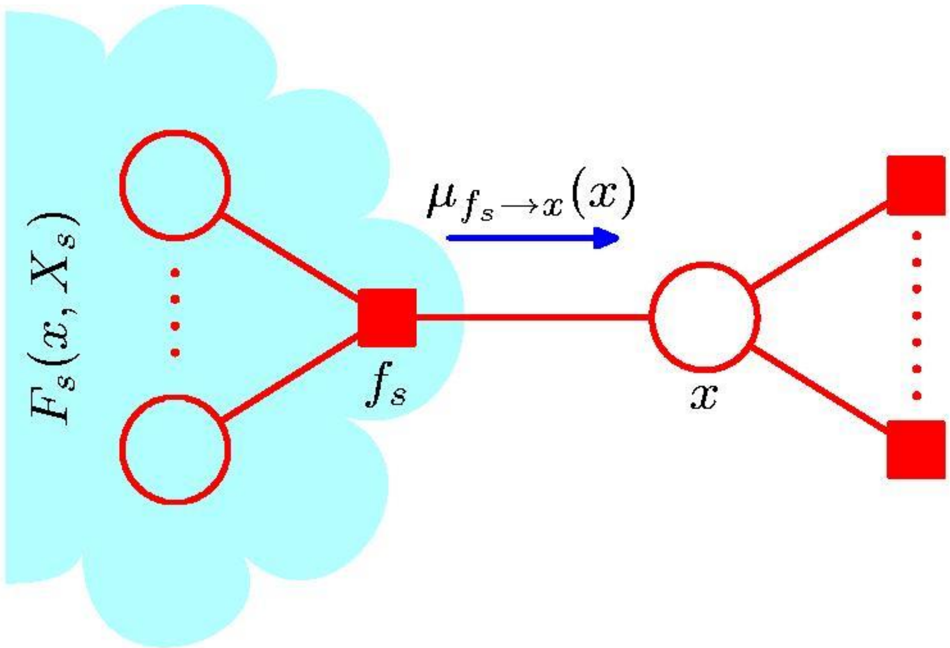
The Sum-Product Algorithm (2)



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

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

The Sum-Product Algorithm (3)

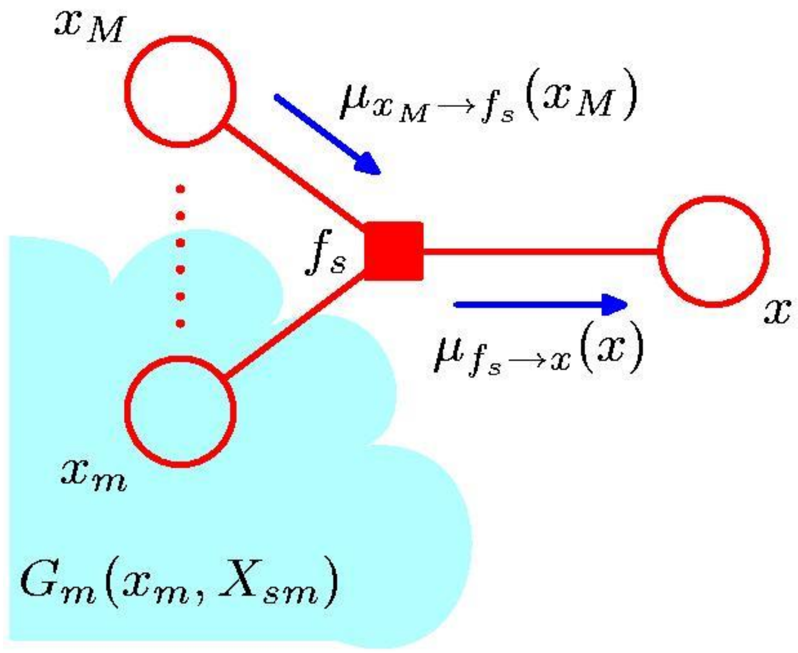


$$p(x) = \prod_{s \in \mathrm{ne}(x)} \left[\sum_{X_s} F_s(x, X_s) \right]$$

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

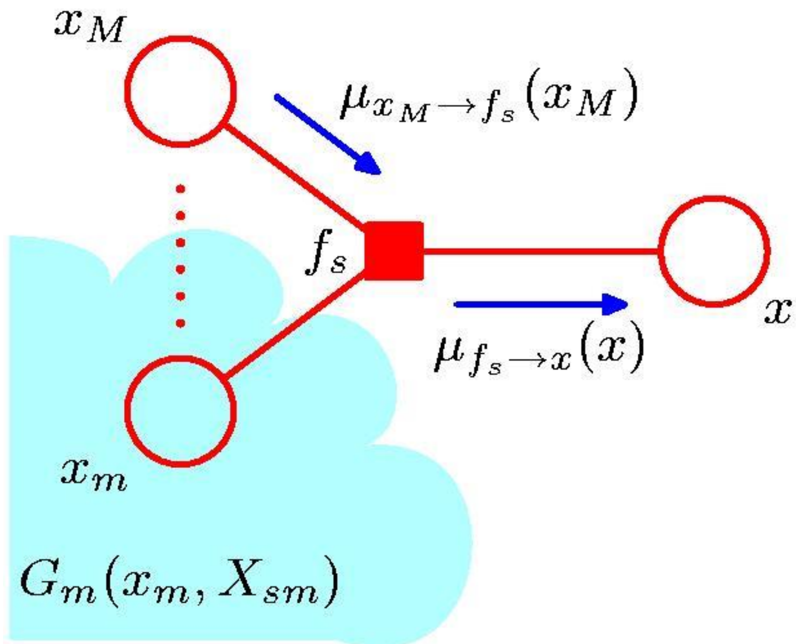
$$\mu_{f_s \to x}(x) \equiv \sum_{X_s} F_s(x, X_s)$$

The Sum-Product Algorithm (4)



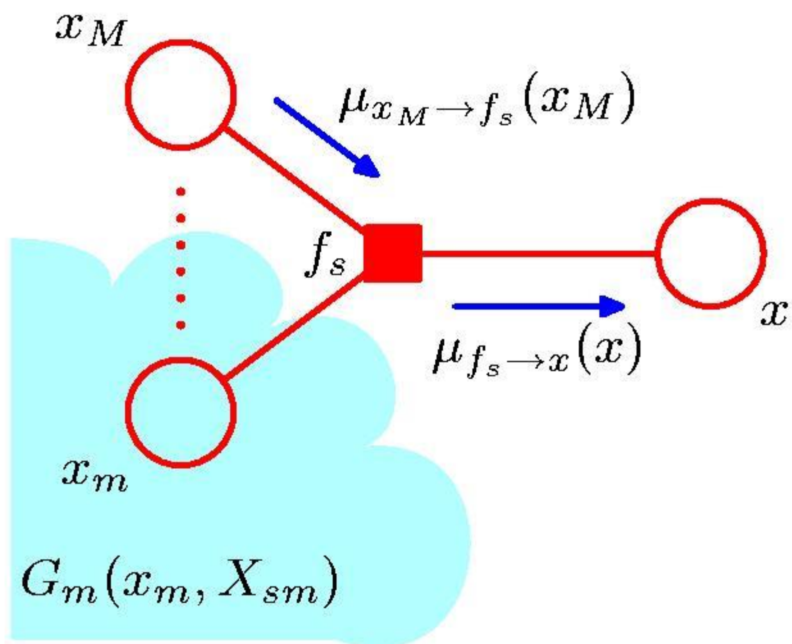
$$F_s(x, X_s) = f_s(x, x_1, \ldots, x_M) G_1(x_1, X_{s1}) \ldots G_M(x_M, X_{sM})$$

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)

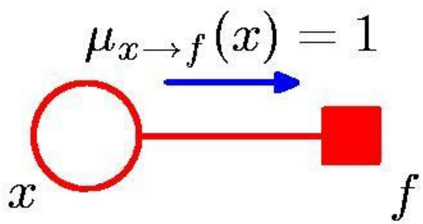


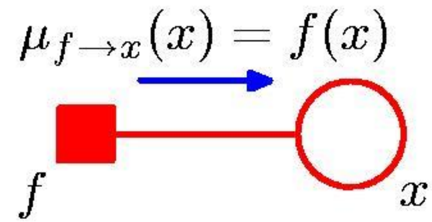
$$\mu_{x_m \to f_s}(x_m) \equiv \sum_{X_{sm}} G_m(x_m, X_{sm}) = \sum_{X_{sm}} \prod_{l \in \mathrm{ne}(x_m) \setminus f_s} F_l(x_m, X_{ml})$$

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

The Sum-Product Algorithm (7)

Initialization

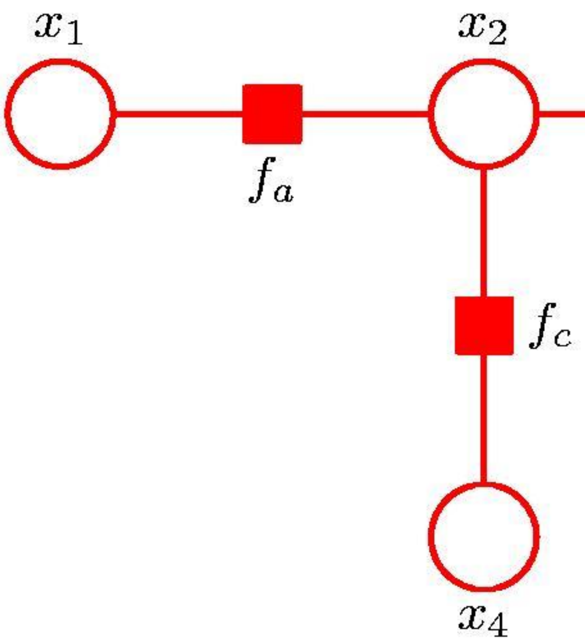




The Sum-Product Algorithm (8)

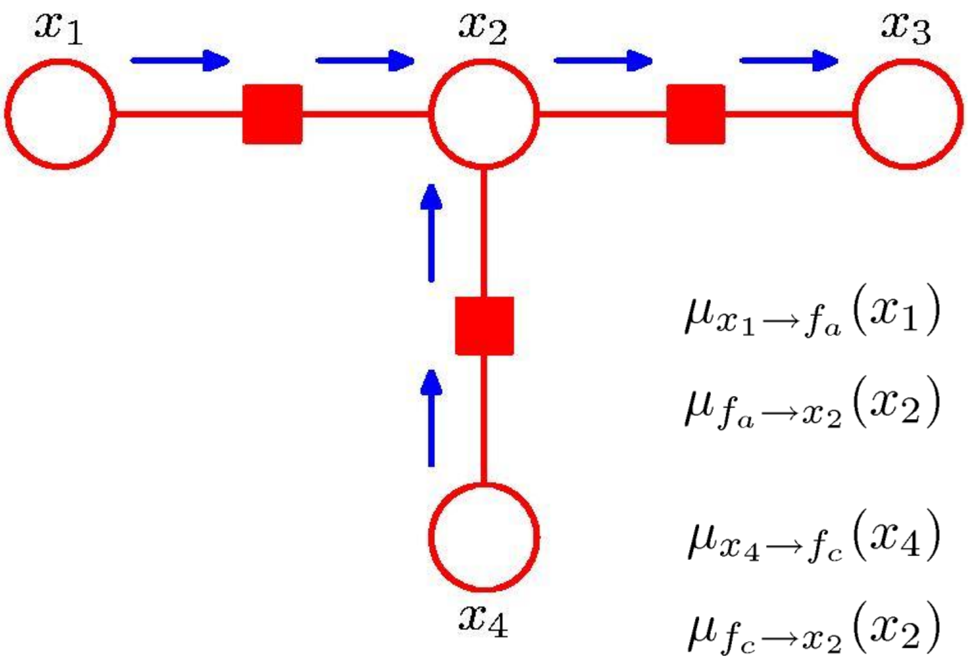
- To compute local marginals:
  - ✓ Pick an arbitrary node as root
  - ✓ Compute and propagate messages from the leaf nodes to the root, storing received messages at every node.
  - ✓ Compute and propagate messages from the root to the leaf nodes, storing received messages at every node.
  - ✓ Compute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

Sum-Product: Example (1)



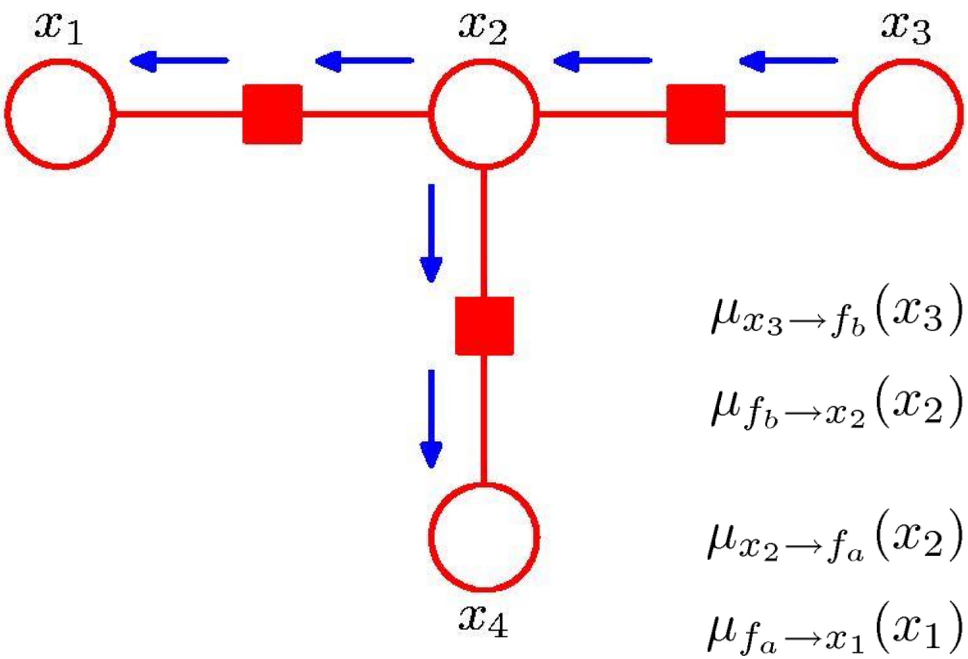
$$\widetilde{p}(\mathbf{x}) = f_a(x_1, x_2) f_b(x_2, x_3) f_c(x_2, x_4)$$

Sum-Product: Example (2)



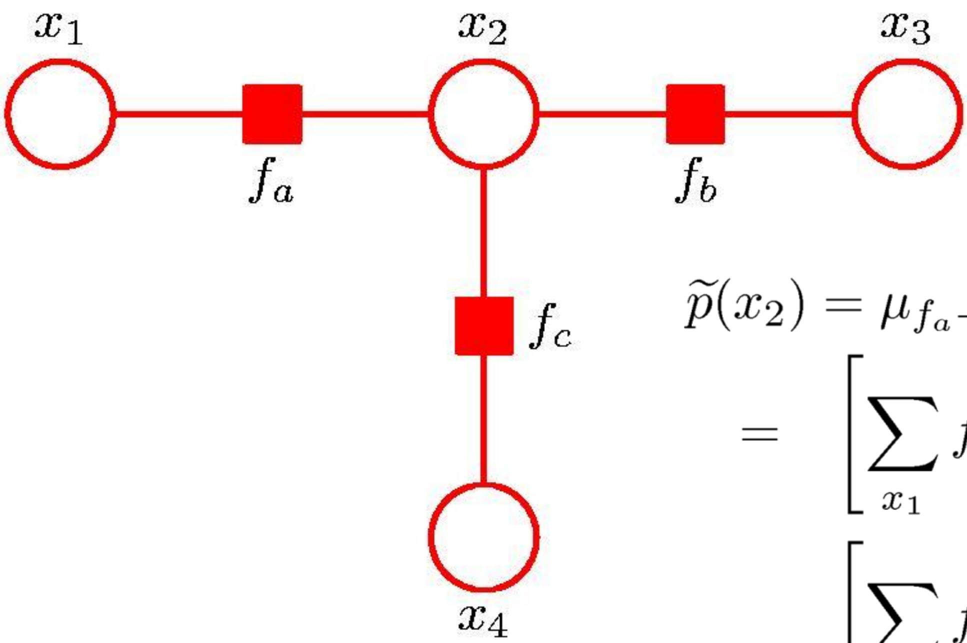
$$
\begin{aligned}
\mu_{x_1 \to f_a}(x_1) &= 1 \\
\mu_{f_a \to x_2}(x_2) &= \sum_{x_1} f_a(x_1, x_2) \\
\mu_{x_4 \to f_c}(x_4) &= 1 \\
\mu_{f_c \to x_2}(x_2) &= \sum_{x_4} f_c(x_2, x_4) \\
\mu_{x_2 \to f_b}(x_2) &= \mu_{f_a \to x_2}(x_2)\mu_{f_c \to x_2}(x_2) \\
\mu_{f_b \to x_3}(x_3) &= \sum_{x_2} f_b(x_2,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

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)



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

$$\begin{aligned} &= \left[\sum_{x_1} f_a(x_1, x_2)\right]\left[\sum_{x_3} f_b(x_2, x_3)\right] \\ &\quad \left[\sum_{x_4} f_c(x_2, x_4)\right] \\ &= \sum_{x_1}\sum_{x_3}\sum_{x_4} f_a(x_1, x_2) f_b(x_2, x_3) f_c(x_2, x_4) \\ &= \sum_{x_1}\sum_{x_3}\sum_{x_4} \widetilde{p}(\mathbf{x}) \end{aligned}$$

The Max-Sum Algorithm (1)

- Objective: an efficient algorithm for finding
  i. the value $\mathbf{x}^{\max}$ that maximizes $p(\mathbf{x})$;
  ii. the value of $p(\mathbf{x}^{\max})$.

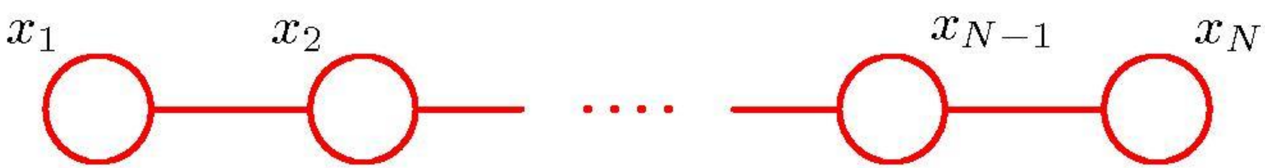
In general, maximum marginals $\neq$ joint maximum.

	$x=0$	$x=1$
$y=0$	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)



$$
\begin{aligned}
p(\mathbf{x}^{\max}) &= \max_{\mathbf{x}} p(\mathbf{x}) = \max_{x_1} \ldots \max_{x_M} p(\mathbf{x}) \\
&= \frac{1}{Z} \max_{x_1} \cdots \max_{x_N} \left[\psi_{1,2}(x_1, x_2) \cdots \psi_{N-1,N}(x_{N-1}, x_N) \right] \\
&= \frac{1}{Z} \max_{x_1} \left[\max_{x_2} \left[\psi_{1,2}(x_1, x_2) \left[\cdots \max_{x_N} \psi_{N-1,N}(x_{N-1}, x_N) \right] \cdots \right] \right]
\end{aligned}
$$

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

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

The Max-Sum Algorithm (6)

- Termination (root node)

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

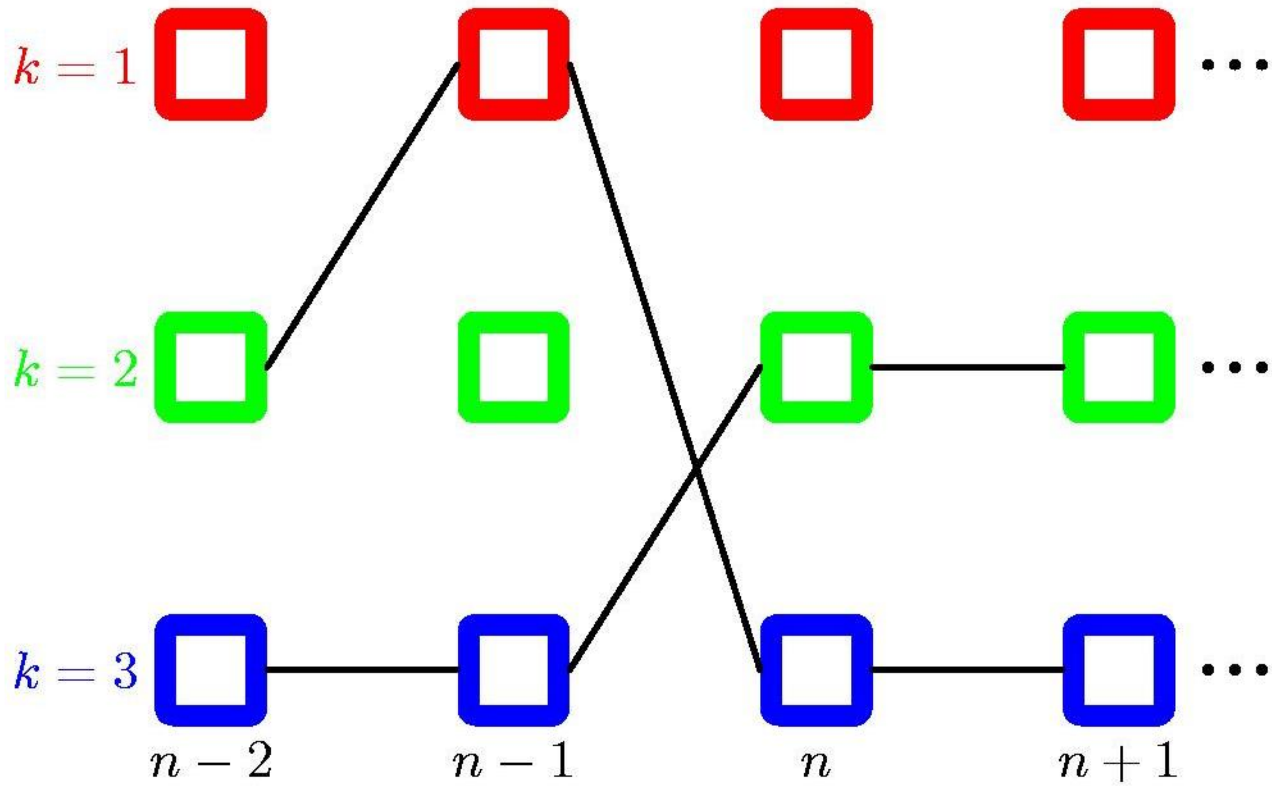
$$x^{\max} = \arg\max_x \left[\sum_{s \in \mathrm{ne}(x)} \mu_{f_s \to x}(x) \right]$$

- 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.

Summary

- Bayesian Networks
- Bayesian Curve Fitting
- Discrete Variables and Linear Gaussian Models
- Conditional Independence
- Markov Random Fields
- Inference in Graphical Models