Exact Inference in Graphical Models

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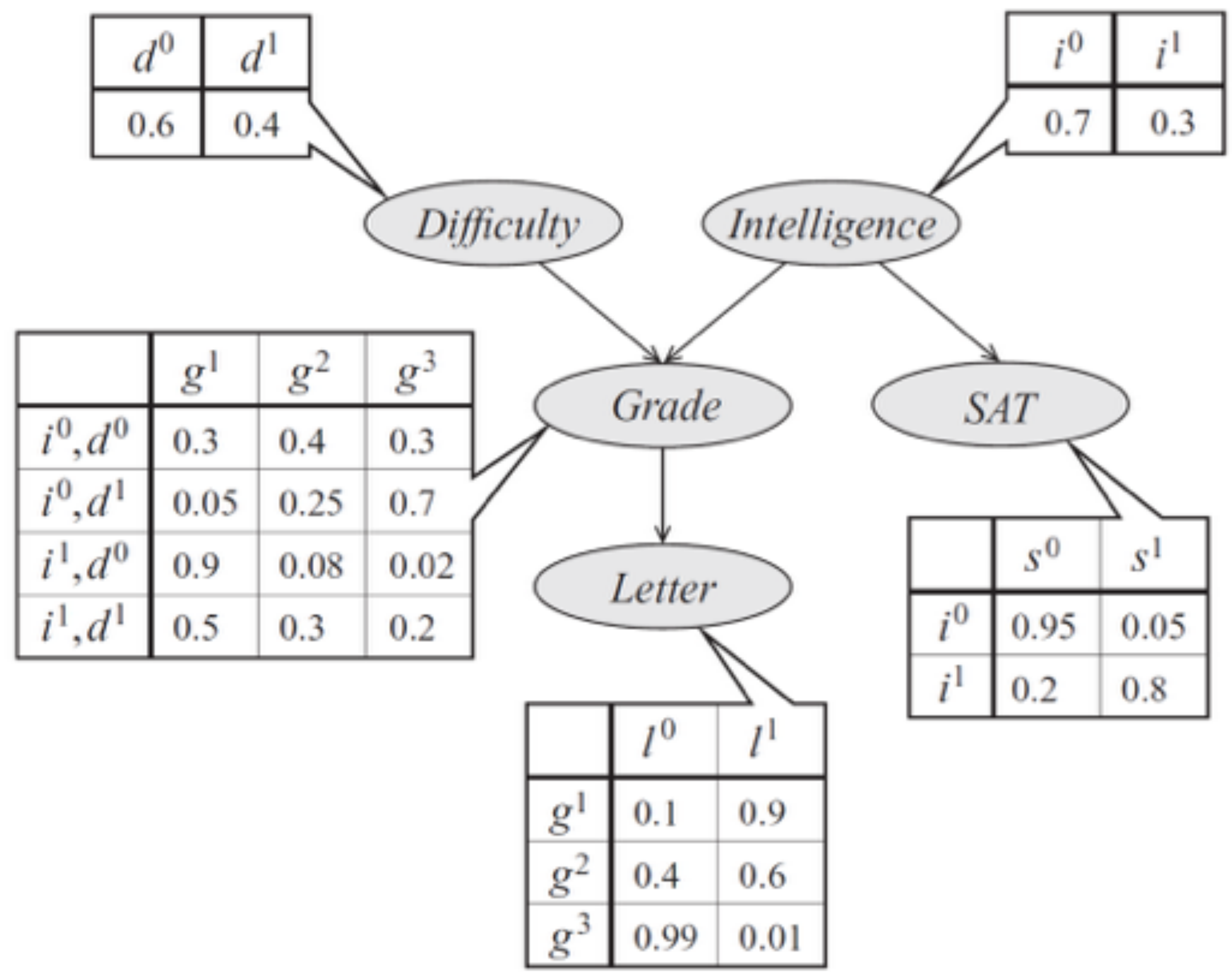
CS 159

(with materials from lectures by Stefano Ermon, Zoubin Gharamani, Bert Huang)

Recap: Graphical Model Representation

Bayesian Networks

Directed Acyclic Graph, a.k.a Belief Networks



d^0	d^1
0.6	0.4

i^0	i^1
0.7	0.3

	g^1	g^2	g^3
i^0,d^0	0.3	0.4	0.3
i^0,d^1	0.05	0.25	0.7
i^1,d^0	0.9	0.08	0.02
i^1,d^1	0.5	0.3	0.2

	s^0	s^1
i^0	0.95	0.05
i^1	0.2	0.8

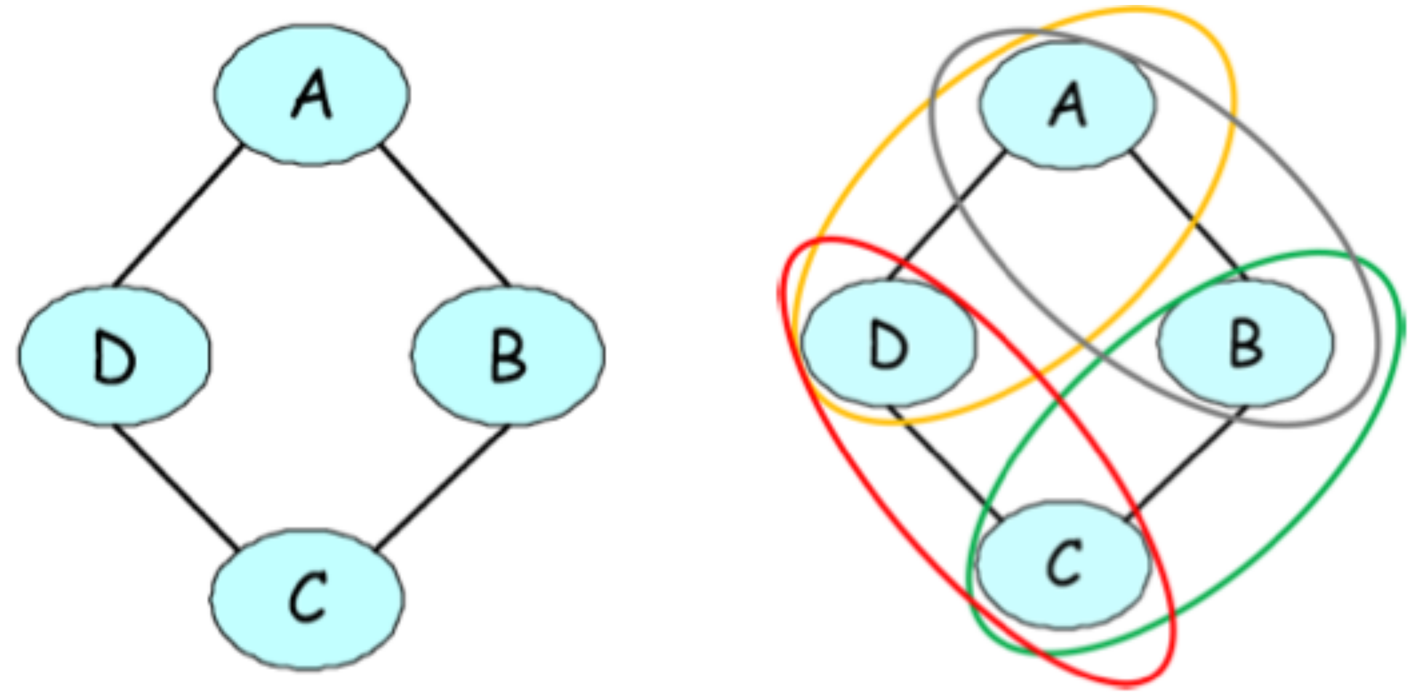
	l^0	l^1
g^1	0.1	0.9
g^2	0.4	0.6
g^3	0.99	0.01

$$p(l, g, i, d, s) = p(l|g)p(g|i, d)p(i)p(d)p(s|i)$$

Markov Random Fields

- Example: voting preference in social networks

- Assign scores to each assignment to these variables and then define a probability as a normalized score



$$\tilde{p}(A,B,C,D) = \phi(A,B)\phi(B,C)\phi(C,D)\phi(D,A),$$

$$\phi(X,Y) = \begin{cases} 10 & \text{if } X = Y = 1 \\ 5 & \text{if } X = Y = 0 \\ 1 & \text{otherwise.} \end{cases}$$

$$p(A,B,C,D) = \frac{1}{Z}\tilde{p}(A,B,C,D),$$

where

$$Z = \sum_{A,B,C,D} \tilde{p}(A,B,C,D)$$

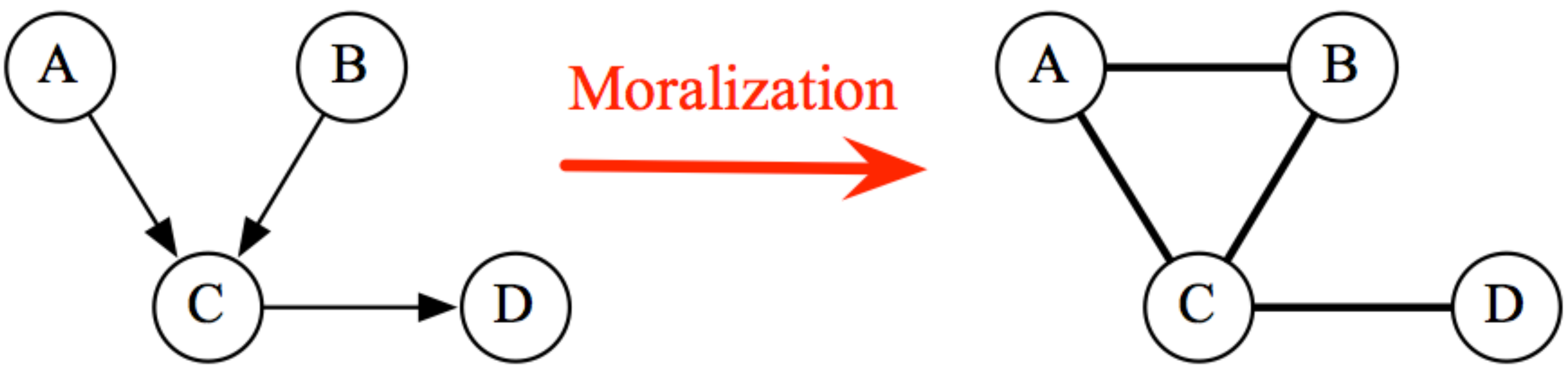
Markov Random Fields

A MRF is a probability distribution p over variables $x_1,\ldots,x_n$ defined by an undirected graph G with nodes correspond to x_i

$$p(x_1,..,x_n) = \frac{1}{Z}\prod_{c\in C}\phi_c(x_c),$$

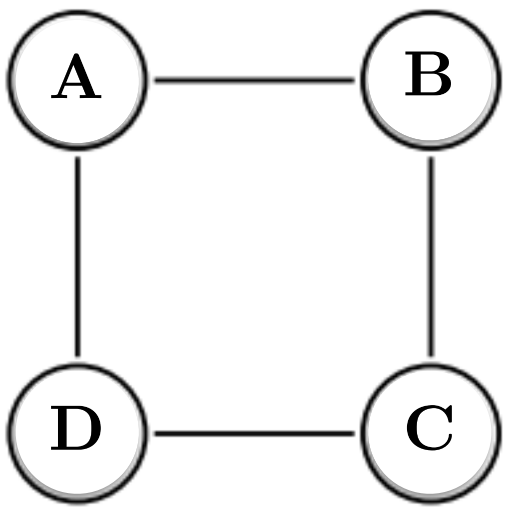
where C is set of cliques

$$Z = \sum_{x_1,..,x_n}\prod_{c\in C}\phi_c(x_c)$$

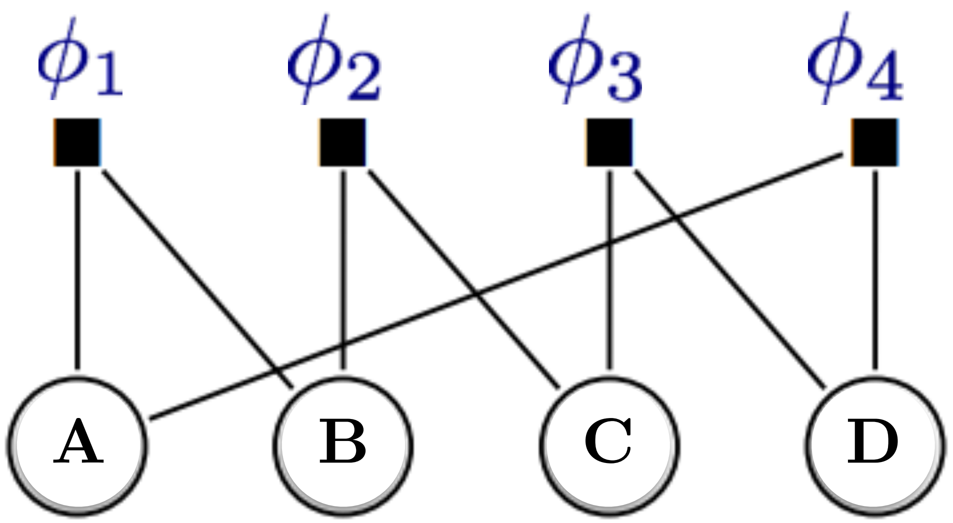

A
B
C
D
Moralization
A
B
C
D

Factor Graph Representation

$$p(A, B, C, D) \propto \phi_1(A, B)\phi_2(B, C)\phi_3(C, D)\phi_4(D, A)$$

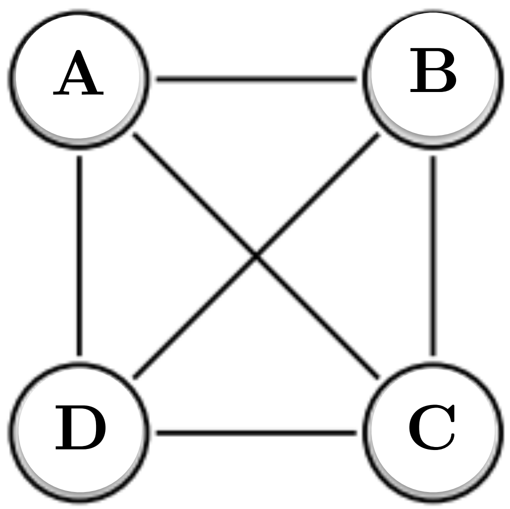


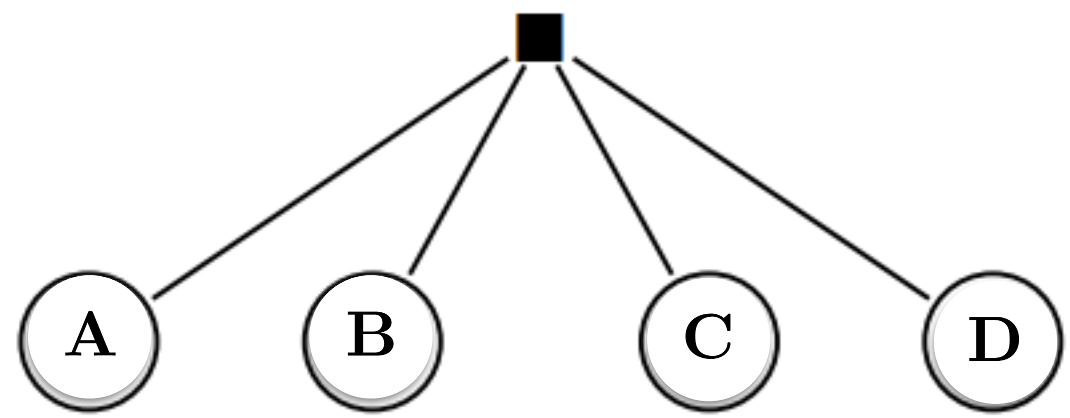
graphical model



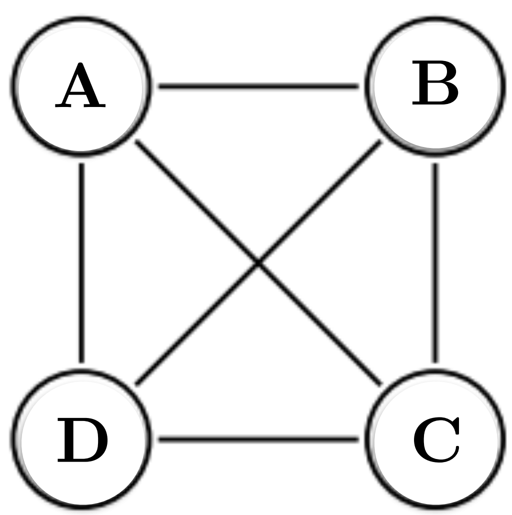
factor graph

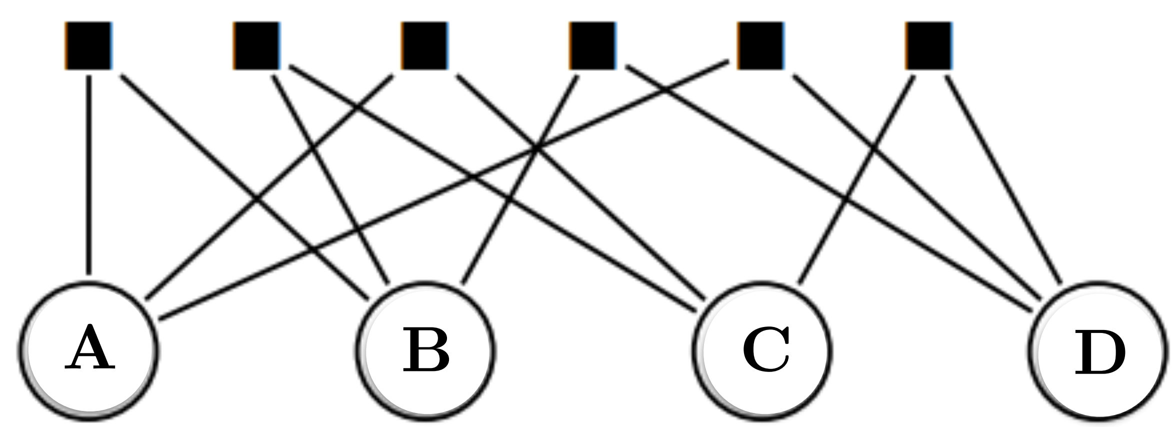
Factor Graph Representation





...instead of





Probabilistic Inference

- Let (E,F) be disjoint subset of node indices of a graphical model. Two basic kinds of inference problems:
  - *Marginal probability inference*

$$p(x_E) = \sum_{x_F} p(x_E, x_F)$$

  - *Maximum a posteriori (MAP) inference*

$$p^*(x_E) = \max_{x_F} p(x_E, x_F)$$

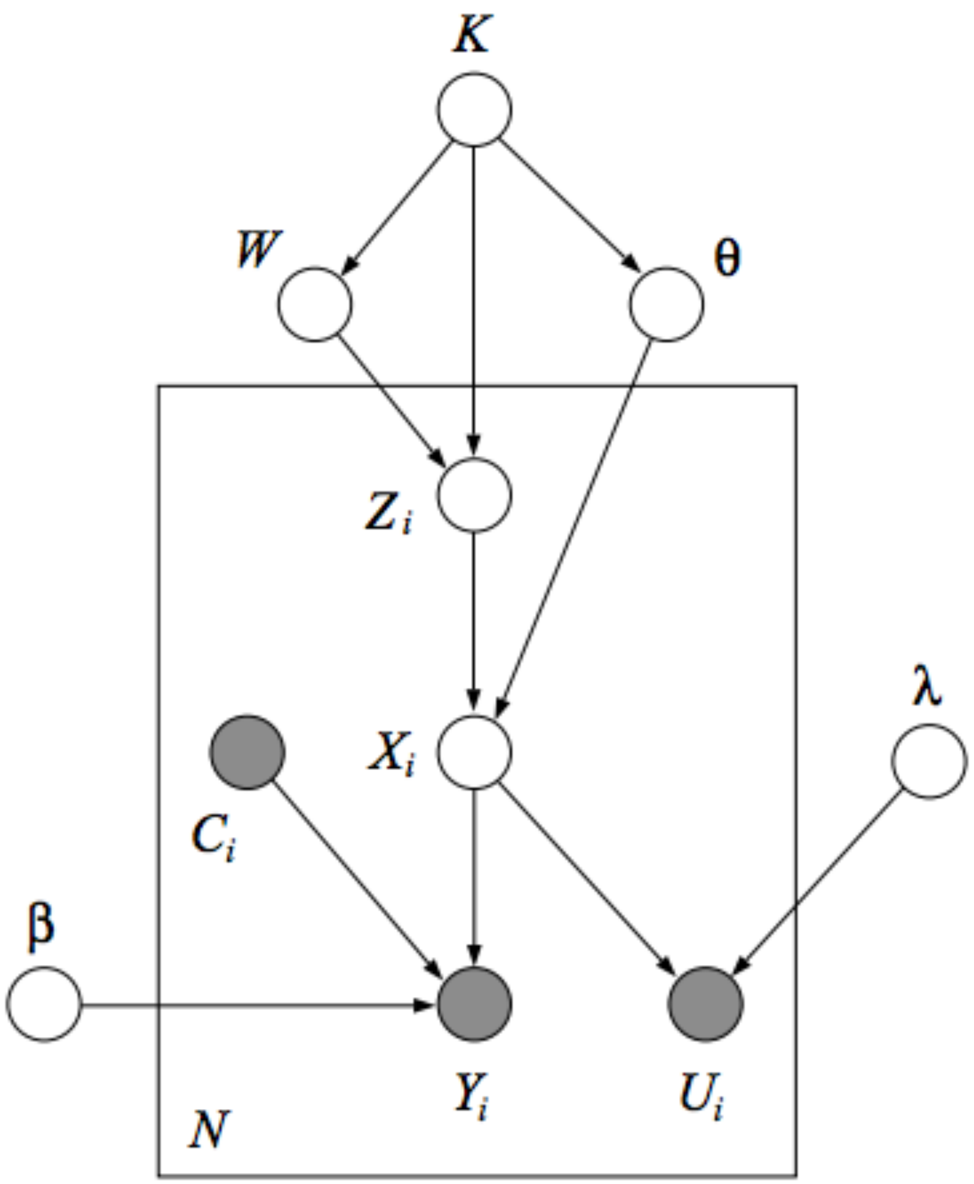
- Conditional probability $p(x_F|x_E)$

$$p(x_F|x_E) = \frac{p(x_E, x_F)}{\sum_{x_F} p(x_E, x_F)}$$

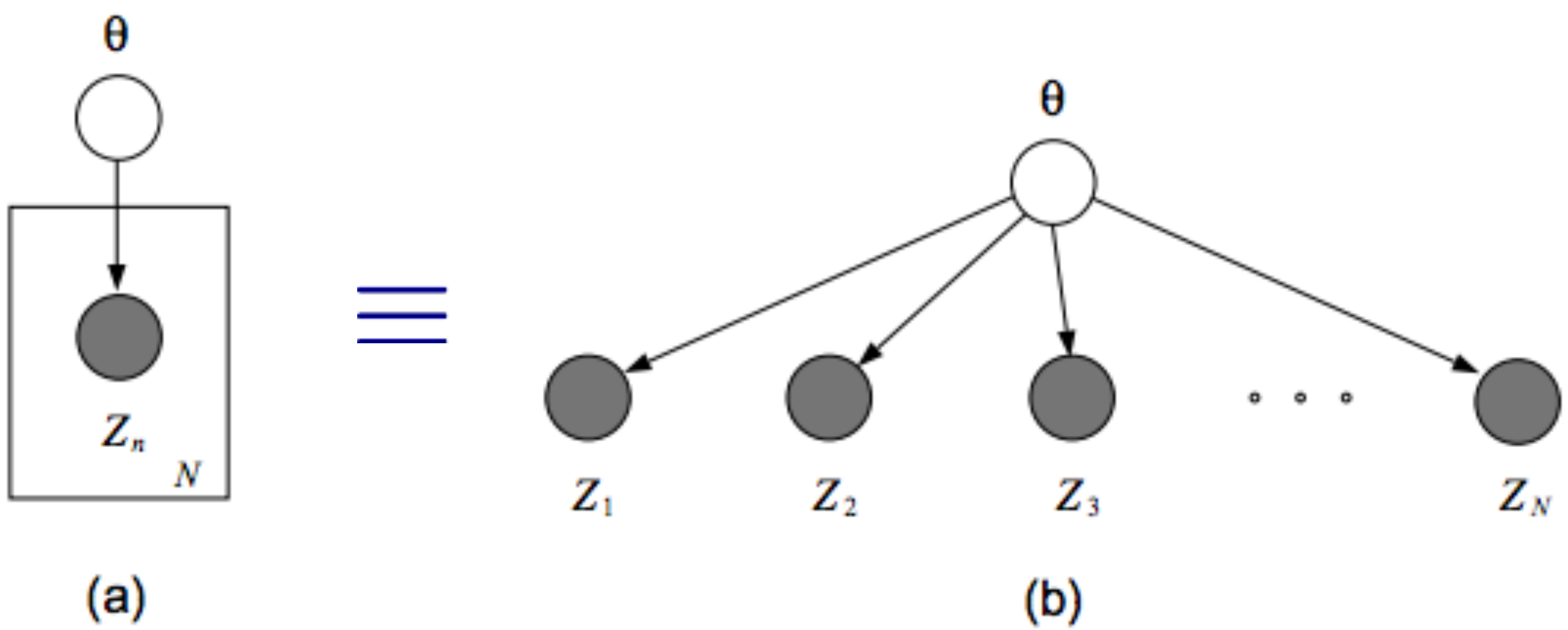
- Combining conditioning and marginalization

$$p(x_F|x_E) = \frac{p(x_E, x_F)}{\sum_{x_F} p(x_E, x_F)} = \frac{\sum_{x_H} p(x_E, x_F, x_H)}{\sum_{x_F} \sum_{x_H} p(x_E, x_F, x_H)}$$

Inference + Learning



Inference + Learning



Roadmap

- Overview of Graphical Model, Inference and Learning, Structured Predictions
- Conditional Random Field and applications
- Graphical Model Inference
    - Exact Inference: Message Passing
    - Approximate Inference: LP Relaxation
    - More approximate inference: Sampling-based methods, Variational Inference
- Graphical Model Learning: Parameter learning & structure learning
- Structured Predictions: Structured SVMs, random forests, deep structured models
- Advanced topics that combine inference and learning

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Exact Inference: Message Passing

Variable Elimination

$$p(x_1, ..., x_n) = p(x_1) \prod_{i=2}^{n} p(x_i \mid x_{i-1}).$$

Inference Goal: calculate $p(x_n)$

Naive Method: $$p(x_n) = \sum_{x_1} \cdots \sum_{x_{n-1}} p(x_1, ..., x_n).$$

Variable Elimination

$$p(x_1, \ldots, x_n) = p(x_1) \prod_{i=2}^{n} p(x_i \mid x_{i-1}).$$

Inference Goal: calculate $p(x_n)$

More efficient method:

$$\begin{aligned} p(x_n) &= \sum_{x_1} \cdots \sum_{x_{n-1}} p(x_1) \prod_{i=2}^{n} p(x_i \mid x_{i-1}) \\ &= \sum_{x_{n-1}} p(x_n \mid x_{n-1}) \sum_{x_{n-2}} p(x_{n-1} \mid x_{n-2}) \cdots \underbrace{\sum_{x_1} p(x_2 \mid x_1) p(x_1)}_{m_{12}(x_2)} \end{aligned}$$

$$p(x_n) = \sum_{x_{n-1}} p(x_n \mid x_{n-1}) \sum_{x_{n-2}} p(x_{n-1} \mid x_{n-2}) \cdots \sum_{x_2} p(x_3 \mid x_2) m_{12}(x_2).$$

Variable Elimination

$$p(x_1, ..., x_n) = p(x_1) \prod_{i=2}^{n} p(x_i \mid x_{i-1}).$$

Inference Goal: calculate $p(x_n)$

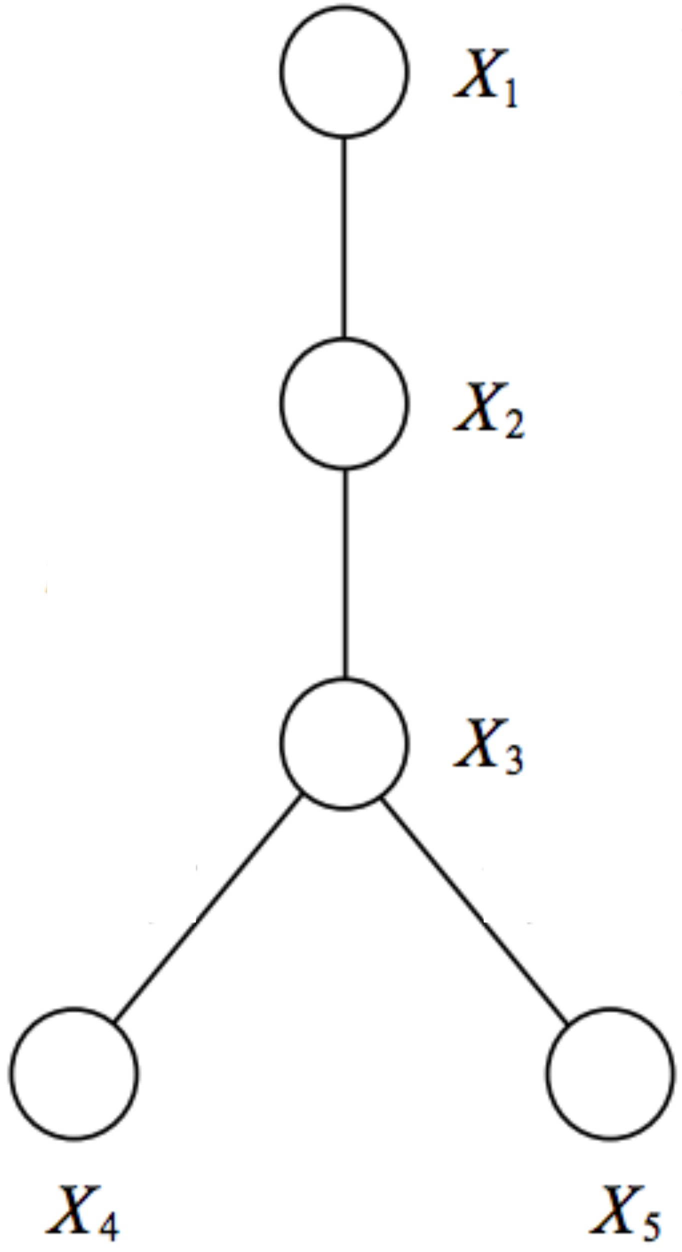
More efficient method:

$$p(x_n) = \sum_{x_{n-1}} p(x_n \mid x_{n-1}) \sum_{x_{n-2}} p(x_{n-1} \mid x_{n-2}) \cdots \underbrace{\sum_{x_2} p(x_3 \mid x_2) m_{12}(x_2)}_{m_{23}(x_3)}$$

$$= \ldots$$

$$= m_{(n-1)n}(x_n)$$

Variable Elimination

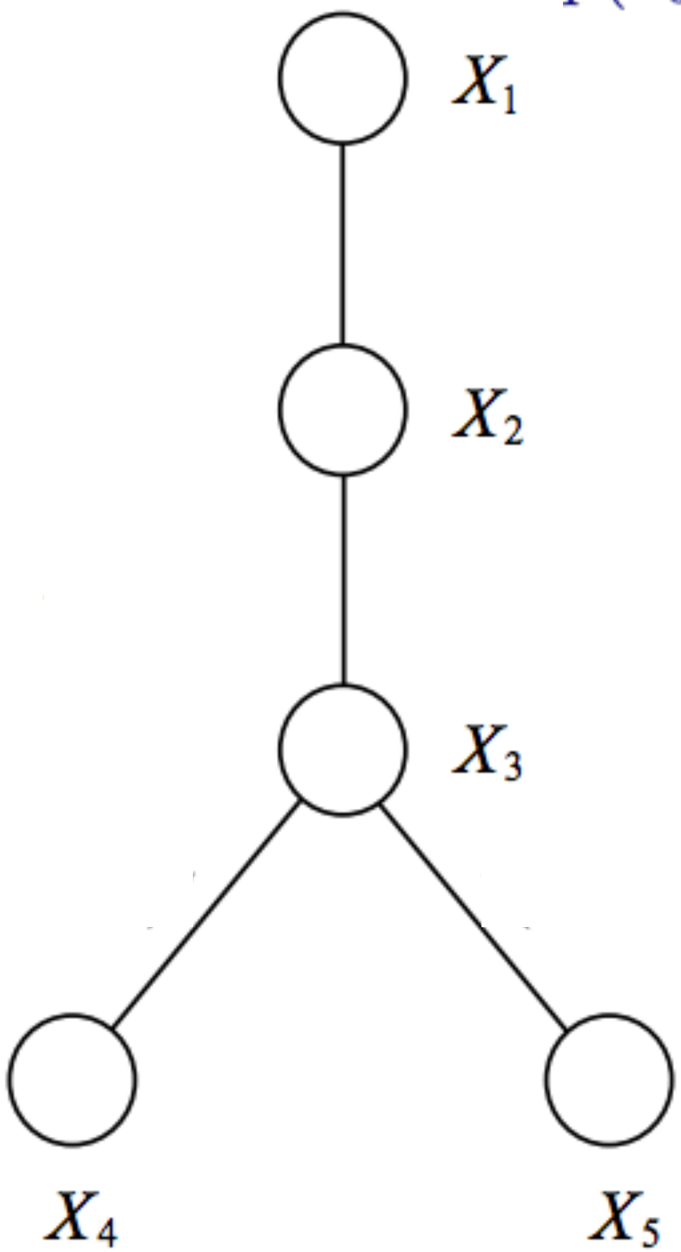


Inference Goal: calculate $p(x_5)$

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

Elimination order: (1,2,4,3)

Variable Elimination



$$p(x_5) = \frac{1}{Z}\sum_{x_3}\phi_{35}(x_3,x_5)\sum_{x_4}\phi_{34}(x_3,x_4)\sum_{x_2}\phi_{23}(x_2,x_3)\underbrace{\sum_{x_1}\phi_{12}(x_1,x_2)}_{m_{12}(x_2)}$$

$$= \frac{1}{Z}\sum_{x_3}\phi_{35}(x_3,x_5)\sum_{x_4}\phi_{34}(x_3,x_4)\underbrace{\sum_{x_2}\phi_{23}(x_2,x_3)m_{12}(x_2)}_{m_{23}(x_3)}$$

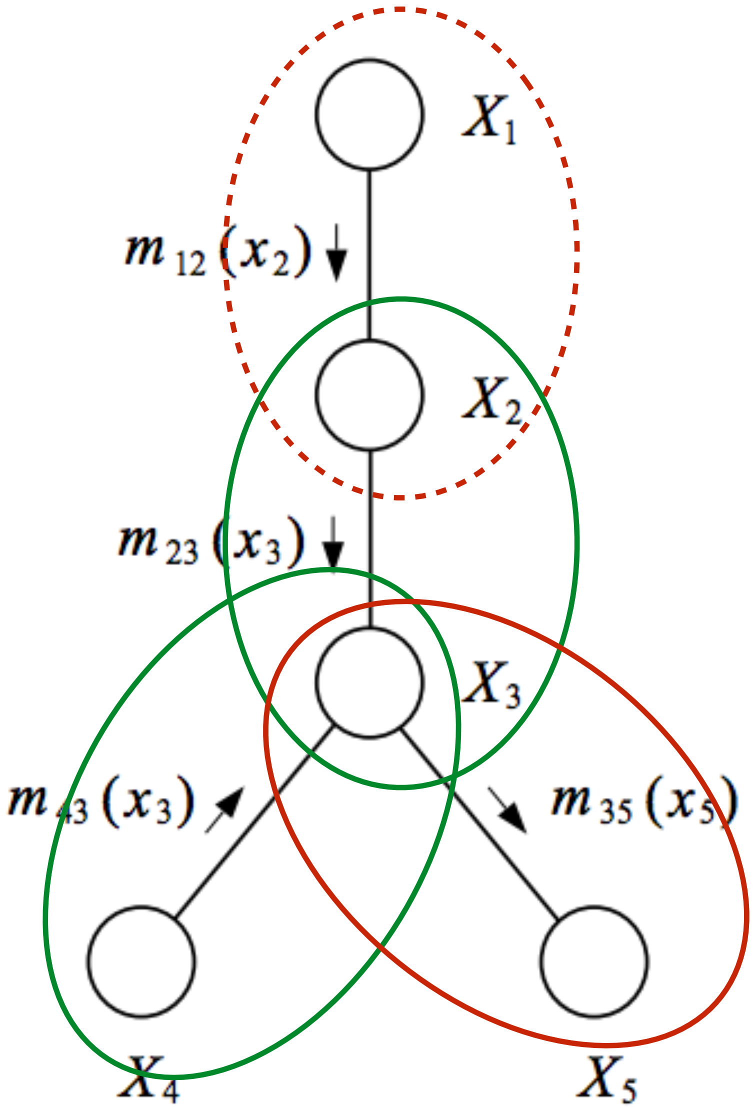
$$= \frac{1}{Z}\sum_{x_3}\phi_{35}(x_3,x_5)\sum_{x_4}\phi_{34}(x_3,x_4)m_{23}(x_3)$$

$$= \frac{1}{Z}\sum_{x_3}\phi_{35}(x_3,x_5)m_{23}(x_3)\underbrace{\sum_{x_4}\phi_{34}(x_3,x_4)}_{m_{43}(x_3)}$$

$$= \frac{1}{Z}\sum_{x_3}\phi_{35}(x_3,x_5)m_{23}(x_3)m_{43}(x_3)$$

$$= \frac{1}{Z}m_{35}(x_5)$$

Variable Elimination Algorithm

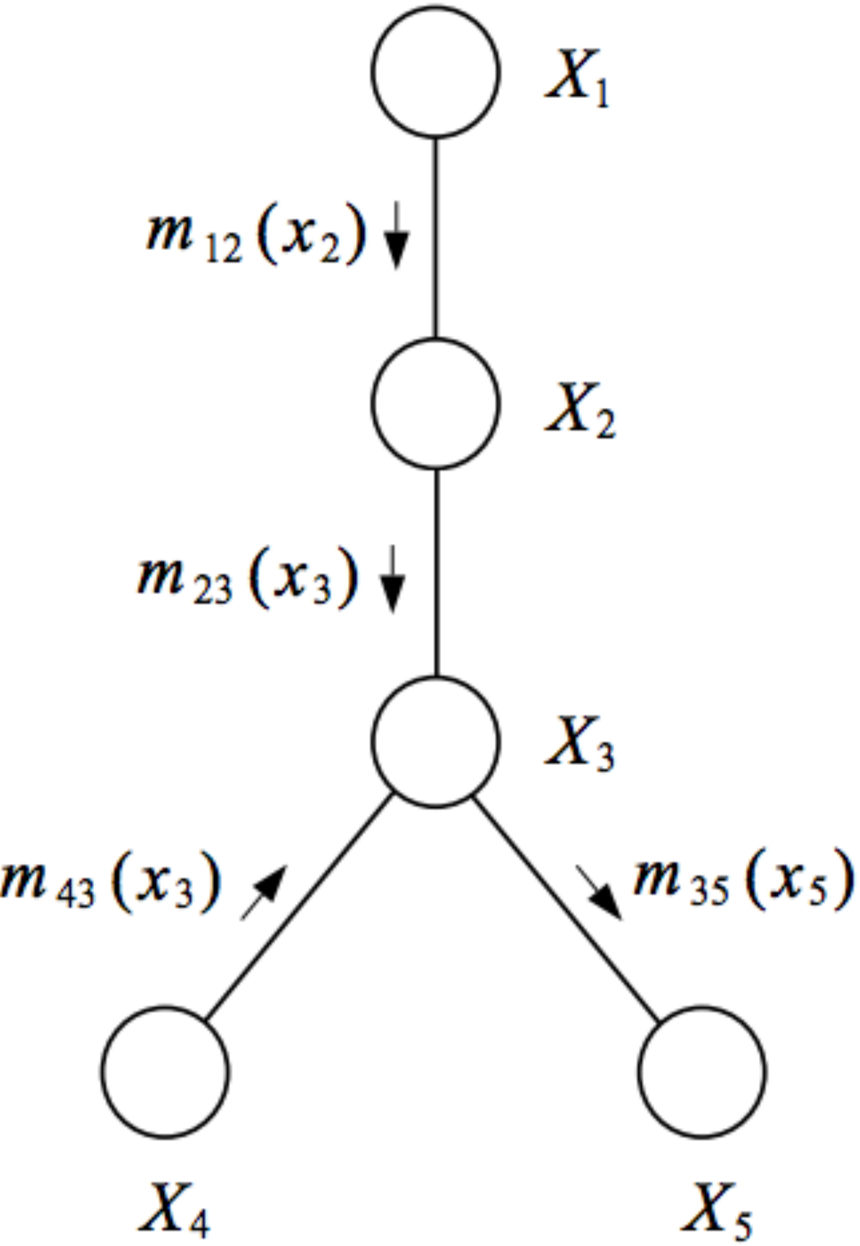


1. Place all potentials $\phi_C(x_C)$ on the active list
2. choose an ordering I of the indices $(1, 2, 4, 3)$
3. **for** each x_i in I
   - A. find all potentials on the active list that reference x_i and remove them from the active list
   - B. define a new potential as the sum (w.r.t x_i) of the product of these potentials
   - C. place the new potential on the active list
4. return the product of the remaining potentials

Variable Elimination

- Two key operations for factors: ***product*** and ***sum*** (marginalization)
- Orderings: matters a lot. NP hard to find the best. Common heuristics: min-neighbors, min-weight, min-fill
- Running time: $O(nd^M)$, where M is the max size of any factor during elimination
- Introducing evidence: $P(Y|E=e) = \frac{P(Y,E=e)}{P(E=e)}$ where $P(X,Y,E)$ is the joint, query variables Y, observed E, and unobserved variables X
  - perform variable elimination once on $P(Y,E=e)$ and once more on $P(E=e)$

Variable Elimination as Message Passing



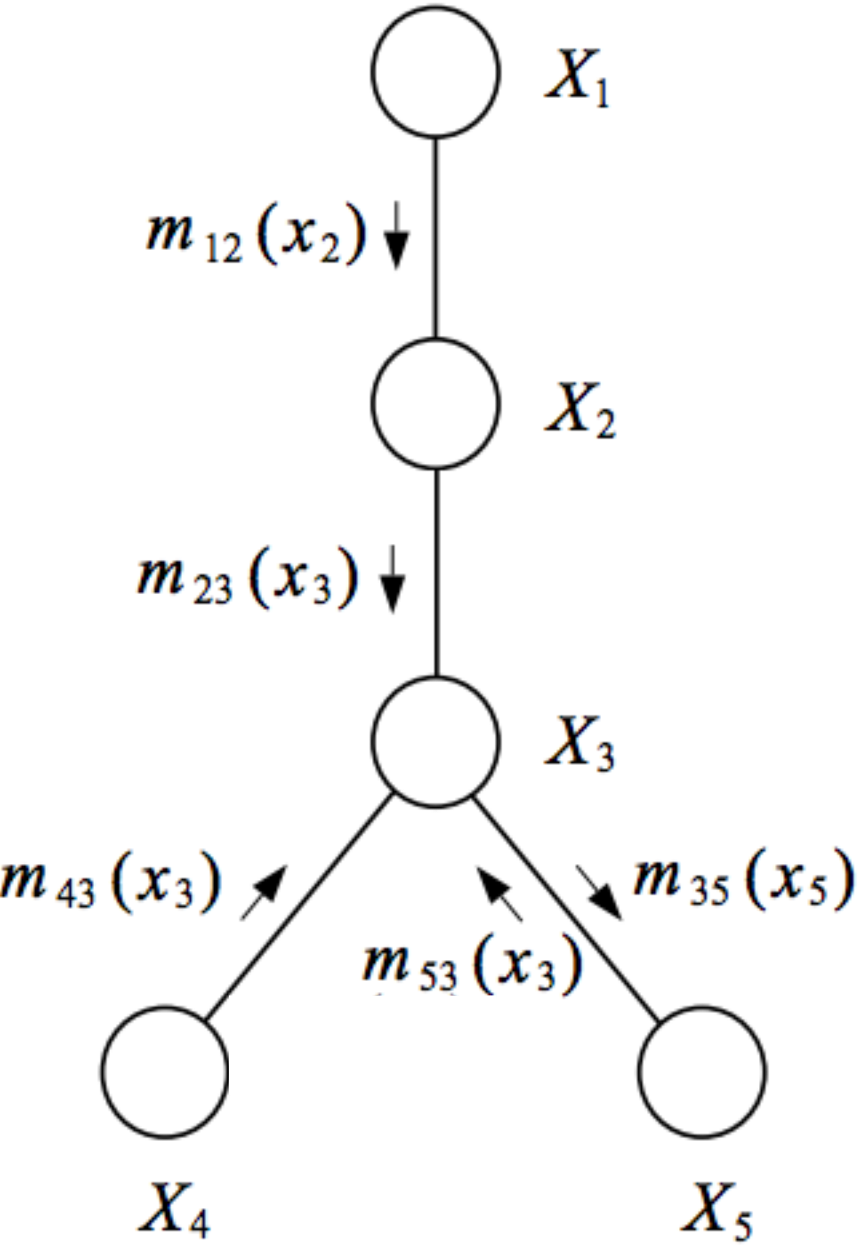
Inference Goal: calculate $p(x_5)$ and $p(x_3)$

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

Elimination order $p(x_5)$: (1,2,4,3)

Elimination order $p(x_3)$: (1,2,5,4)

Variable Elimination as Message Passing



Inference Goal: calculate $p(x_5)$ and $p(x_3)$

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

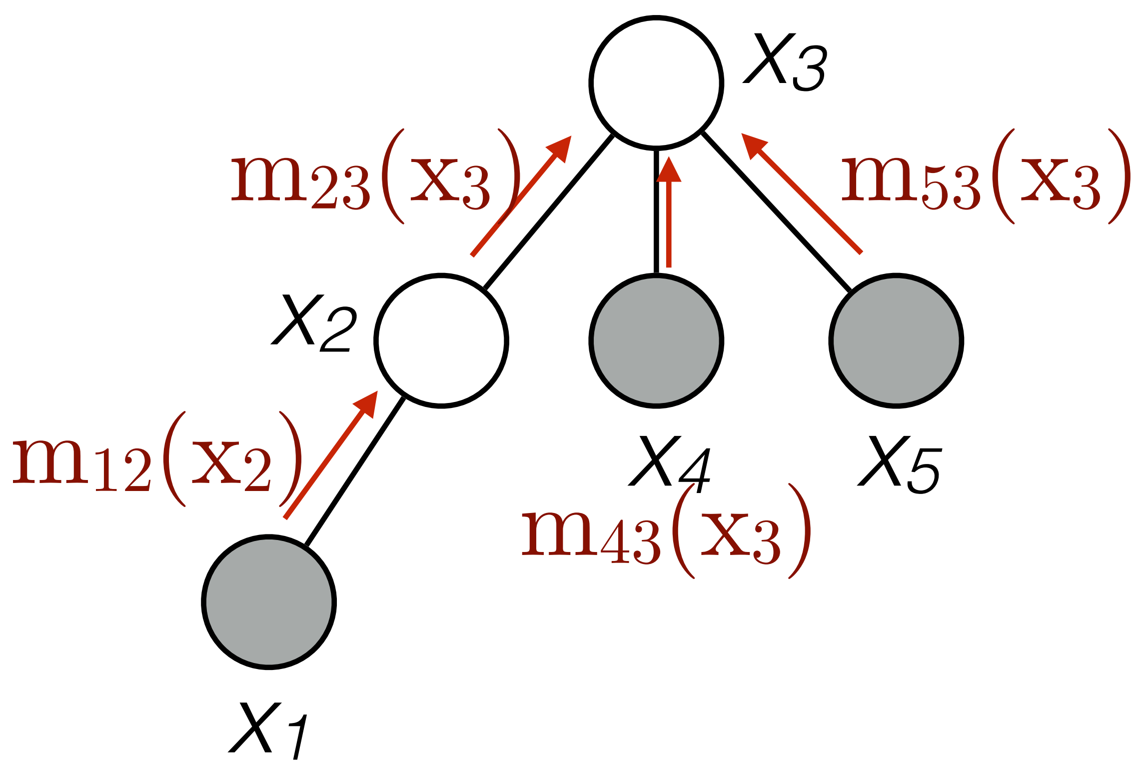
Elimination order $p(x_5)$: (1,2,4,3)

Elimination order $p(x_4)$: (1,2,5,4)

Problem: Naive method wasteful and computationally burdensome

Solution: Reuse intermediate terms efficiently!

Message Passing on Trees



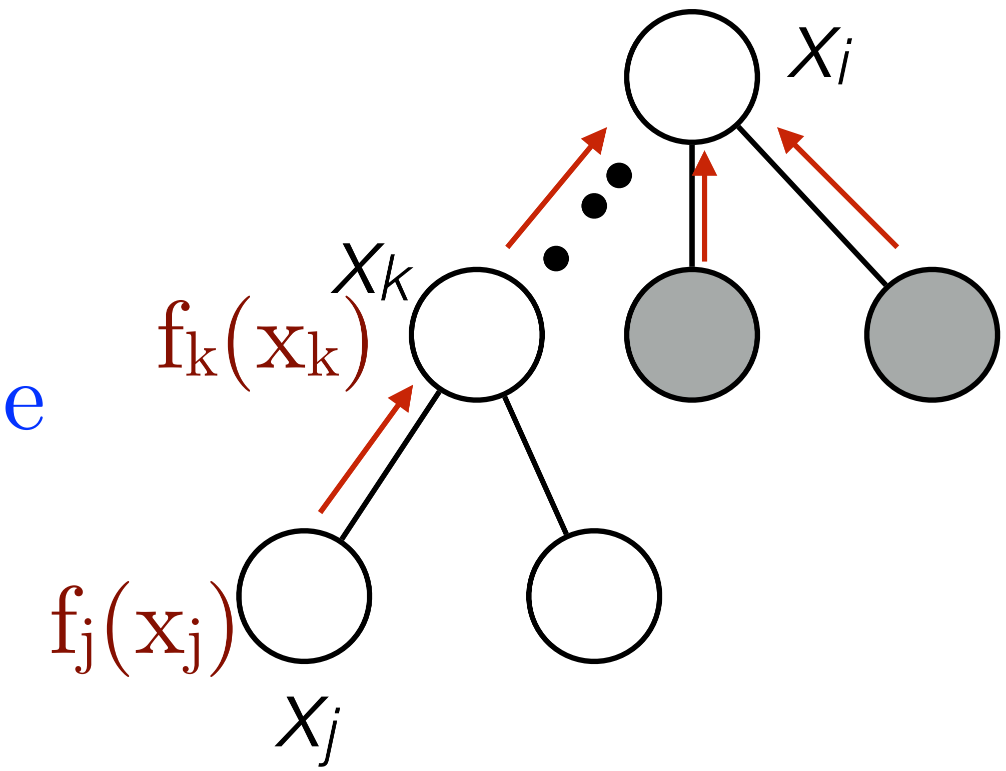
Message Passing on Trees

At each step, eliminate x_j by

$$f_k(x_k) = \sum_{x_j} \phi(x_k, x_j) f_j(x_j)$$

where x_k is parent of x_j in the tree

$f_j(xj)$ is a message that x_j sends to x_k to summarize all it knows about its children



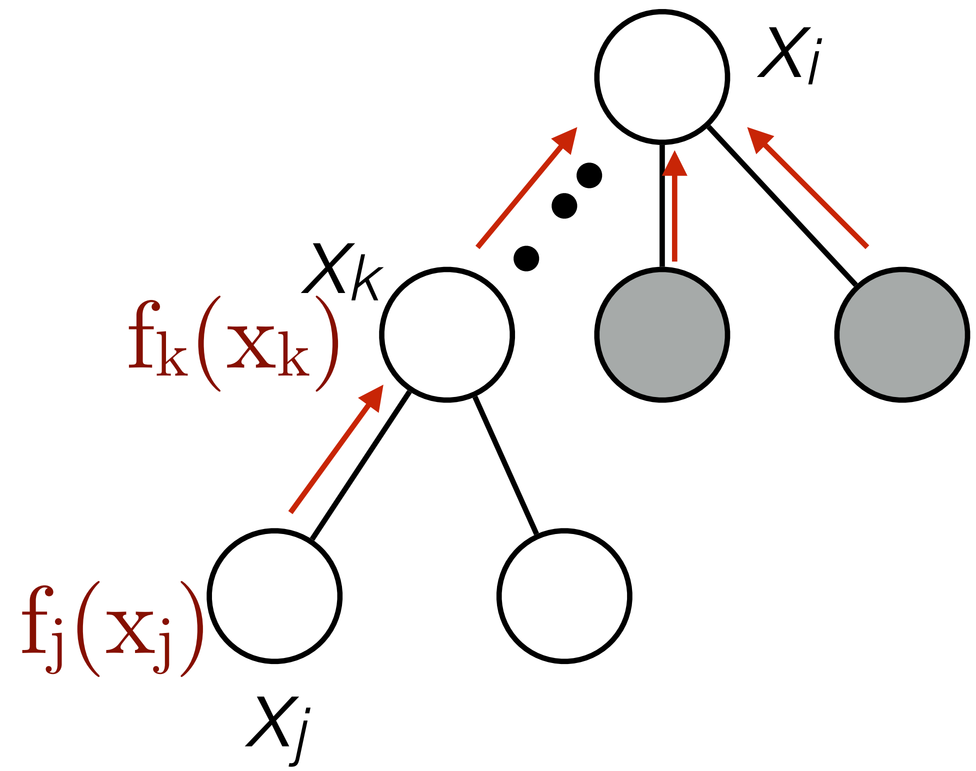
Message Passing on Trees

Now compute $p(x_k)$ as well:

<u>Key insight:</u>

messages x_k will receive from x_j

will the same as when x_i was the root

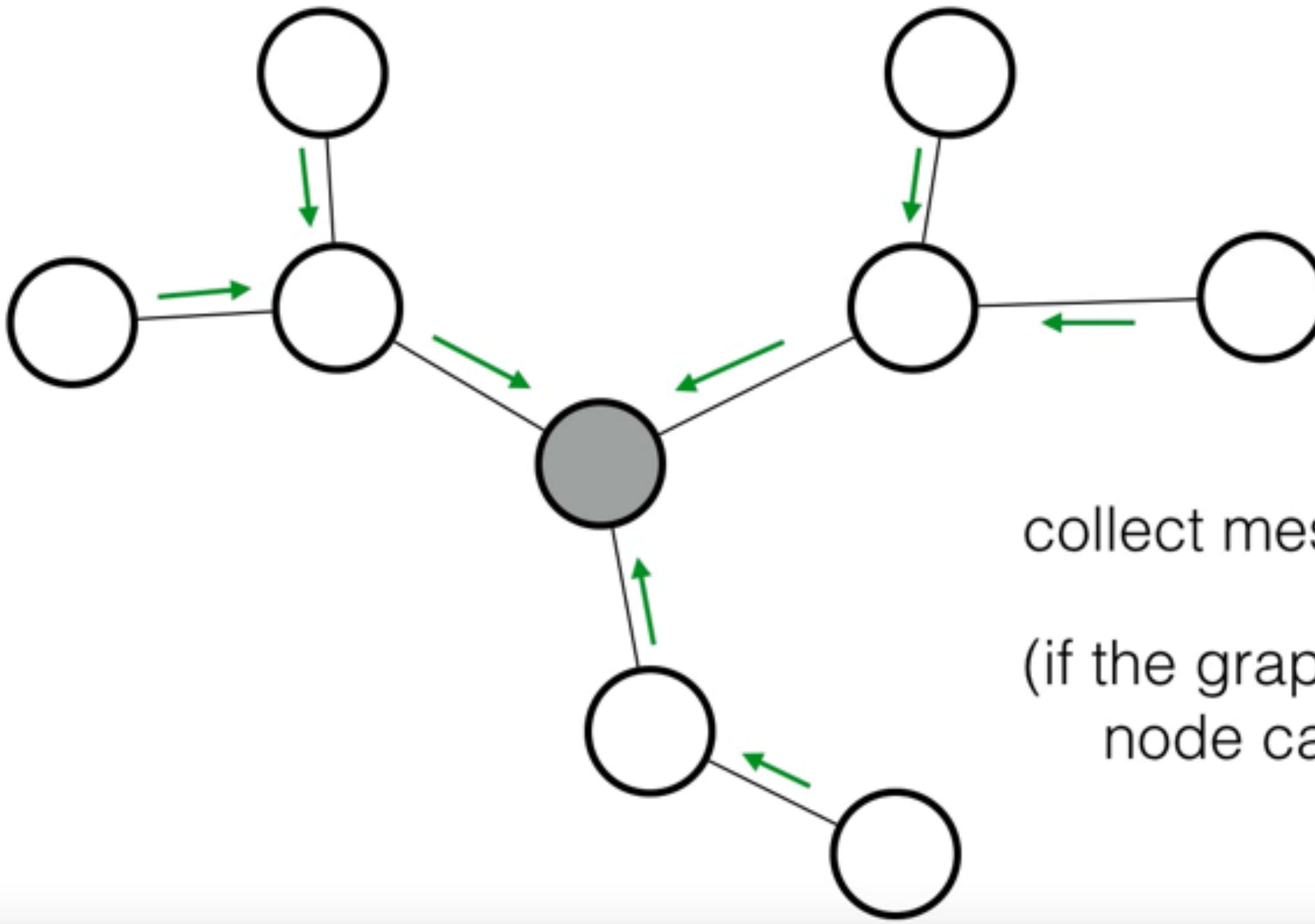


How do we compute all the message we need?

<u>Solution:</u>

A node x_i sends a message to a neighbor x_j whenever it has received messages from all nodes beside x_j

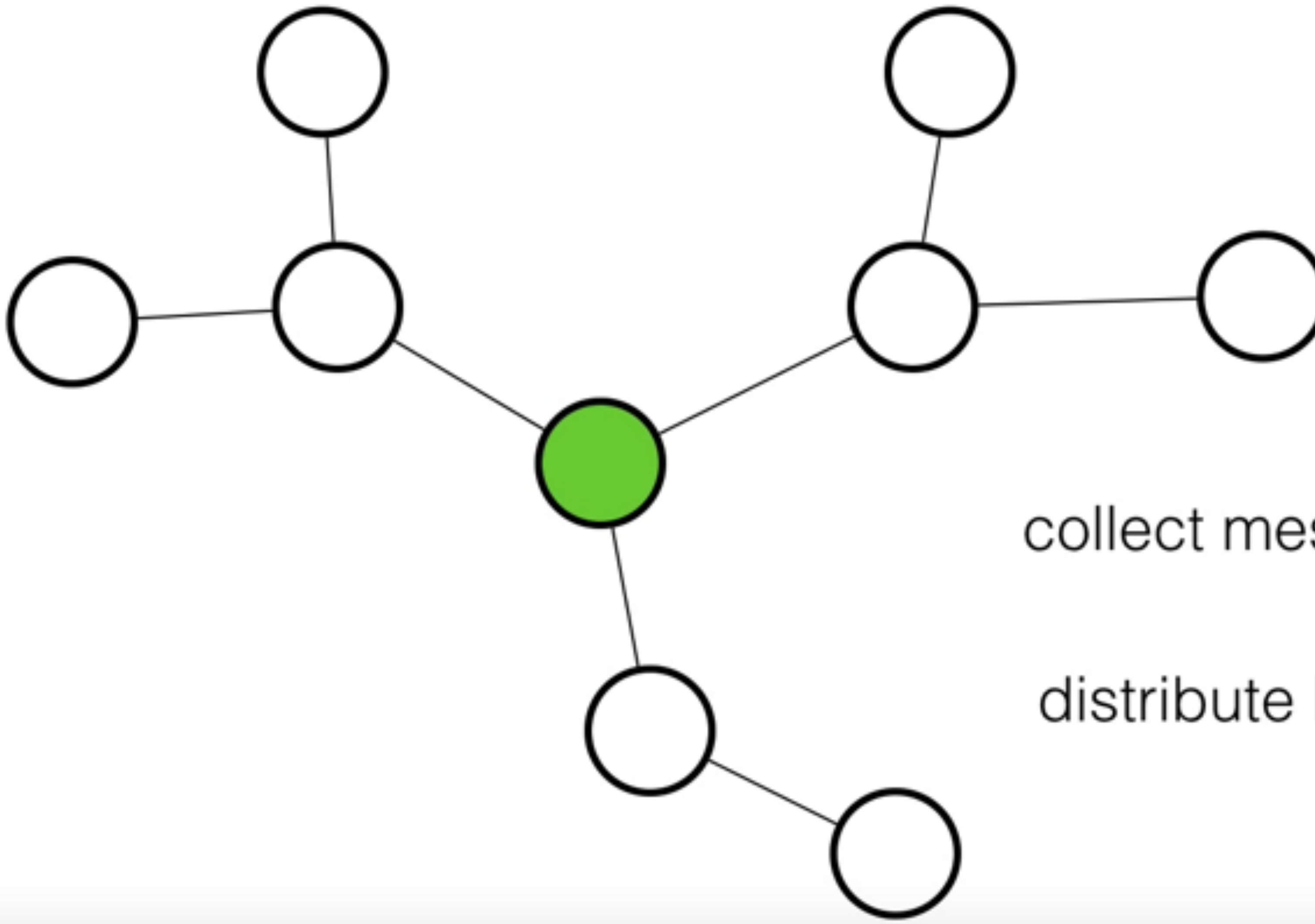
Message Passing on Trees



collect messages to root

(if the graph is a tree, any node can be a root)

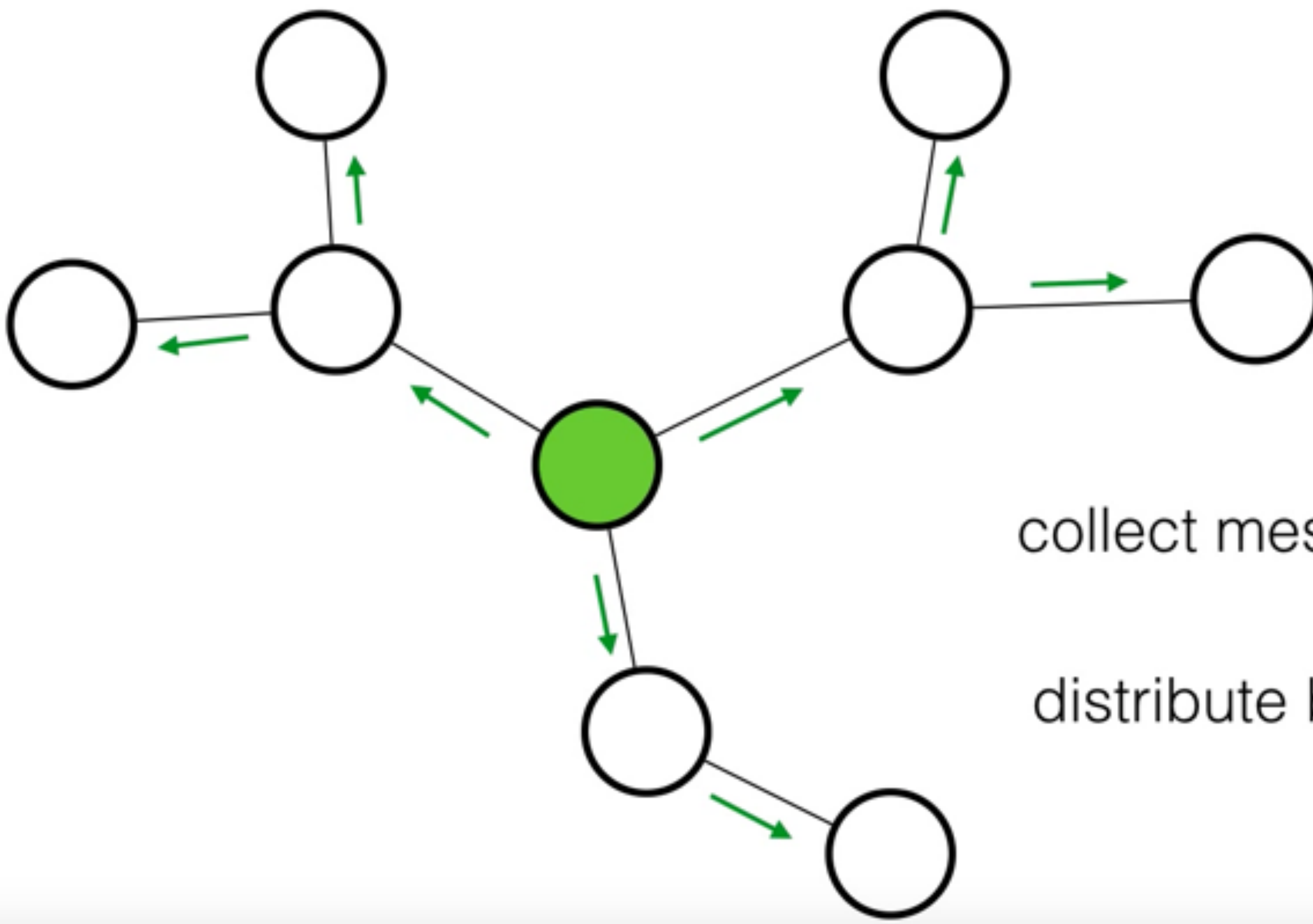
Message Passing on Trees



collect messages to root

distribute back to leaves

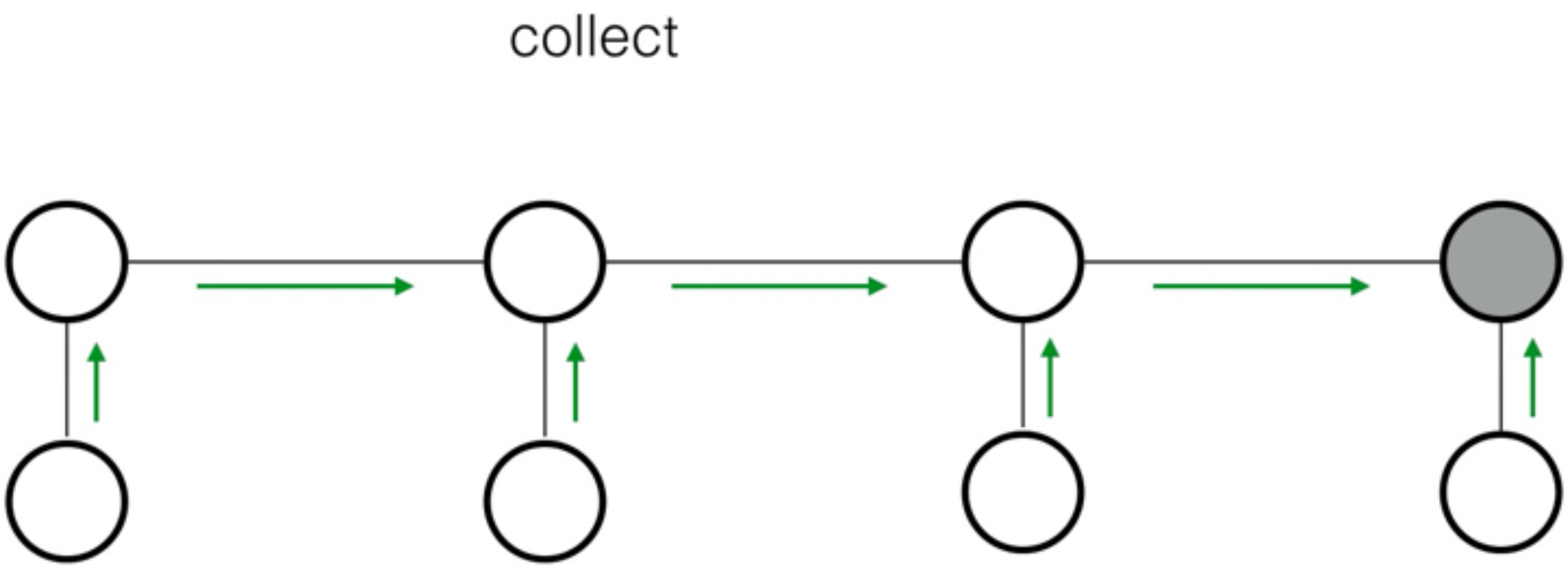
Message Passing on Trees



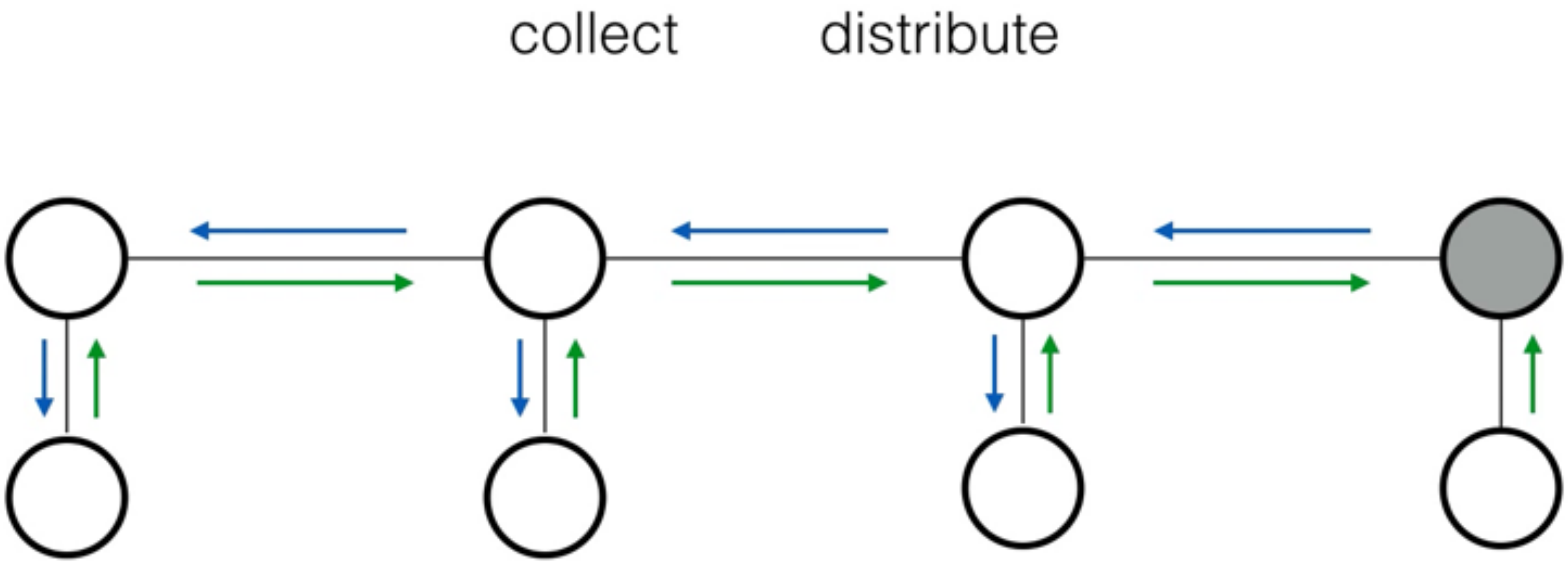
collect messages to root

distribute back to leaves

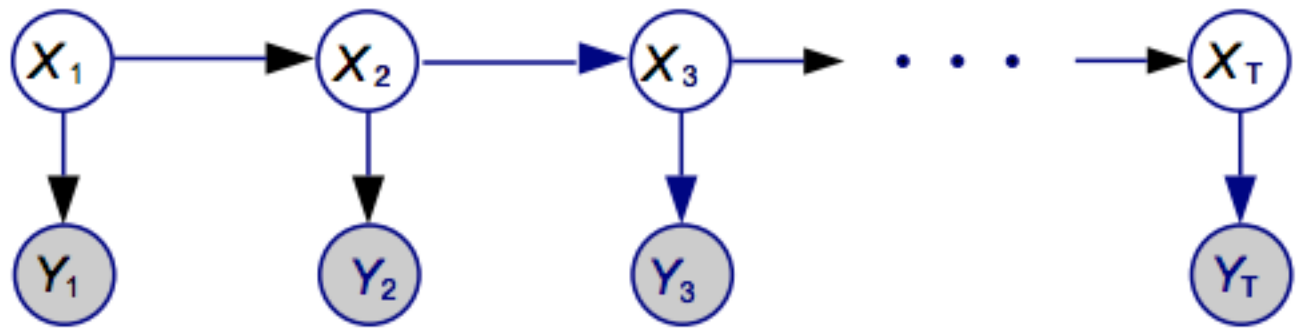
Forward-Backward in HMM



Forward-Backward in HMM



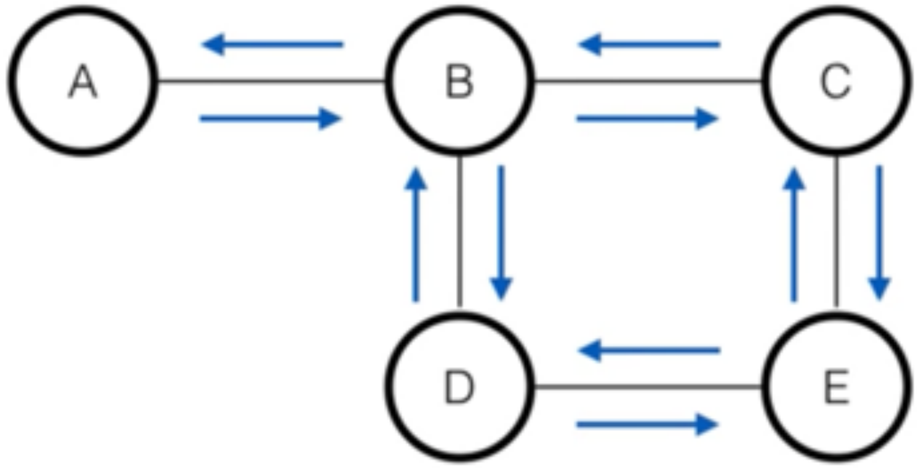
Inference in Hidden Markov Models and Linear Gaussian state-space models



$$p(X_{1,\ldots,T}, Y_{1,\ldots,T}) = p(X_1)p(Y_1|X_1)\prod_{t=2}^{T}[p(X_t|X_{t-1})p(Y_t|X_t)]$$

- In HMMs, the states X_t are discrete.
- In linear Gaussian SSMs, the states are real Gaussian vectors.
- Both HMMs and SSMs can be represented as singly connected DAGs.
- The forward–backward algorithm in hidden Markov models (HMMs), and the Kalman smoothing algorithm in SSMs are both instances of belief propagation / factor graph propagation.

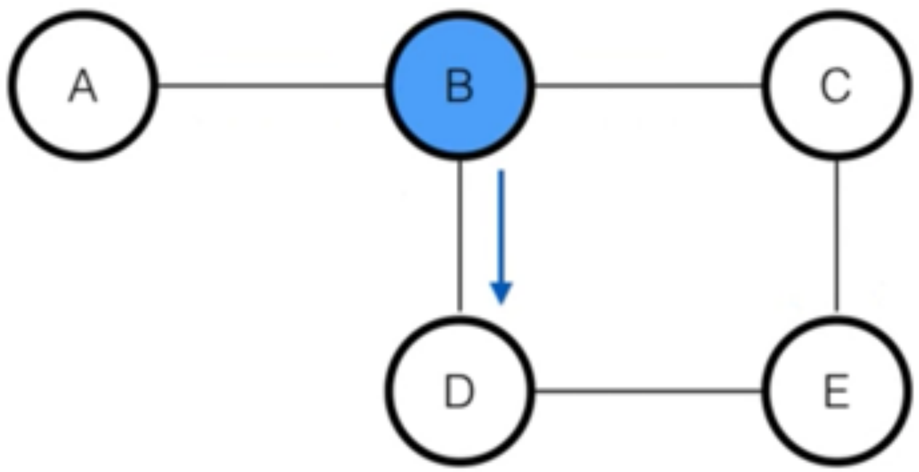
Loopy Belief Propagation



$$b_t(x_t) \propto \prod_{s \in \text{neighbors}(t)} m_{t \to s}(x_s)$$

$$m_{s \to t}(x_t) := \sum_{x_s} \left(\phi_{st}(x_s, x_t) \prod_{u \in \text{neighbors}(s) \setminus t} m_{u \to s}(x_s) \right)$$

Loopy Belief Propagation



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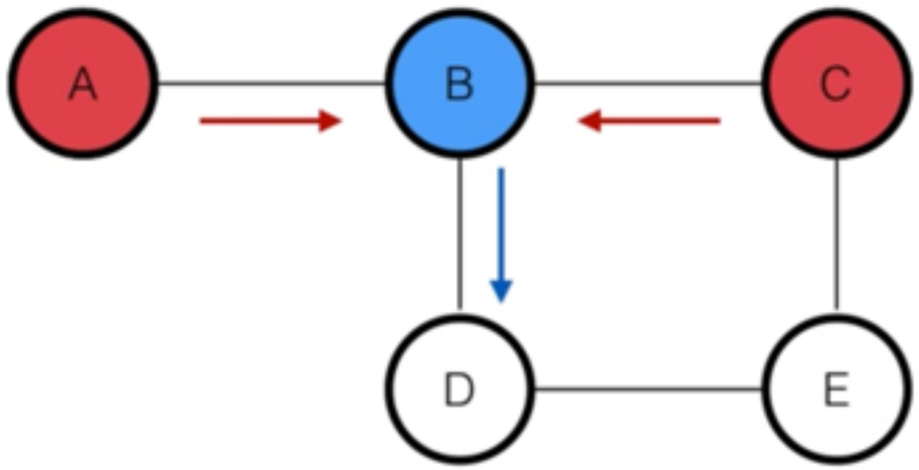
Loopy Belief Propagation

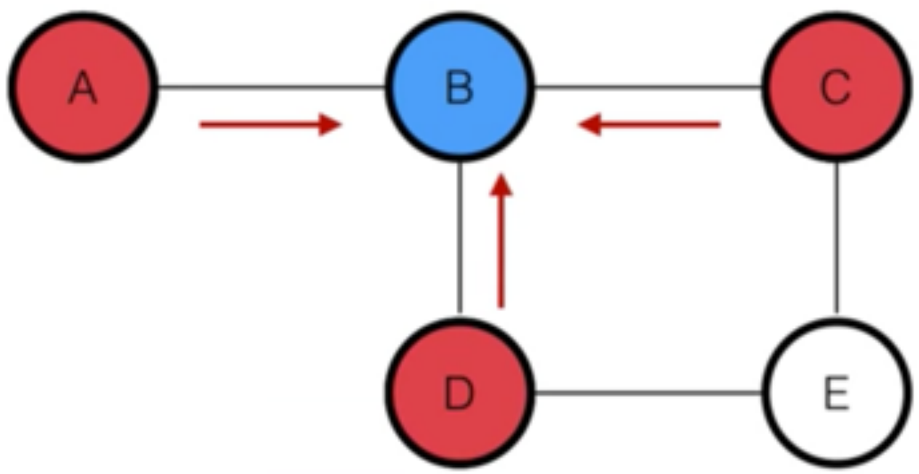


$$b_t(x_t) \propto \prod_{s \in \text{neighbors}(t)} m_{t \to s}(x_s)$$

$$m_{s \to t}(x_t) := \sum_{x_s} \left(\phi_{st}(x_s, x_t) \prod_{u \in \text{neighbors}(s) \setminus t} m_{u \to s}(x_s) \right)$$

$$m_{B \to D}(x_D) = \sum_{x_B} \phi(x_B, x_C) \times m_{A \to B}(x_B) \times m_{C \to B}(x_B)$$

Loopy Belief Propagation



$$b_t(x_t) \propto \prod_{s \in \text{neighbors}(t)} m_{t\to s}(x_s)$$

$$b_B(x_B) \propto (m_{A\to B}(x_B))(m_{C\to B}(x_B))(m_{D\to B}(x_B))$$

$$m_{s\to t}(x_t) := \sum_{x_s} \left(\phi_{st}(x_s, x_t) \prod_{u \in \text{neighbors}(s)\setminus t} m_{u\to s}(x_s) \right)$$

$$m_{B\to D}(x_D) = \sum_{x_B} \phi(x_B, x_D) \times m_{A\to B}(x_B) \times m_{C\to B}(x_B)$$

Sum-Product Message Passing

- While there is node x_s ready to transmit to x_t, send the message

$$m_{s\to t}(x_t) := \sum_{x_s} \left(\phi(x_s)\phi(x_s, x_t) \prod_{u\in\mathcal{N}(s)-t} m_{u\to s}(x_s) \right)$$

- After computing all messages, any marginal query can be computed in *O(1)*:

$$p(x_t) \equiv b_t(x_t) \propto \prod_{s\in\mathcal{N}(t)} m_{t\to s}(x_s)$$

Sum-Product Messages

- Function of receiving node's variable
- Vectors for discrete variables
- Should be normalized (by taking log)
- Alternate form explicitly encodes **unary** and **pairwise** potentials

$$p(\mathbf{x}) \propto \prod_{s \in \mathcal{V}} \phi_s(x_s) \prod_{(s,t) \in \mathcal{E}} \phi_{st}(x_s, x_t)$$

Max-Product Message Passing

Consider MAP query $$\max_{x_1,\ldots,x_n} p(x_1, ..., x_n)$$

Chain MRF, partition function

$$\begin{aligned} Z &= \sum_{x_1} \cdots \sum_{x_n} \phi(x_1) \prod_{i=2}^{n} \phi(x_i, x_{i-1}) \\ &= \sum_{x_n} \sum_{x_{n-1}} \phi(x_n, x_{n-1}) \sum_{x_{n-2}} \phi(x_{n-1}, x_{n-2}) \cdots \sum_{x_1} \phi(x_2, x_1) \phi(x_1). \end{aligned}$$

To compute the mode of $\tilde{p}(x_1, ..., x_n)$

$$\begin{aligned} \tilde{p}^* &= \max_{x_1} \cdots \max_{x_n} \phi(x_1) \prod_{i=2}^{n} \phi(x_i, x_{i-1}) \\ &= \max_{x_n} \max_{x_{n-1}} \phi(x_n, x_{n-1}) \max_{x_{n-2}} \phi(x_{n-1}, x_{n-2}) \cdots \max_{x_1} \phi(x_2, x_1) \phi(x_1). \end{aligned}$$

Message Passing

- a.k.a Belief Propagation (BP)
- Trees: Guaranteed to converge to marginals
- Trees: Takes just one update per message
- Guarantees not as nice in non-trees
  - only provably converges on trees and on graphs with at most one cycle
  - general graph: treat loopy BP as approximate inference

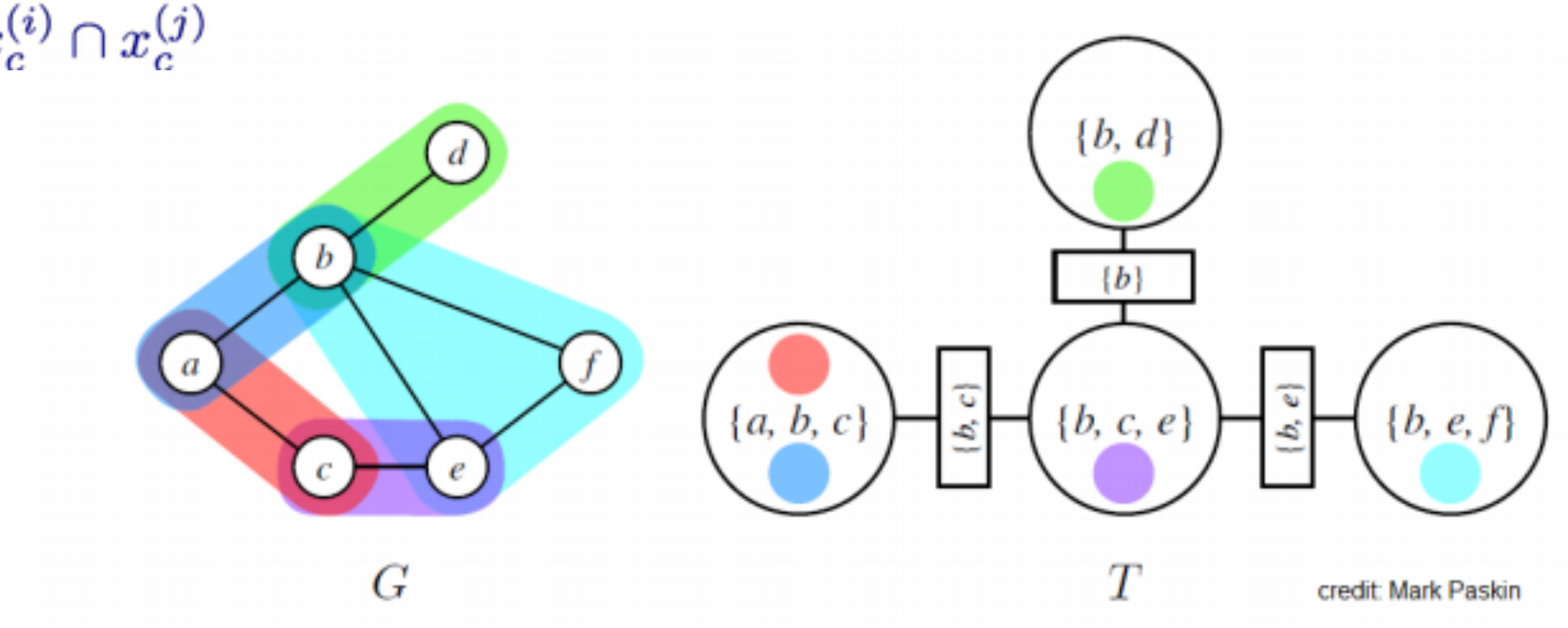
Junction Tree Algorithm

Main idea: Turn graph into a tree of clusters that are amenable to the variable elimination algorithm

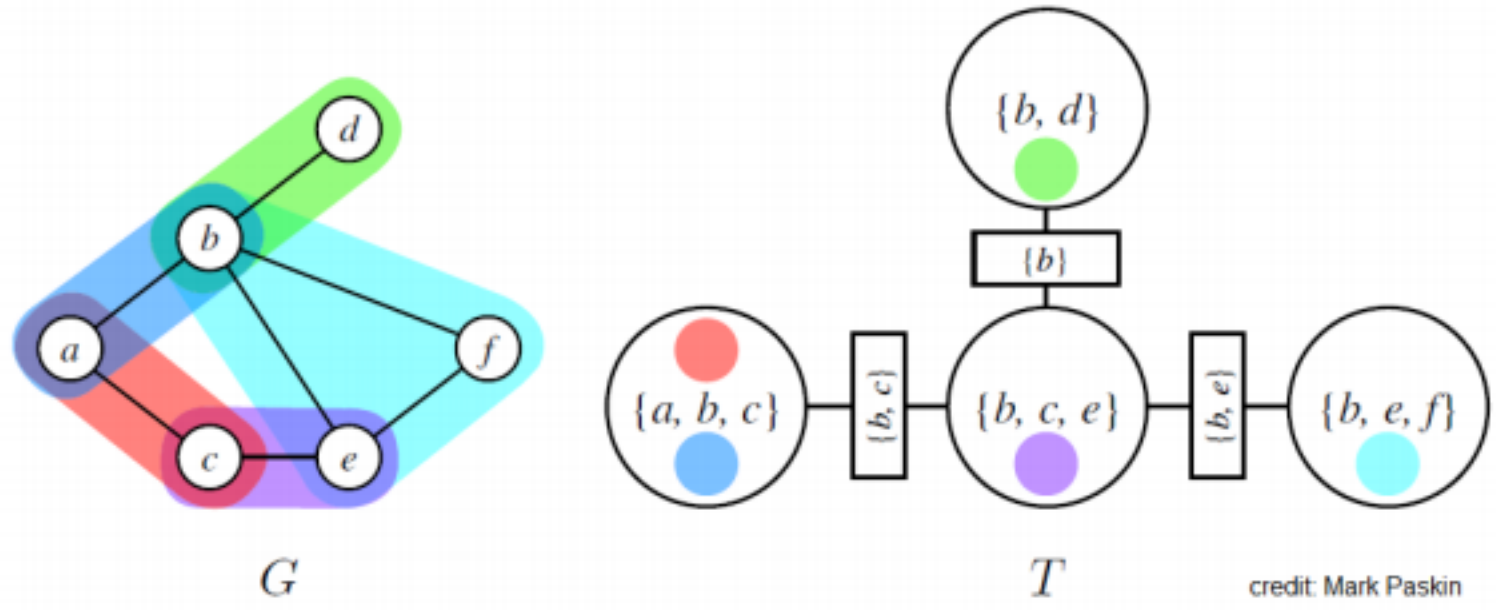
A junction tree $T = (C, E_T)$ over $G = (\mathcal{X}, E_G)$ is a tree whose nodes $c \in C$ are associated with subsets $x_c \in \mathcal{X}$of the graph vertices (i.e. sets of variables); the junction tree must satisfy the following properties:

Family preservation: For each factor ϕ, there exists a cluster c such that $Scope[\phi] \subset x_c$

Running intersection: for every pair of clusters $c^{(i)}, c^{(j)}$, every cluster on the path between $c^{(i)}, c^{(j)}$ contains $x_c^{(i)} \cap x_c^{(j)}$



Junction Tree Algorithm



Redefine potential $\psi_c(x_c) =$ product of all the factors ϕ in G that have been assigned to c

$$p(x_1, .., x_n) = \frac{1}{Z} \prod_{c \in C} \psi_c(x_c).$$

Message Passing between Clique Potentials

- Choose a pair of adjacent clusters c(i), c(j) in T and compute a message whose scope if the sep-set Sij between the two clusters

$$m_{i\to j}(S_{ij}) = \sum_{x_c \setminus S_{ij}} \psi(x_c) \prod_{\ell \in N(i)\setminus j} m_{\ell\to i}(S_{\ell i})$$

- Belief computation: define the belief of each cluster based on all the messages that it receives

$$\beta_c(x_c) = \psi(x_c) \prod_{\ell \in N(i)} m_{\ell\to i}(S_{\ell i}).$$

- Finally marginalizing out the variables in its belief

$$\tilde{p}(x) \propto \sum_{x_c \setminus x} \beta_c(x_c)$$

Finding A Good Junction Tree

- Again NP-Hard
  - By hand: Typically, our models will have a very regular structure, for which there will be an obvious solution. For example, very often our model is a grid, in which case clusters will be associated with pairs of adjacent rows (or columns) in the grid
  - Using variable elimination: One can show that running the VE elimination algorithm implicitly generates a junction tree over the variables. Thus it is possible to use the heuristics we previously discussed to define this ordering