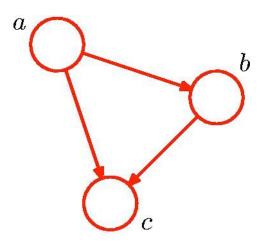
PATTERN RECOGNITION AND MACHINE LEARNING

CHAPTER 8: GRAPHICAL MODELS

Bayesian Networks

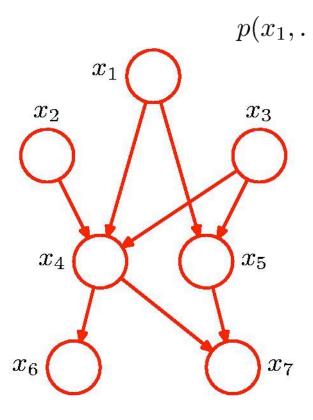
Directed Acyclic Graph (DAG)



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

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

Bayesian Networks



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

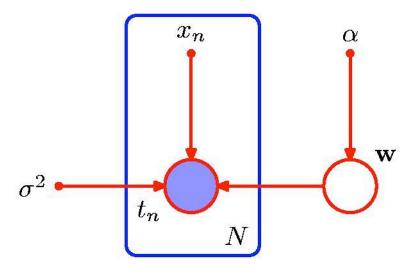
General Factorization

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

Bayesian Curve Fitting—Learning

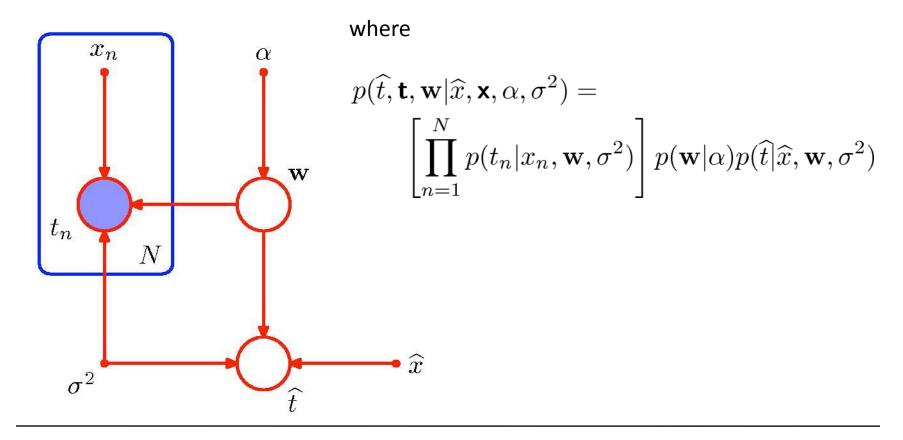
Condition on data

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



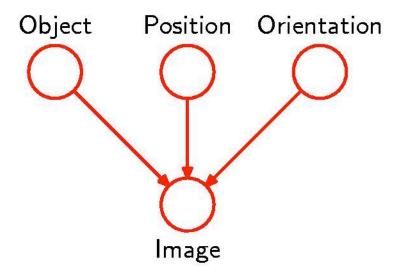
Bayesian Curve Fitting—Prediction

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



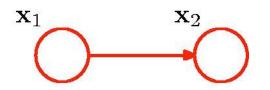
Generative Models

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

$$\mathbf{x}_1$$

$$\sum_{i=1}^{n} x_{i}$$

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

Discrete Variables (2)

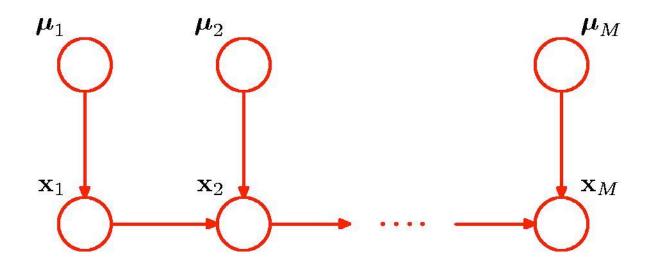
General joint distribution over M variables:

 K^M-1 parameters

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



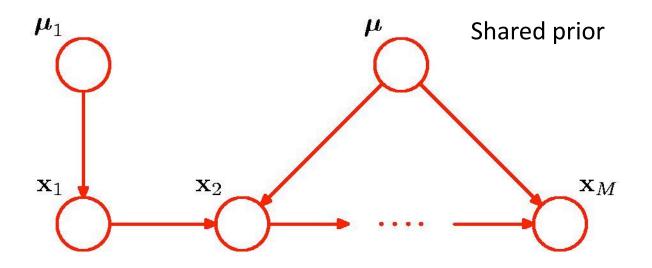
Discrete Variables: Bayesian Parameters (1)



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

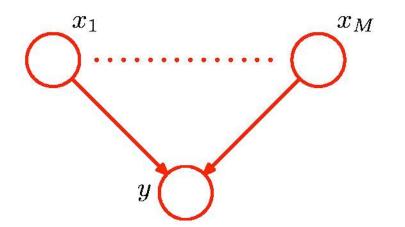
$$p(\boldsymbol{\mu}_m) = \operatorname{Dir}(\boldsymbol{\mu}_m | \boldsymbol{\alpha}_m)$$

Discrete Variables: Bayesian Parameters (2)



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

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

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

requires only M+1 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

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

Conditional Independence

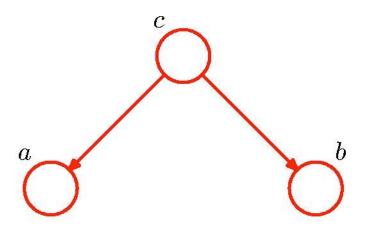
a is independent of b given c

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

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

Notation

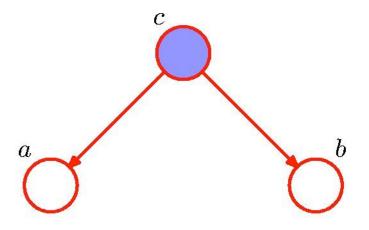
$$a \perp \!\!\!\perp b \mid c$$



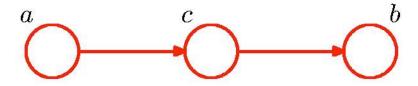
$$p(a, b, c) = p(a|c)p(b|c)p(c)$$

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

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



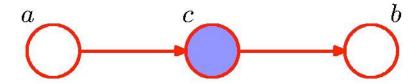
$$p(a, b|c) = \frac{p(a, b, c)}{p(c)}$$
$$= p(a|c)p(b|c)$$
$$a \perp \!\!\!\perp b \mid c$$



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

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

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

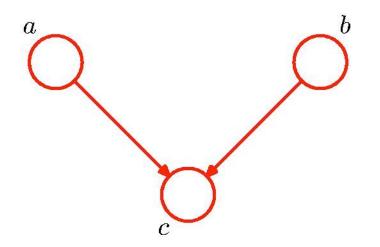


$$p(a,b|c) = \frac{p(a,b,c)}{p(c)}$$

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

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

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

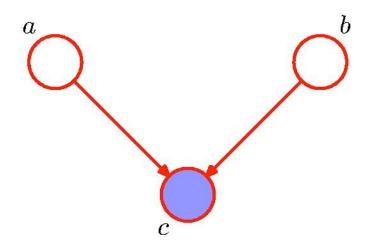


$$p(a,b,c) = p(a)p(b)p(c|a,b)$$

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

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

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



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

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

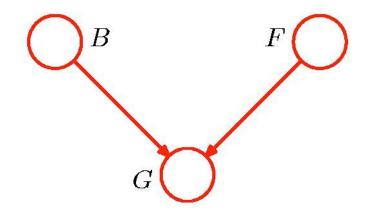
$$a \not\perp \!\!\! \perp b \mid c$$

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

"Am I out of fuel?"

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

 $p(G = 1|B = 1, F = 0) = 0.2$
 $p(G = 1|B = 0, F = 1) = 0.2$
 $p(G = 1|B = 0, F = 0) = 0.1$



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

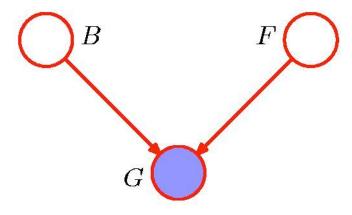
 $p(F=1) = 0.9$
and hence
 $p(F=0) = 0.1$

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

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

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

"Am I out of fuel?"

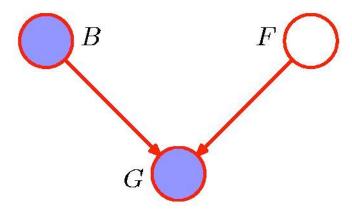


$$p(F = 0|G = 0) = \frac{p(G = 0|F = 0)p(F = 0)}{p(G = 0)}$$

\$\sim 0.257\$

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

"Am I out of fuel?"



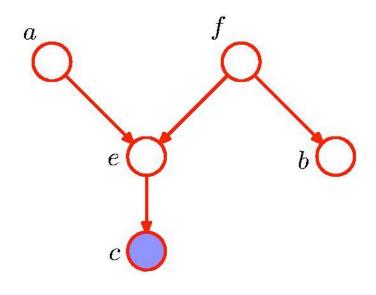
$$p(F=0|G=0,B=0) = \frac{p(G=0|B=0,F=0)p(F=0)}{\sum_{F\in\{0,1\}}p(G=0|B=0,F)p(F)} \simeq 0.111$$

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

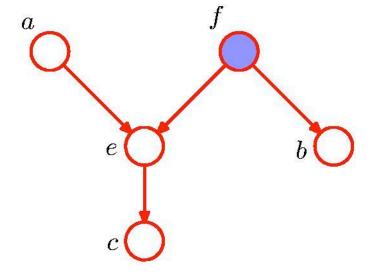
D-separation

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

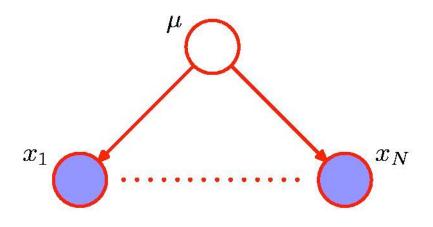


$$a \not\perp\!\!\!\perp b \mid c$$



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

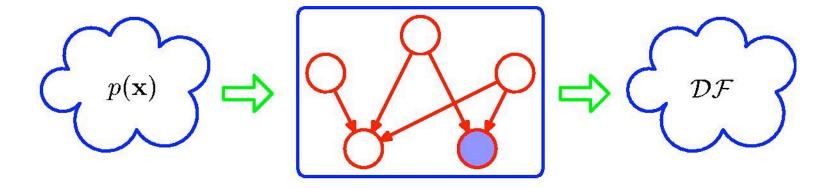
D-separation: I.I.D. Data



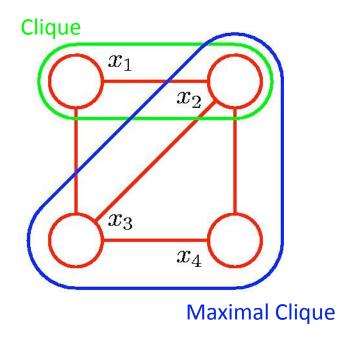
$$p(\mathcal{D}|\mu) = \prod_{n=1}^{N} p(x_n|\mu)$$

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

Directed Graphs as Distribution Filters



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

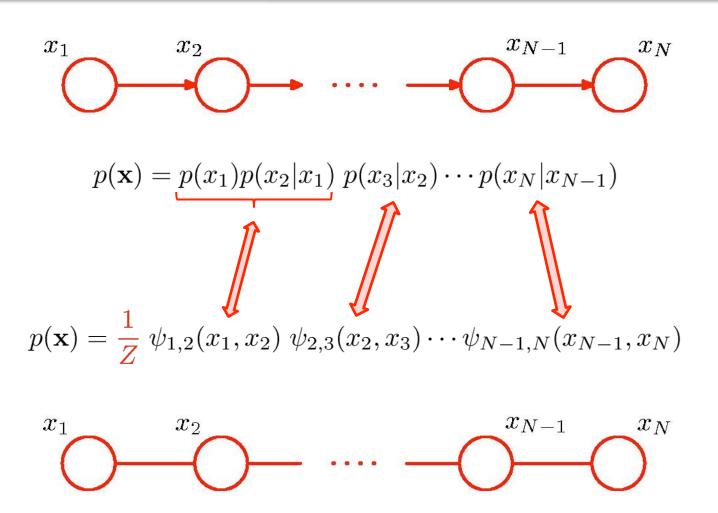
$$Z = \sum_{\mathbf{x}} \prod_{C} \psi_{C}(\mathbf{x}_{C})$$

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

Energies and the Boltzmann distribution

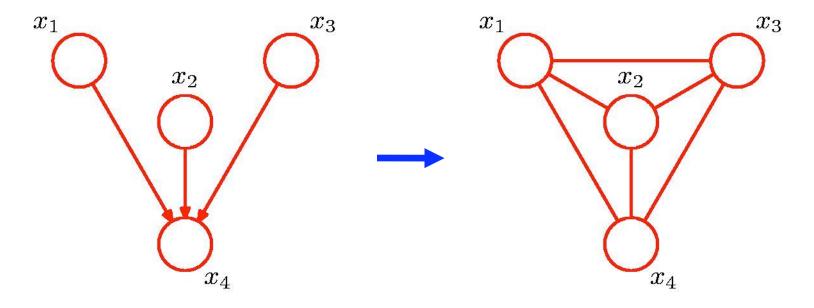
$$\psi_C(\mathbf{x}_C) = \exp\left\{-E(\mathbf{x}_C)\right\}$$

Converting Directed to Undirected Graphs (1)



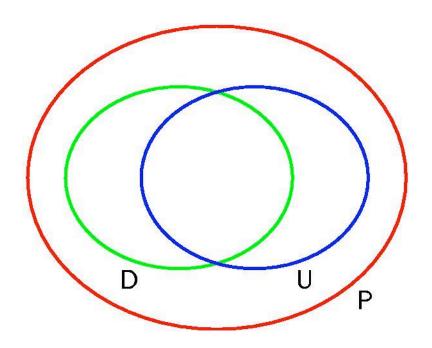
Converting Directed to Undirected Graphs (2)

Additional links

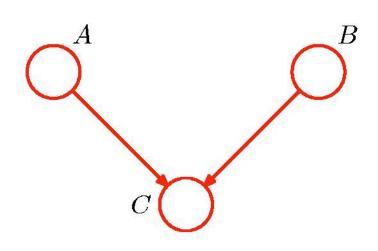


$$p(\mathbf{x}) = p(x_1)p(x_2)p(x_3)p(x_4|x_1, x_2, x_3)$$
$$= \frac{1}{Z}\psi_A(x_1, x_2, x_3)\psi_B(x_2, x_3, x_4)\psi_C(x_1, x_2, x_4)$$

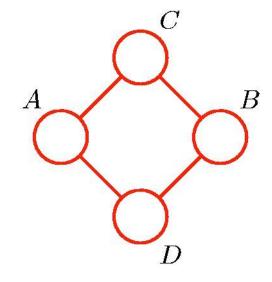
Directed vs. Undirected Graphs (1)



Directed vs. Undirected Graphs (2)



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

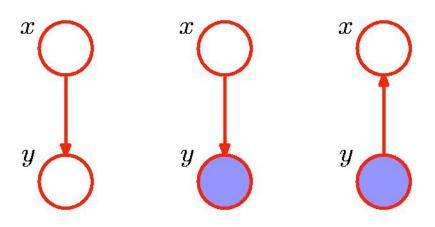


$$A \not\perp \!\!\!\perp B \mid \emptyset$$

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

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

Inference in Graphical Models



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

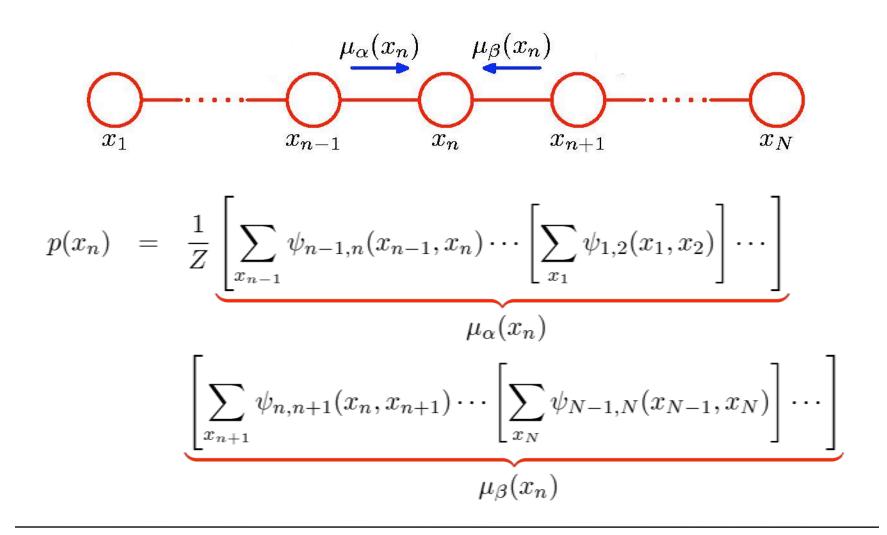
Inference on a Chain



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

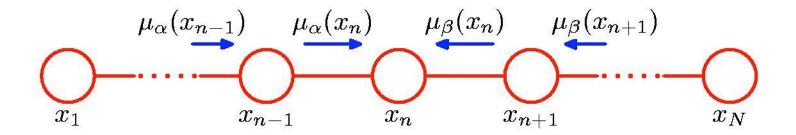
$$p(x_n) = \sum_{x_1} \cdots \sum_{x_{n-1}} \sum_{x_{n+1}} \cdots \sum_{x_N} p(\mathbf{x})$$

Inference on a Chain



Inference on a Chain

Inference on a Chain



$$\mu_{\alpha}(x_2) = \sum_{x_1} \psi_{1,2}(x_1, x_2)$$

$$\mu_{\beta}(x_{N-1}) = \sum_{x_N} \psi_{N-1,N}(x_{N-1}, x_N)$$

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

Inference on a Chain

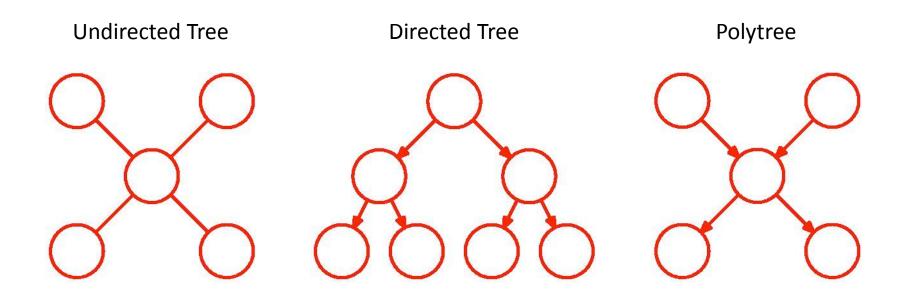
To compute local marginals:

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

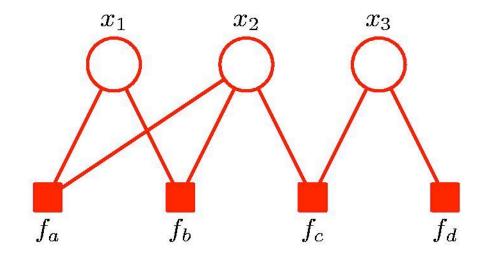
$$p(x_n) = \frac{1}{Z} \mu_{\alpha}(x_n) \mu_{\beta}(x_n)$$

for all variables required.

Trees



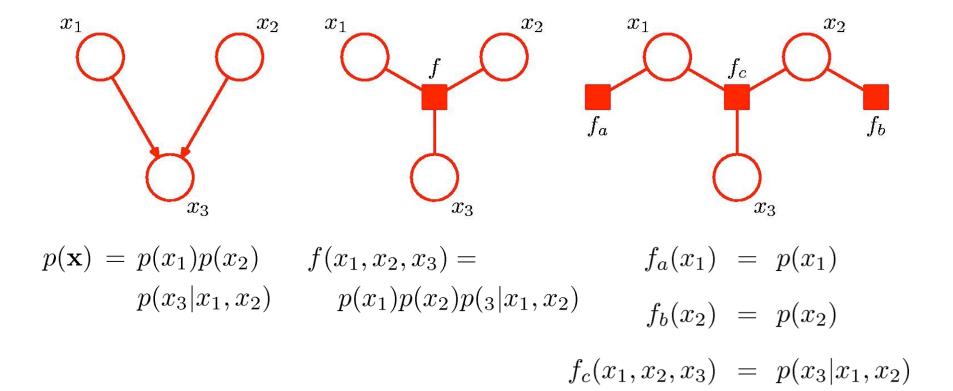
Factor Graphs



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

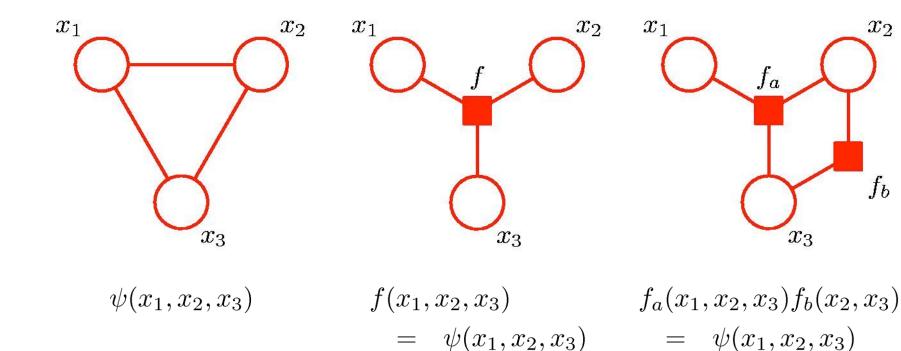
$$p(\mathbf{x}) = \prod_{s} f_s(\mathbf{x}_s)$$

Factor Graphs from Directed Graphs



Factor Graphs from Undirected Graphs

 x_2



The Sum-Product Algorithm (1)

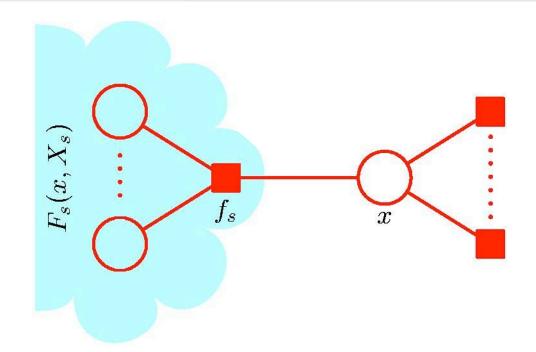
Objective:

- 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

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

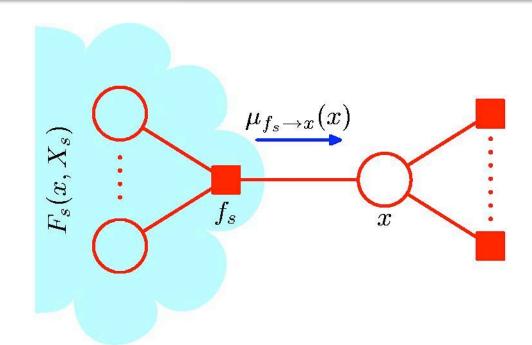
The Sum-Product Algorithm (2)



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

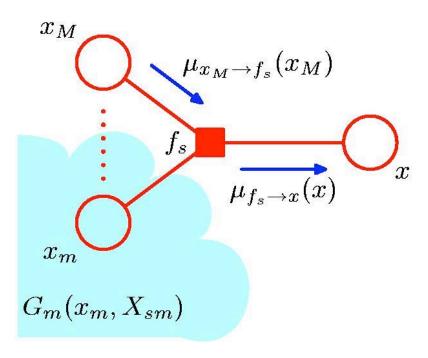
$$p(\mathbf{x}) = \prod_{s \in \text{ne}(x)} F_s(x, X_s)$$

The Sum-Product Algorithm (3)



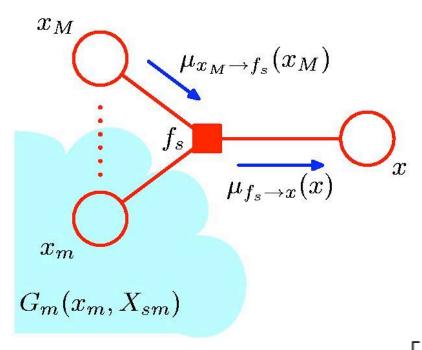
$$p(x) = \prod_{s \in ne(x)} \left[\sum_{X_s} F_s(x, X_s) \right]$$
$$= \prod_{s \in ne(x)} \mu_{f_s \to x}(x). \qquad \mu_{f_s \to x}(x) \equiv \sum_{X_s} F_s(x, X_s)$$

The Sum-Product Algorithm (4)



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

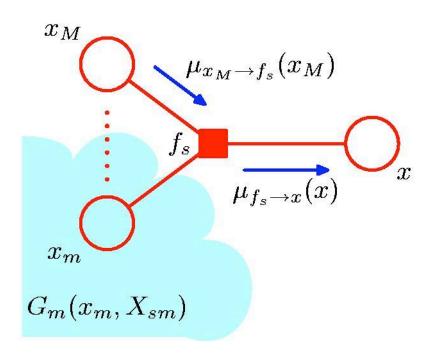
The Sum-Product Algorithm (5)



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

$$= \sum_{x_1} \dots \sum_{x_M} f_s(x, x_1, \dots, x_M) \prod_{m \in \text{ne}(f_s) \setminus x} \mu_{x_m \to f_s}(x_m)$$

The Sum-Product Algorithm (6)

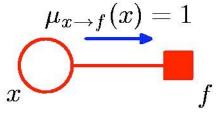


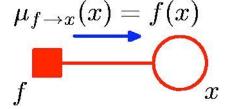
$$\mu_{x_m \to f_s}(x_m) \equiv \sum_{X_{sm}} G_m(x_m, X_{sm}) = \sum_{X_{sm}} \prod_{l \in \text{ne}(x_m) \setminus f_s} F_l(x_m, X_{ml})$$

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

The Sum-Product Algorithm (7)

Initialization



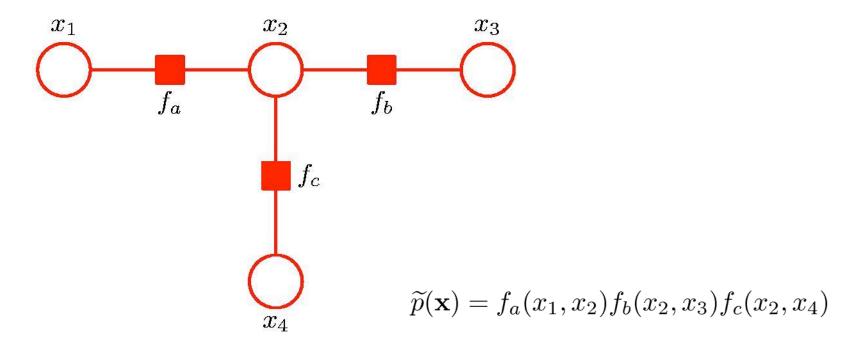


The Sum-Product Algorithm (8)

To compute local marginals:

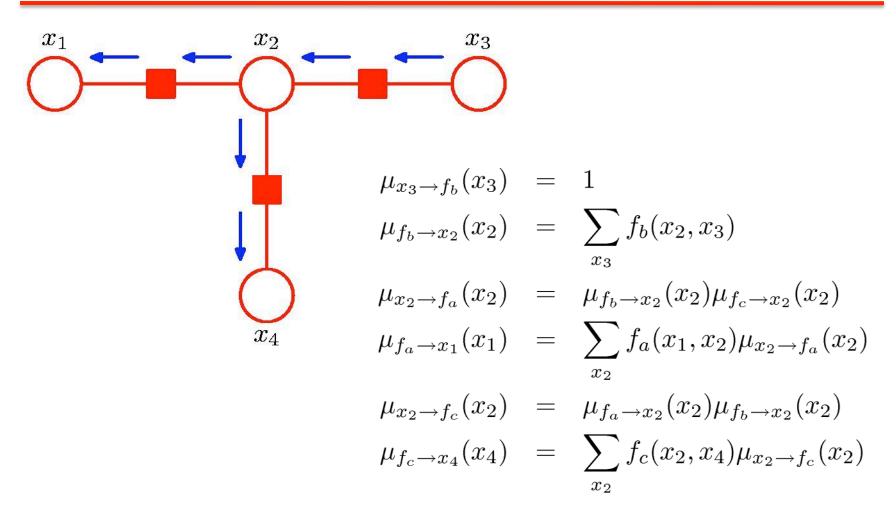
- Pick an arbitrary node as root
- Compute and propagate messages from the leaf nodes to the root, storing received messages at every node.
- Compute and propagate messages from the root to the leaf nodes, storing received messages at every node.
- Compute the product of received messages at each node 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 \mathbf{x}^{\max} that maximises $p(\mathbf{x})$;
- ii. the value of $p(\mathbf{x}^{\text{max}})$.

In general, maximum marginals \neq joint maximum.

$$\operatorname{arg\,max}_{x} p(x, y) = 1 \qquad \operatorname{arg\,max}_{x} p(x) = 0$$

The Max-Sum Algorithm (2)

Maximizing over a chain (max-product)



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

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

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

The Max-Sum Algorithm (3)

Generalizes to tree-structured factor graph

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

maximizing as close to the leaf nodes as possible

The Max-Sum Algorithm (4)

Max-Product → 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

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

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

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

The Max-Sum Algorithm (6)

Termination (root node)

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

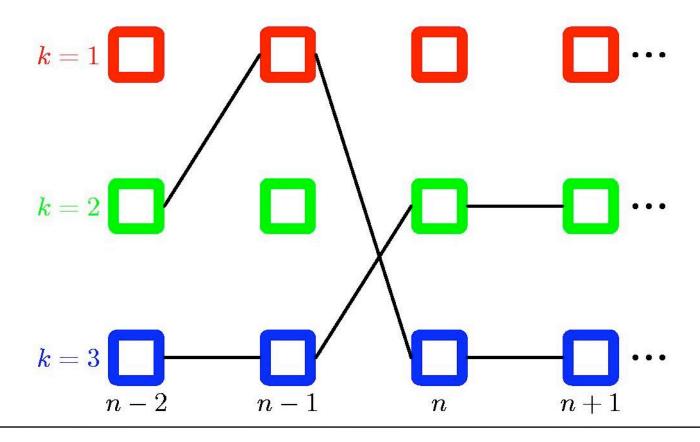
$$x^{\max} = \arg\max_{x} \left[\sum_{s \in ne(x)} \mu_{f_s \to x}(x) \right]$$

Back-track, for all nodes i with 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 sumproduct-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.