COMP9418: Advanced Topics in Statistical Machine Learning

Belief Propagation

Instructor: Gustavo Batista

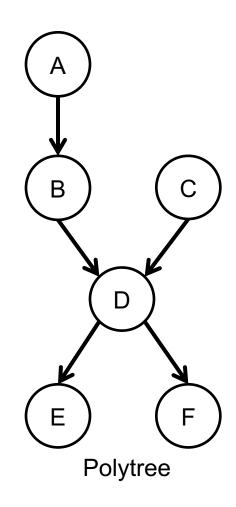
University of New South Wales

Introduction

- In this lecture, we discuss a class of approximate inference algorithms based on belief propagation
 - Belief propagation was introduced as an exact algorithm for networks with polytree structure
 - Later, applied to networks with arbitrary structure and produced high-quality approximations in certain cases
- We introduce generalization of the algorithm with a full spectrum of approximations
 - Belief propagation approximation at one end
 - Exact results at the other

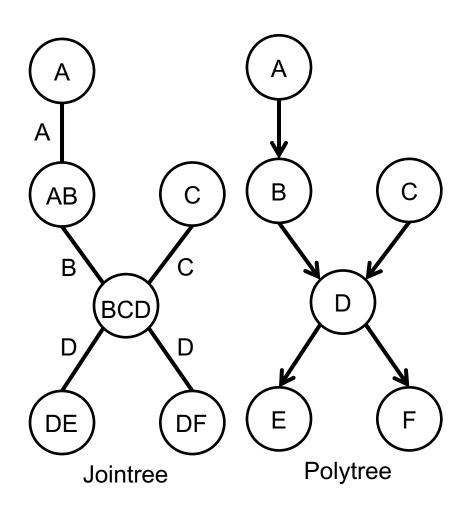
Belief Propagation

- Belief propagation is a messaging-passing algorithm
 - Originally developed for exact inference in polytrees networks
 - A polytree is a network with only one undirected path between any two nodes
- The exact algorithm is a variation of the jointree
 - It computes P(X, e) for every variable in the polytree
 - We discuss the approximate algorithm later on



Belief Propagation

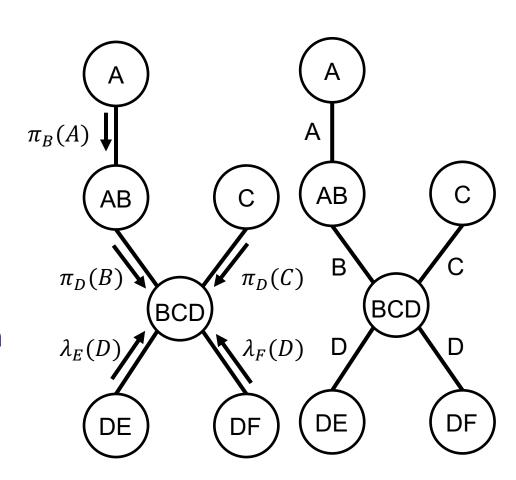
- Suppose we want to apply the jointree algorithm under evidence E = true
 - In this case, we can create a "special" jointree has the same structure as the polytree
 - A node i in the jointree has cluster $C_i = XU$, where U are the parents of X
 - Edge $U \to X$ in the jointree has separator $S_{ij} = U$
- Therefore
 - Jointree width equals polytree treewidth
 - Each jointree message is over a single variable



Belief Propagation

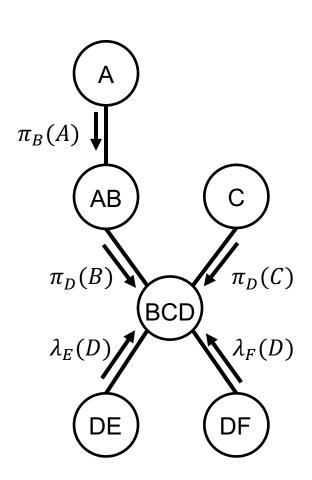
- Belief propagation is the jointree algorithm under these circumstances
 - Messages are notated differently based on the polytree
 - Message from node U to child X is denoted $\pi_X(U)$ (causal support)
 - Messages from node Y to parent X is denoted $\lambda_Y(X)$ (diagnostic support)
- The joint marginal for the family of variable X with parents U_i and children Y_i is given by

$$P(X\boldsymbol{U}) = \phi_X(X, \boldsymbol{U}) \prod_i \pi_X(U_i) \prod_i \lambda_{Y_i}(X)$$



- In the presence of evidence, the belief propagation uses an evidence indicator $\lambda_e(X)$
 - $\lambda_e(x) = 1$ if x is consistent with the evidence e and zero otherwise
 - We can rewrite the joint marginal for the family of variable X with parents U_i , children Y_i and evidence e as

$$P(X\boldsymbol{U},\boldsymbol{e}) = \lambda_{\boldsymbol{e}}(X) \, \phi_{X}(X,\boldsymbol{U}) \prod_{i} \pi_{X}(U_{i}) \prod_{j} \lambda_{Y_{j}}(X)$$



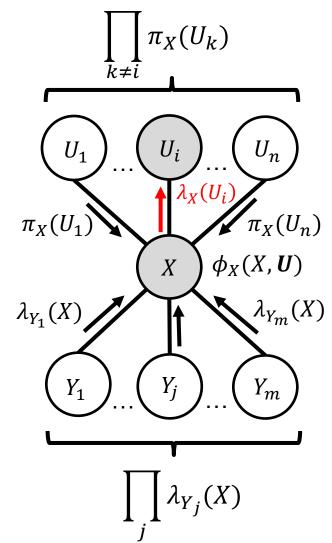
Using this notation, diagnostic messages can be defined as

$$\lambda_X(U_i) = \sum_{X \mathbf{U} \setminus \{U_i\}} \lambda_e(X) \, \phi_X(X, \mathbf{U}) \prod_{k \neq i} \pi_X(U_k) \prod_j \lambda_{Y_j}(X)$$

And causal messages as

$$\pi_{Y_j}(X) = \sum_{\boldsymbol{U}} \lambda_e(X) \, \phi_X(X, \boldsymbol{U}) \prod_i \pi_X(U_i) \prod_{k \neq j} \lambda_{Y_k}(X)$$

 A node can send a message to a neighbour only after it has received messages from all other neighbours



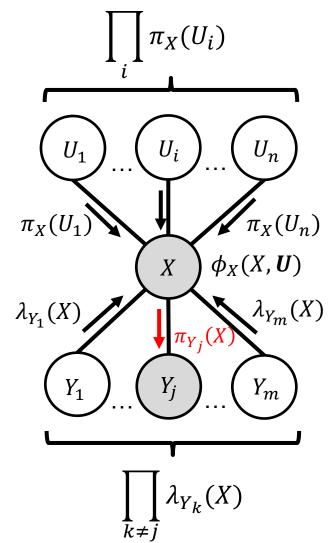
Using this notation, diagnostic messages can be defined as

$$\lambda_X(U_i) = \sum_{X \mathbf{U} \setminus \{U_i\}} \lambda_e(X) \, \phi_X(X, \mathbf{U}) \prod_{k \neq i} \pi_X(U_k) \prod_j \lambda_{Y_j}(X)$$

And causal messages as

$$\pi_{Y_j}(X) = \sum_{\boldsymbol{U}} \lambda_e(X) \, \phi_X(X, \boldsymbol{U}) \prod_i \pi_X(U_i) \prod_{k \neq j} \lambda_{Y_k}(X)$$

 A node can send a message to a neighbour only after it has received messages from all other neighbours



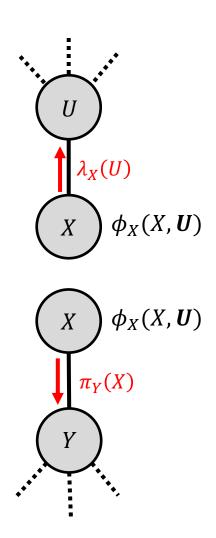
- When a node has a single neighbour, it can immediately send a message to that neighbour
 - This includes a leaf node X with a single parent U

$$\lambda_X(U) = \sum_X \lambda_e(X) \, \phi_X(X, U)$$

And a root node X with a single child Y

$$\pi_Y(X) = \lambda_e(X)\phi_X(X, U)$$

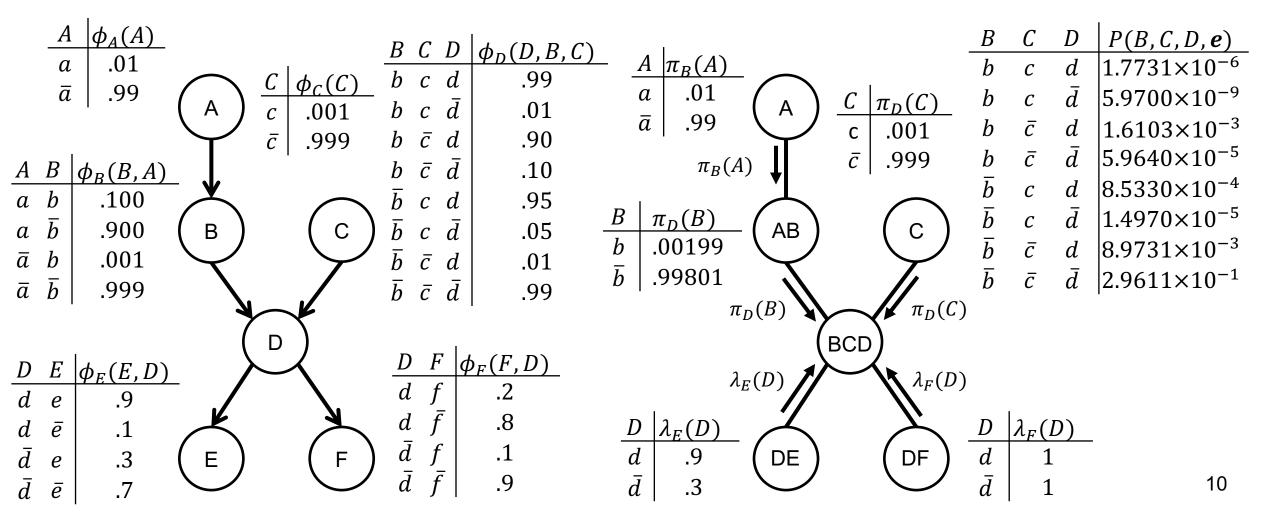
- These are the base cases for belief propagation
 - These messages can be computed immediately as they do not depend on any other messages
 - Typically, messages are first propagated toward a root and them pushed away from root



Belief Propagation: Example

$$P(B, C, D, \mathbf{e}) = \phi_D(D, B, C)\pi_D(B)\pi_D(C)\lambda_E(D)\lambda_F(D)$$

e: $\{E = true\}$



Belief Propagation: Example

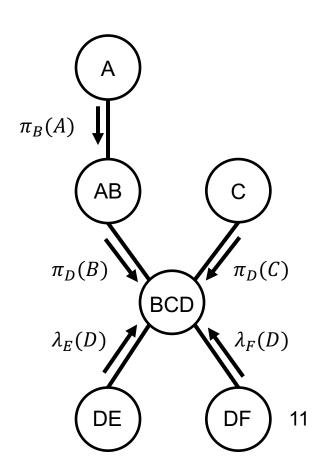
- We can use P(B, C, D, e) to compute marginals for the variables B, C and D. For instance
- $\begin{array}{c|c}
 C & P(C, e) \\
 \hline
 c & .0009 \\
 \hline
 \bar{c} & .3067
 \end{array}$

- We can also compute the joint marginal for C once we compute the message from D to C
- To compute conditional marginals, we simply normalize joint marginals
- Another approach is to use a constant η that normalizes the factor to sum to one

$$P(X\boldsymbol{U}|\boldsymbol{e}) = \eta \ \lambda_{\boldsymbol{e}}(X) \ \phi_{X}(X,\boldsymbol{U}) \prod_{i} \pi_{X}(U_{i}) \prod_{j} \lambda_{Y_{j}}(X)$$

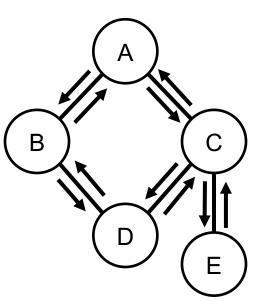
$$\lambda_{X}(U_{i}) = \eta \sum_{X\boldsymbol{U}\setminus\{U_{i}\}} \lambda_{\boldsymbol{e}}(X) \ \phi_{X}(X,\boldsymbol{U}) \prod_{k\neq i} \pi_{X}(U_{k}) \prod_{j} \lambda_{Y_{j}}(X)$$

$$\pi_{Y_{j}}(X) = \eta \sum_{\boldsymbol{U}} \lambda_{\boldsymbol{e}}(X) \ \phi_{X}(X,\boldsymbol{U}) \prod_{i} \pi_{X}(U_{i}) \prod_{k\neq j} \lambda_{Y_{k}}(X)$$



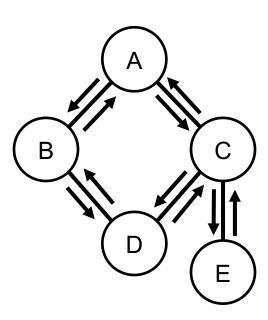
Belief Propagation in Connected Networks

- Belief propagation was designed as an exact algorithm for polytrees
 - However, it was later applied to connected networks
- This application poses some difficulties
 - A message can be sent from X to Y only when X has received all messages from other neighbours
 - The correctness of belief propagation depends on the underlying polytree
- The results can be incorrect if applied to connected networks
 - The algorithm is no longer always correct
 - But can still provide some high-quality approximations in many cases
- In the figure, after node *E* send a message to *C* no other message can be propagated
 - Since each is dependent on others that are waiting to be propagated



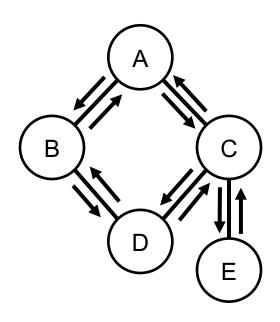
Iterative Belief Propagation (IBP)

- Iterative or Loopy Belief Propagation assumes some initial value to each message in the network
 - Given these initial values, each node is ready to send a message to each of its neighbours
 - At each iteration t, every node X send a message to its neighbours using the messages received from its other neighbours in t-1
- The algorithm iterates until message convergence
 - The value of messages at the current iteration are within some threshold from their values at the previous iteration
 - When IBP converges, the values of the messages at convergence are called fixed point
 - IBP may have multiple fixed points on a given network



Message Schedule

- For some networks, IBP can oscillate and never converge
- The convergence rate can depend on the order the messages are propagated, which is known as message schedule
 - Parallel schedule: the order of the messages does not affect the algorithm
 - Sequential schedule: messages are propagates as soon as they are computed
- Sequential schedules are flexible in when and how quickly information is propagated
- Although one schedule may converge and other may not, all schedules have the same fixed points



Parallel Iterative Belief Propagation

```
t \leftarrow 0
initialize all messages
while messages have not converged do
         t \leftarrow t + 1
         for each node X with parents U do
                  for each parent U_i do
                             \lambda_X^t(U_i) = \eta \sum_{X \mathbf{U} \setminus \{U_i\}} \lambda_e(X) \, \phi_X(X, \mathbf{U}) \prod_{k \neq i} \pi_X^{t-1}(U_k) \prod_j \lambda_{Y_i}^{t-1}(X)
                  for each child Y_i do
                             \pi_{Y_i}^t(X) = \eta \sum_{U} \lambda_e(X) \phi_X(X, U) \prod_i \pi_X^{t-1}(U_i) \prod_{k \neq j} \lambda_{Y_k}^{t-1}(X)
return \beta(X\boldsymbol{U}) = P(X\boldsymbol{U}|\boldsymbol{e}) = \eta \ \lambda_{\boldsymbol{e}}(X) \ \phi_{X}(X,\boldsymbol{U}) \prod_{i} \pi_{X}^{t}(U_{i}) \prod_{j} \lambda_{Y_{i}}^{t}(X)
```

The Kullback-Leibler Divergence

The Kullback-Leibler divergence, known as KL divergence, between two distributions P
and P' conditioned on e

$$KL(P'(X|e), P(X|e)) \stackrel{\text{def}}{=} \sum_{x} P'(x|e) \log \frac{P'(x|e)}{P(x|e)}$$

- KL(P'(X|e), P(X|e)) is non-negative and equal to zero if and only if P'(X|e) and P(X|e) are equivalent
 - However, KL divergence is not a true distance since it is not symmetric. In general $KL(P'(X|e), P(X|e)) \neq KL(P(X|e), P'(X|e))$
 - We say we are weighting the KL divergence by the approximate distribution
 - This variation has some useful computational properties

Optimizing KL Divergence

- The approximate inference can be posed as an optimization problem
 - The goal is to search for an approximate distribution P' that minimizes KL divergence with P
 - We can assume a parametrized form for P' and search for the best instance, i.e., the best set of parameters
- The Iterative Belief Propagation algorithm presented before assumes that the approximate distribution P'(X) factors as

$$P'(X|e) = \prod_{XU} \frac{P'(XU|e)}{\prod_{U \in U} P'(U|e)}$$

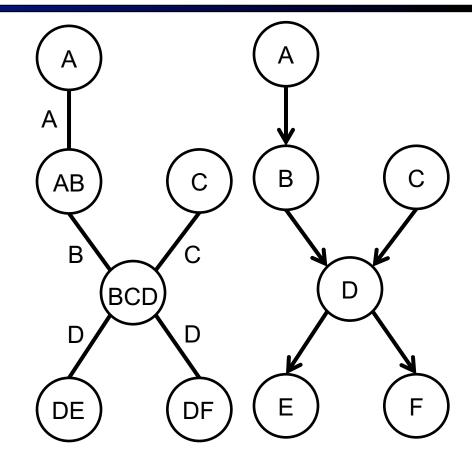
- XU ranges over the families of the network N
- U ranges over nodes that appear as parents in N

Optimizing KL Divergence

• The approximate distribution P'(X) factors as

$$P'(X|e) = \prod_{XU} \frac{P'(XU|e)}{\prod_{U \in U} P'(U|e)}$$

- XU ranges over the families of the network N
- U ranges over nodes that appear as parents in N
- Some observations about this assumption
 - This choice of P'(X|e) is expressive enough to describe distributions induced by polytree networks
 - If the network N is a polytree then P(X|e) does factor according to this equation (see figure for an example)
 - If N is not a polytree, then we are trying to fit P(X|e) into an approximation P'(X|e) as if it were generated by a polytree



$$\frac{P(A,B,C,D,E,F) =}{P(A)P(C)P(B,A)P(D,B,C)P(E,D)P(F,D)}$$
$$\frac{P(A)P(B)P(C)P(D)P(D)}{P(A)P(B)P(C)P(D)P(D)}$$

Optimizing KL Divergence

- The previous correspondence that IBP fixed points are stationary points of the KL divergence
 - They may or may not be local minima
 - When IBP performs well, it often has fixed points that are minima of the KL divergence
 - Otherwise, we need to seek approximations P' whose factorizations are more expressive than the polytree-based factorization
- If we do not insist on marginals being over families and individual variables, we can have a more general form that covers every distribution

Generalized Belief Propagation

 We saw in the previous lecture that a network can be factorized according to this this expression if

 $P'(X|e) = \frac{\prod_{C} P'(C|e)}{\prod_{S} P'(S|e)}$

- C corresponds to the clusters of a jointree
- S corresponds to the separators
- If we base our factorization in a jointree
 - Solving the previous optimization problem yields the same update equations of the jointree algorithm
- Therefore, the factorizations used by IBP and the factorization based on jointrees can be viewed as two extremes
 - One efficient but approximate
 - The other expensive but exact

Joingraphs

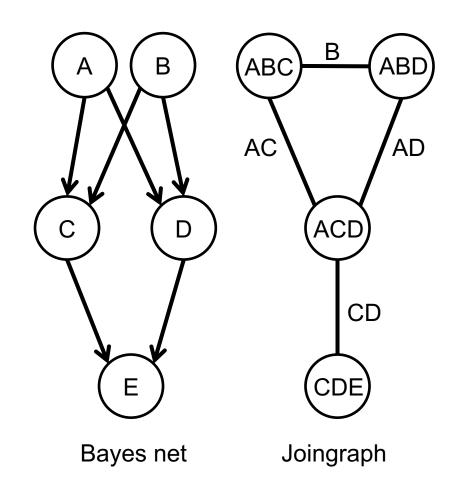
- There is a spectrum of factorizations that fall in between these two extremes
 - This allows a trade-off quality and efficiency
 - The notion of joingraph is one way to obtain such a spectrum

- Joingraphs are generalizations of jointrees
 - They can be used to obtain factorizations according to $P'(X|e) = \frac{\prod_{C} P'(C|e)}{\prod_{S} P'(S|e)}$
 - They are used to formulate a message-passing algorithm similar to IBF, known as iterative joingraph propagation

Joingraphs

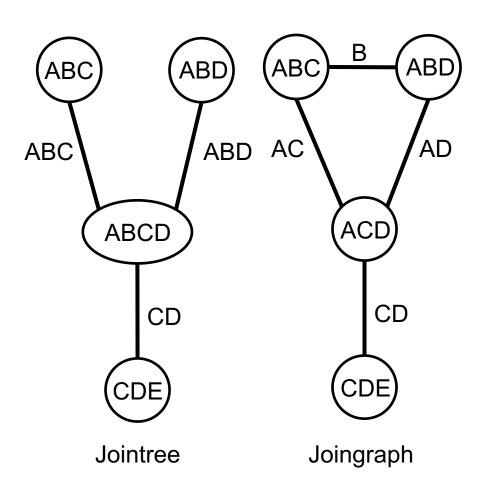
- A joingraph G for a network N is a graph where nodes i are labelled by cluster C_i , and edges i-j are labelled by separators S_{ij} .

 Moreover, G satisfies the following properties
 - Clusters C_i and separators S_{ij} are sets of nodes from N
 - Each factor in N must appear in some cluster C_i
 - If a variable X appears in two clusters C_i and C_j , then there exists a unique path connecting i and j in the joingraph such that X appears in every cluster and separator on that path
 - For every edge i-j in the joingraph, $m{S}_{ij} \subseteq m{C}_i \cap m{C}_j$



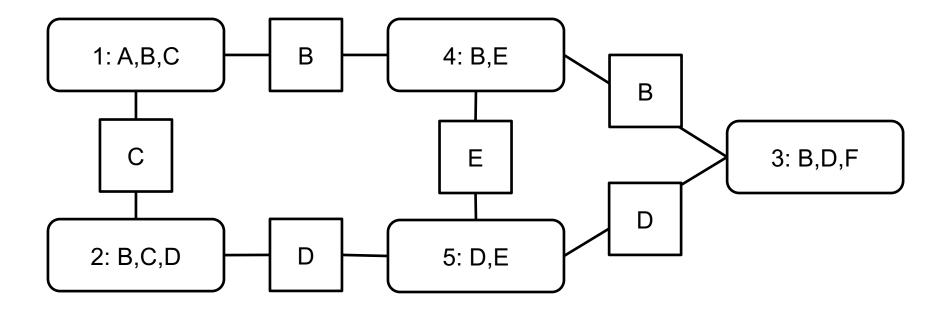
Jointrees and Joingraphs

- We can think of a jointgraph as a way of relaxing some constraints of jointrees
 - In a jointree, if two clusters C_i and C_j share a set of variables X then every cluster and separator on the path connecting C_i and C_j must contain X
 - In a joingraph, we assert each variable $X \in X$ be contained in clusters and separators of some path connecting C_i and C_j
 - We do not require separators S_{ij} to be precisely the intersection of C_i and C_j , as in the case of jointrees



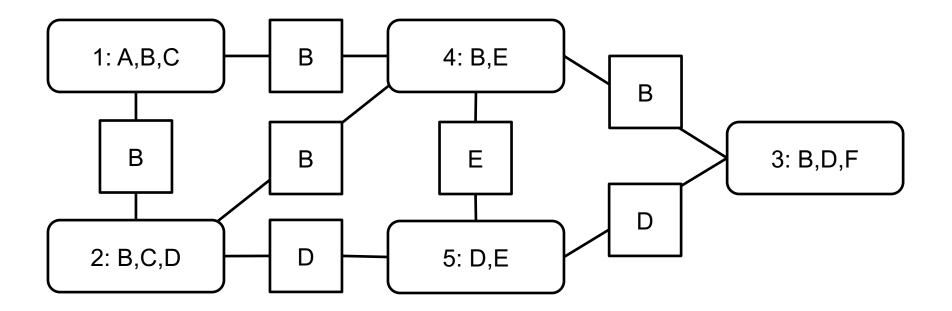
Valid Joingraph?

 $\phi_1(A,B,C), \phi_2(B,C), \phi_3(B,D), \phi_4(D,E), \phi_5(B,E), \phi_6(B,D), \phi_7(B,D,F)$



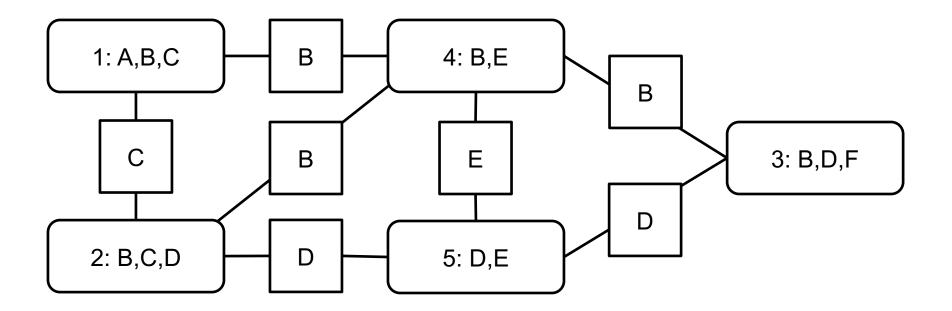
Valid Joingraph?

 $\phi_1(A,B,C), \phi_2(B,C), \phi_3(B,D), \phi_4(D,E), \phi_5(B,E), \phi_6(B,D), \phi_7(B,D,F)$



Valid Joingraph?

 $\phi_1(A,B,C), \phi_2(B,C), \phi_3(B,D), \phi_4(D,E), \phi_5(B,E), \phi_6(B,D), \phi_7(B,D,F)$

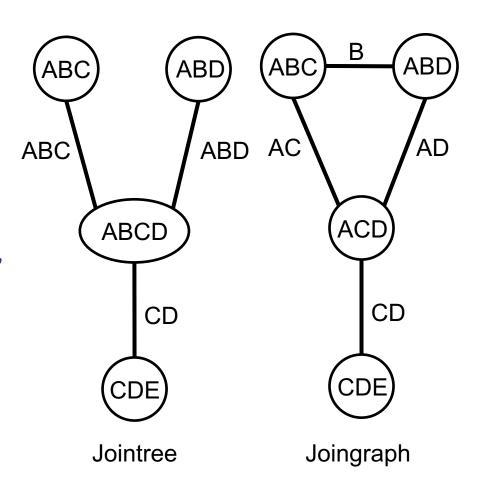


Joingraph Factorization

A joingraph induces an approximate factorization

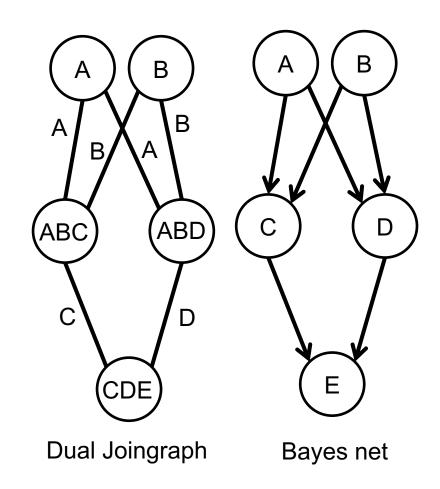
$$P'(X|e) = \frac{\prod_{i} P'(C_i|e)}{\prod_{ij} P'(S_{ij}|e)}$$

 When the joingraph corresponds to a jointree, the factorization is exact



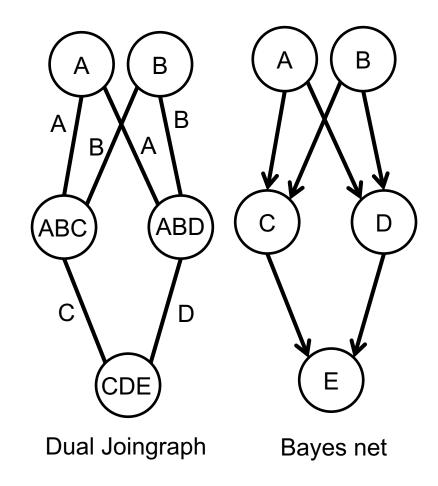
Dual Joingraph

- A dual joingraph is a special joingraph whose factorization reduces to the one used by IBP
- A dual joingraph G for a network N is obtained as follows
 - G has the same undirected structure as N
 - For each family XU in N, the corresponding node i in G has the cluster $C_i = XU$
 - For each $U \to X$ in N, the corresponding edge i-j in G has separator $\mathbf{S}_{ij} = U$



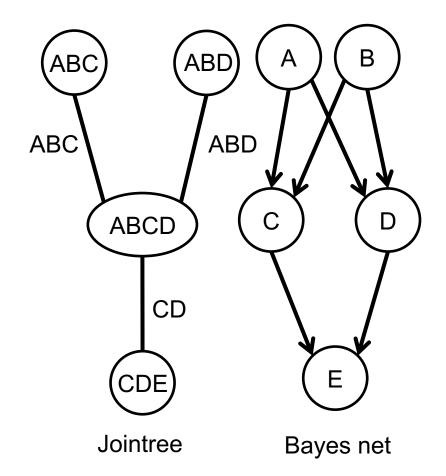
28

Dual jointgraph (approximate, same as IBP) $P'(X|e) = \frac{P'(A|e)P'(B|e)P'(A,B,C|e)P'(A,B,D|e)P'(C,D,E|e)}{P'(A|e)^2P'(B|e)^2P'(C|e)P'(D|e)}$

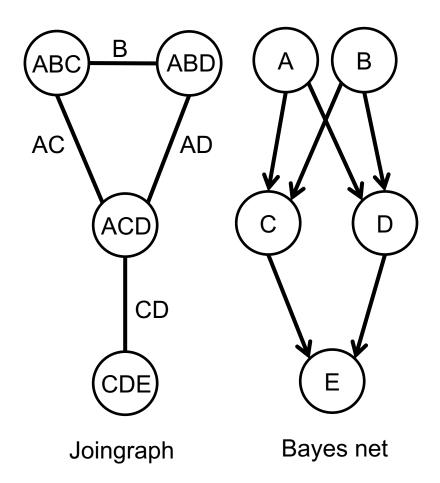


- Dual jointgraph (approximate, same as IBP) $P'(X|e) = \frac{P'(A|e)P'(B|e)P'(A,B,C|e)P'(A,B,D|e)P'(C,D,E|e)}{P'(A|e)^2P'(B|e)^2P'(C|e)P'(D|e)}$
- Jointree (exact)

$$P'(\boldsymbol{X}|\boldsymbol{e}) = \frac{P'(A,B,C|\boldsymbol{e})P'(A,B,D|\boldsymbol{e})P'(A,B,C,D|\boldsymbol{e})P'(C,D,E|\boldsymbol{e})}{P'(A,B,C|\boldsymbol{e})P'(A,B,D|\boldsymbol{e})P'(C,D|\boldsymbol{e})}$$

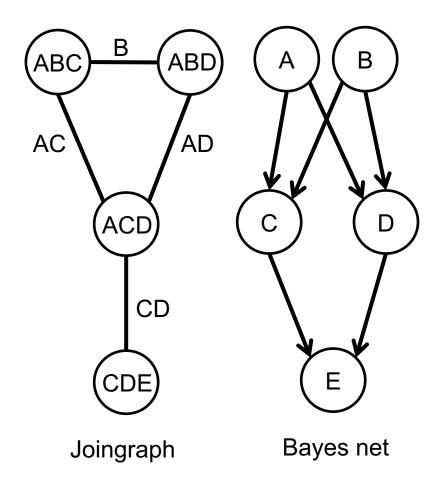


- Dual jointgraph (approximate, same as IBP) $P'(X|e) = \frac{P'(A|e)P'(B|e)P'(A,B,C|e)P'(A,B,D|e)P'(C,D,E|e)}{P'(A|e)^2P'(B|e)^2P'(C|e)P'(D|e)}$
- Jointree (exact) $P'(X|e) = \frac{P'(A,B,C|e)P'(A,B,D|e)P'(A,B,C,D|e)P'(C,D,E|e)}{P'(A,B,C|e)P'(A,B,D|e)P'(C,D|e)}$
- Joingraph (trade complexity and quality) $P'(X|e) = \frac{P'(A,B,C|e)P'(A,B,D|e)P'(A,C,D|e)P'(C,D,E|e)}{P'(B|e)P'(A,C|e)P'(A,D|e)P'(C,D|e)}$



Joingraph (trade complexity and quality)

$$P'(\boldsymbol{X}|\boldsymbol{e}) = \frac{P'(A,B,C|\boldsymbol{e})P'(A,B,D|\boldsymbol{e})P'(A,C,D|\boldsymbol{e})P'(C,D,E|\boldsymbol{e})}{P'(B|\boldsymbol{e})P'(A,C|\boldsymbol{e})P'(A,D|\boldsymbol{e})P'(C,D|\boldsymbol{e})}$$



Iterative Joingraph Propagation

- Suppose we have a network N that induces a distribution P
 - And a corresponding joingraph that induces a factorization P'
 - Also, we want to compute cluster marginals $P'(C_i|e)$ and separator marginals $P'(S_{ij}|e)$ that minimize the KL divergence between P(X|e) and P'(X|e)
- This optimization problem can be solved with a generalization of IBP called interactive joingraph propagation (IJGP)

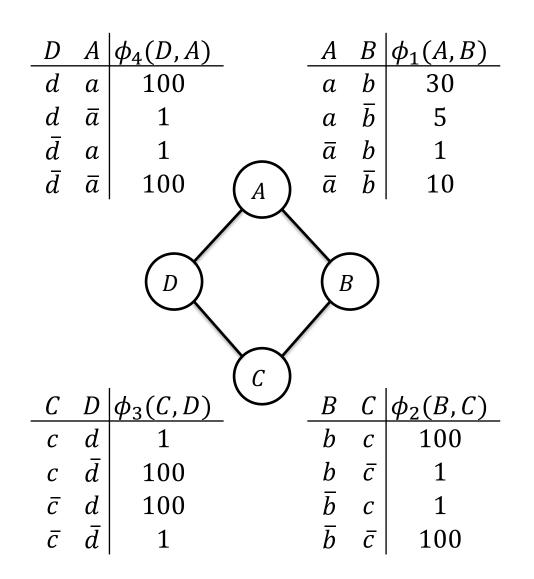
Iterative Joingraph Propagation

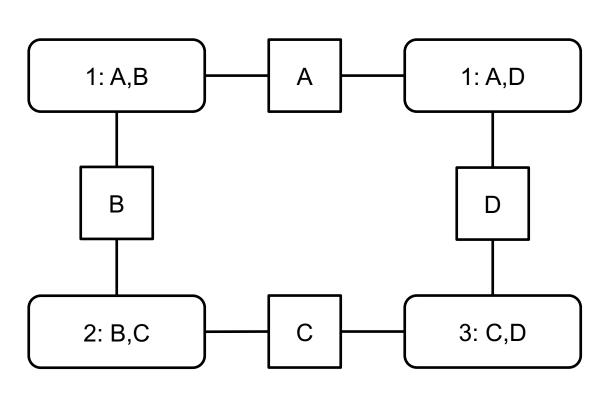
- The algorithm starts assigning each network factor ϕ and evidence indicator λ_e to some cluster C_i that contains variables in ϕ
 - All factors are associated to some cluster (no information loss)
 - No factor is present in more than one cluster (no overcounting of information)
- It propagates messages with the equations
 - $M_{ij} = \eta \sum_{C_i \setminus S_{ij}} \psi_i \prod_{k \neq j} M_{ki}$
 - where ψ_i is the product of all CPTs and evidence indicators assigned to cluster \pmb{C}_i
 - M_{ij} is the message sent from cluster i to cluster j

Parallel Iterative Joingraph Propagation

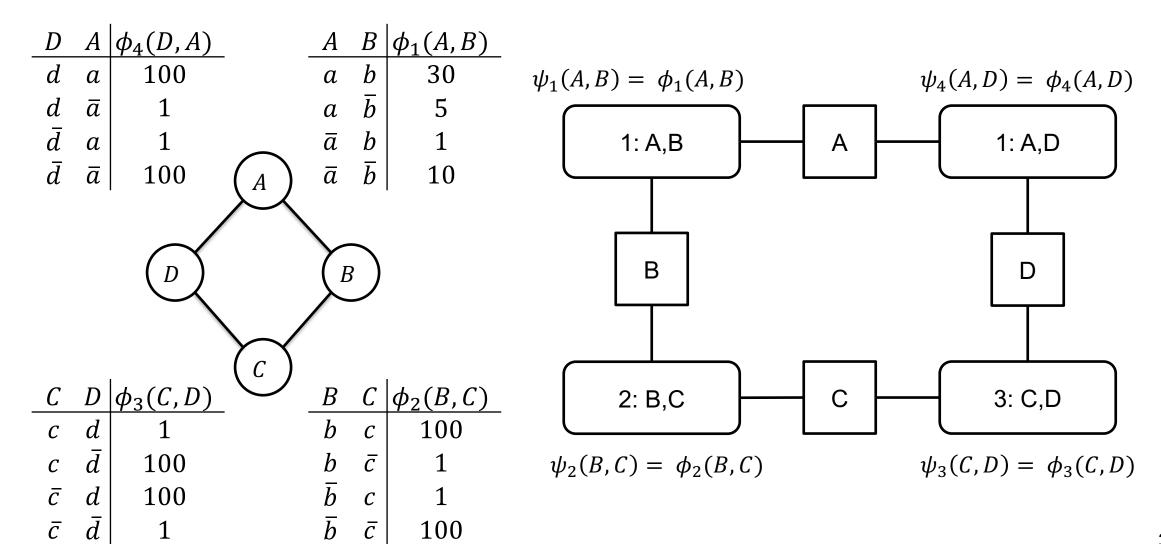
```
initialize all messages  \begin{aligned} \textbf{while} & \text{ messages have not converged } \textbf{do} \\ & t \leftarrow t+1 \\ & \textbf{ for each joingraph edge } i-j \textbf{ do} \\ & M_{ij}^t = \eta \sum_{\boldsymbol{C}_i \backslash \boldsymbol{S}_{ij}} \psi_i \prod_{k \neq j} M_{ki}^{t-1} \\ & M_{ji}^t = \eta \sum_{\boldsymbol{C}_i \backslash \boldsymbol{S}_{ij}} \psi_i \prod_{k \neq i} M_{kj}^{t-1} \\ & \textbf{return } \boldsymbol{\beta}(\boldsymbol{C}_i) = \eta \ \psi_i \prod_k M_{ki}^t \ \text{for each node } i \end{aligned}
```

Joingraph Example with Markov Nets

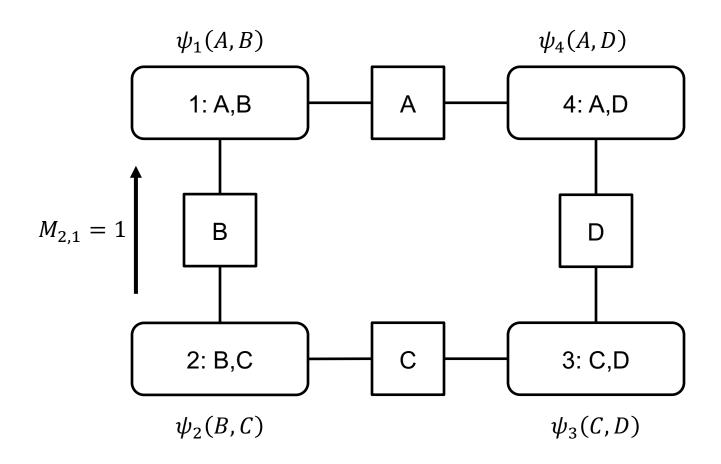




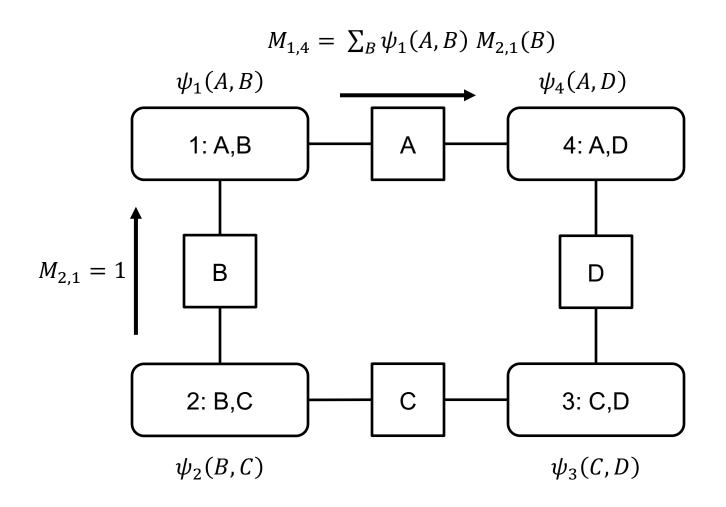
Joingraph Example with Markov Nets



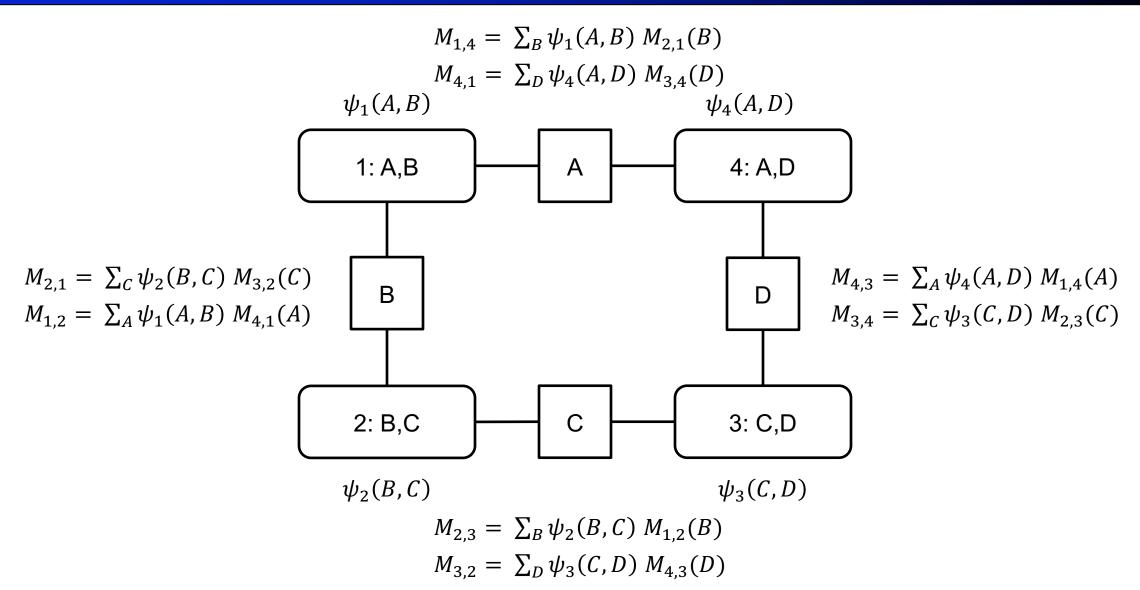
Joingraph Example with Markov Nets



Message Passing with Markov Nets



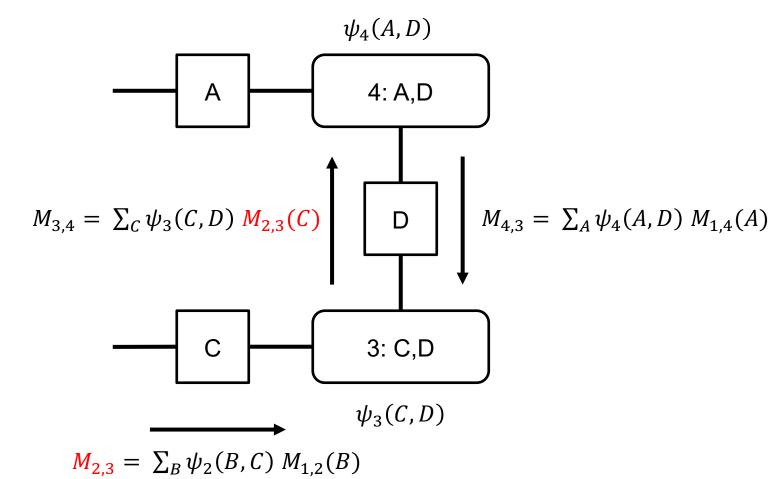
Message Passing with Markov Nets



Message Passing: Avoid Self-Beliefs

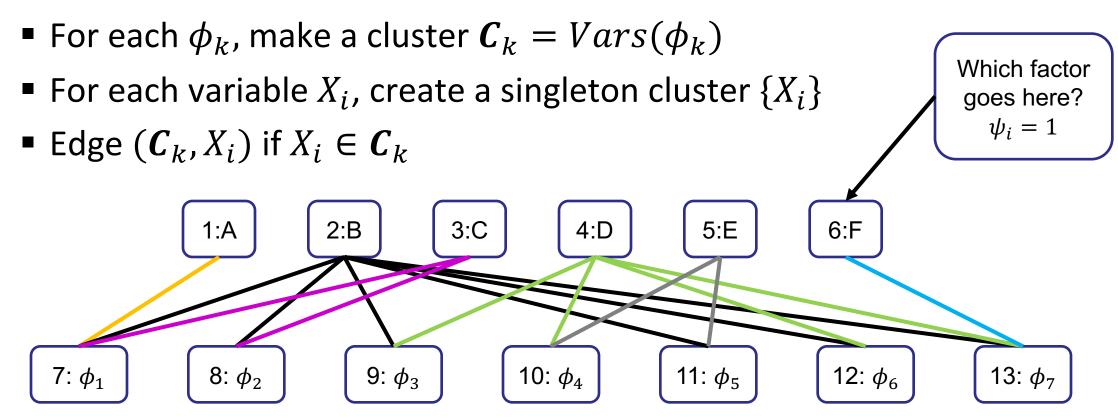
Notice that

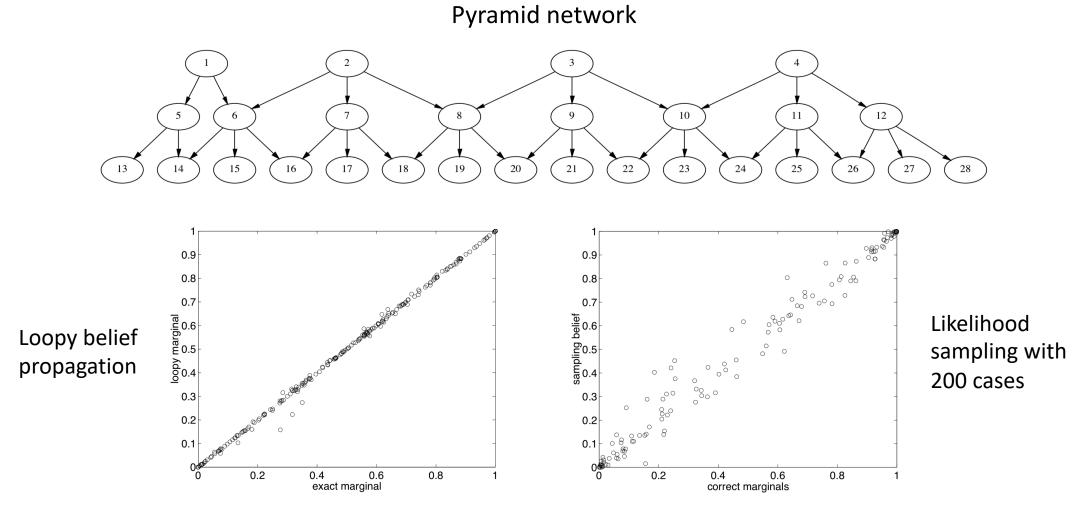
- $M_{3,4}$ only considers information received from 2 $(M_{2,3})$
- Therefore, ignoring information from 4
- This helps to avoid reinforcing selfbeliefs



Bethe Graph

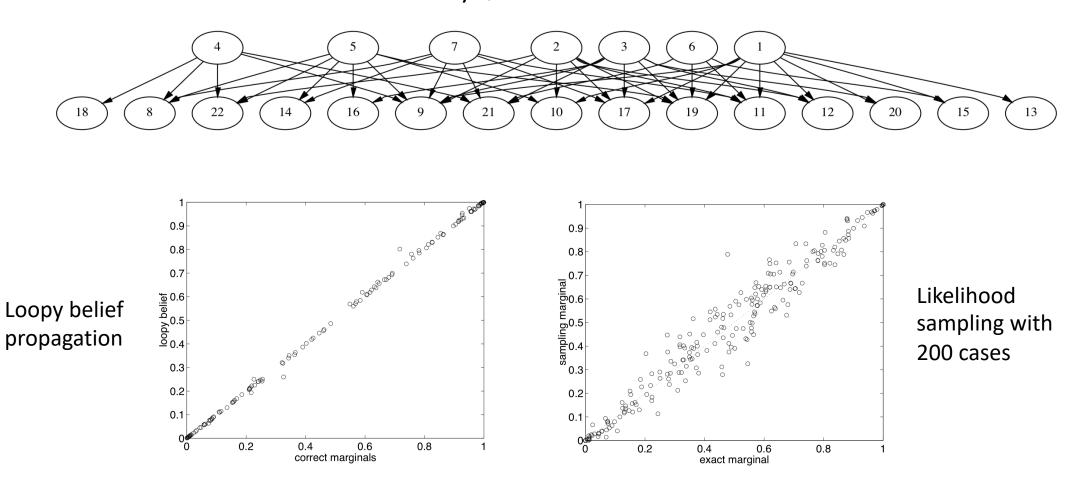
A simple way to generate a valid joingraph



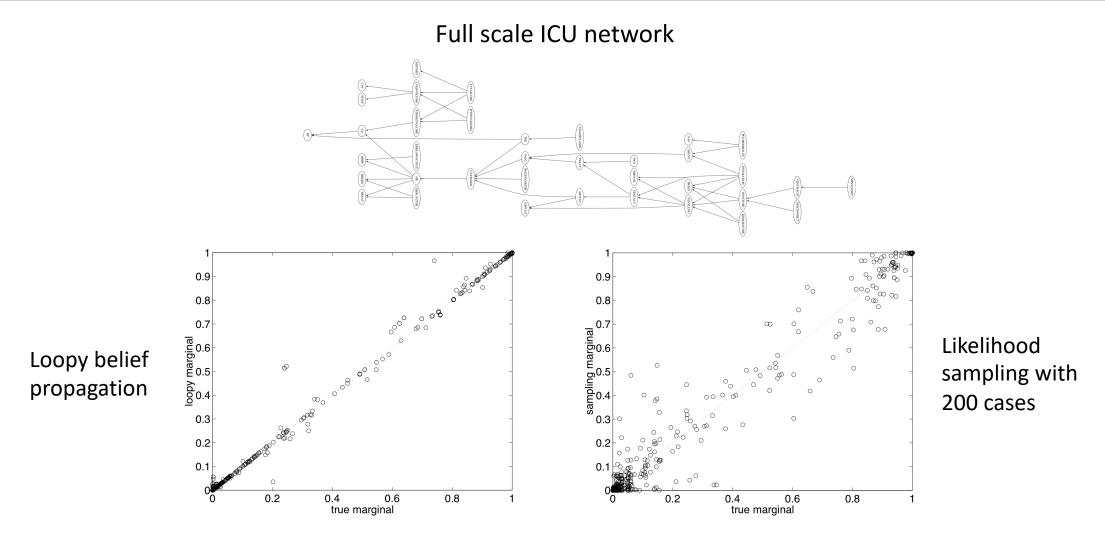


Murphy, K., Weiss, Y., & Jordan, M. I. (2013). Loopy belief propagation for approximate inference: An empirical study. *arXiv* preprint *arXiv*:1301.6725.

toyQMR network

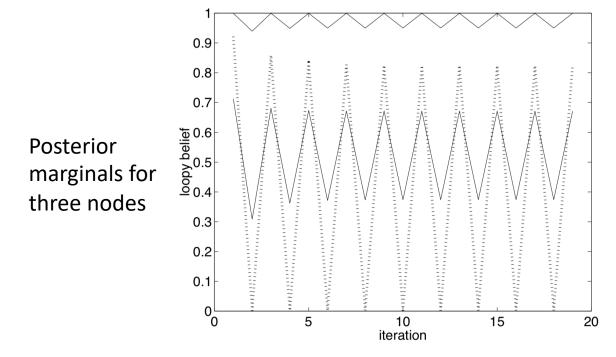


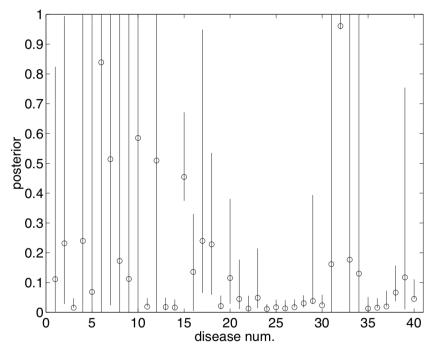
Murphy, K., Weiss, Y., & Jordan, M. I. (2013). Loopy belief propagation for approximate inference: An empirical study. *arXiv* preprint *arXiv*:1301.6725.



Murphy, K., Weiss, Y., & Jordan, M. I. (2013). Loopy belief propagation for approximate inference: An empirical study. *arXiv* preprint *arXiv*:1301.6725.

QMR-DT network



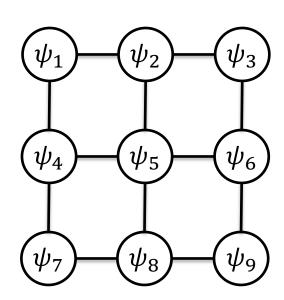


Exact marginals (circles) and error bars

Murphy, K., Weiss, Y., & Jordan, M. I. (2013). Loopy belief propagation for approximate inference: An empirical study. *arXiv preprint arXiv:1301.6725*.

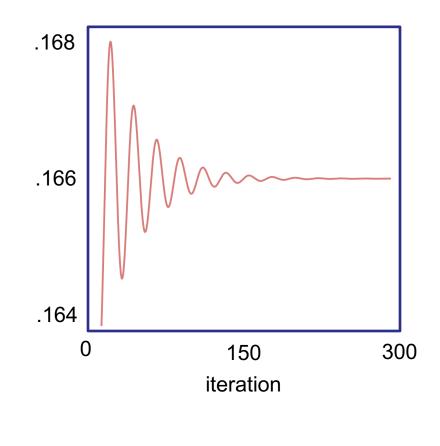
Convergence and Message Schedule

- In their analysis, Murphy, Weiss & Jordan used synchronous (parallel) message passaging
 - However, convergence can be improved with asynchronous approaches
- Some approaches for asynchronous message scheduling
 - Tree reparameterization (TRP): Choose a tree (spanning tree is a good choice) and pass messages. The trees must cover all edges
 - Residual belief propagation (RBP): Pass messages between two clusters whose beliefs over separators disagree the most. Usually organised with a priority queue
- Smoothing messages
 - $M_{ij} = \lambda \left(\eta \sum_{C_i \setminus S_{ij}} \psi_i \prod_{k \neq j} M_{ki} \right) + (1 \lambda) M_{ij}^{old}$

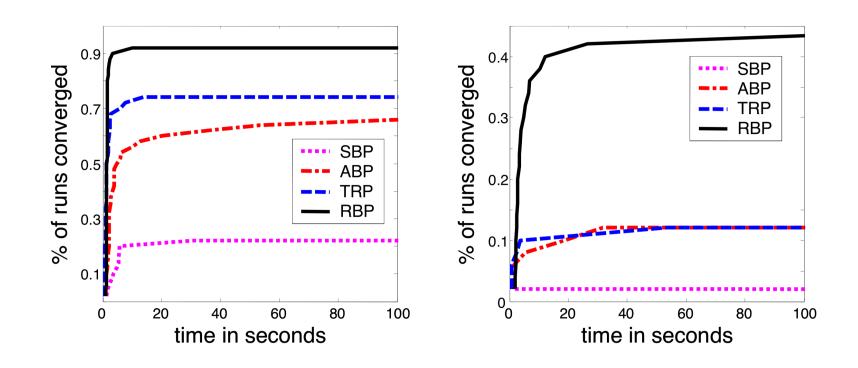


Joingraph Example with Markov Nets

D	A	$\phi_4(D,A)$	_	A	В	$\phi_1(A,B)$
\overline{d}	a	100		а	b	100
d	\bar{a}	1		а	\overline{b}	2
$egin{array}{c} d \ ar{d} \ ar{d} \end{array}$	a	1		\bar{a}	b	1
$ar{d}$	\bar{a}	100	(A)	\bar{a}	\overline{b}	100
			$\nearrow \checkmark$			
		\sim		\		
		(D)		(E)	
		\sim				
			\searrow			
_	_	l. (a.s.	(c)	_	_	l. (5 a)
<u></u>	D	$\phi_3(C,D)$	_	<u>B</u>	<u>C</u>	$\phi_2(B,C)$
С	d	1		b	С	100
С	$ar{d}$	100		b	\bar{C}	1
$ar{c}$ $ar{c}$	d	100		\overline{b}	С	1
\bar{C}	$ar{d}$	1		\overline{b}	\bar{c}	100



Convergence and Message Schedule



50 random grids of size 11×11 and C = 11 (left) and C = 13 (right)

Conclusion

- Belief propagation extends the paradigm of message passing
 - It provides a full spectrum of possibilities from exact to approximate inference
- Interactive joingraph propagation (IJGP) algorithm
 - Can be interpreted as an approach that minimizes the KL divergence between
 - The factorization induced by the network
 - The factorization induced by the joingraph
- IJGP messages convergence
 - Guaranteed in a single iteration if the joingraph is a tree (jointree)
 - Otherwise, convergence is not guaranteed
 - Even if the messages converge, its beliefs may not be necessarily equal the true marginals
 - Although very often in practice they will be close
- Task
 - Read chapter 14 (but 14.8)