# COMP9418: Advanced Topics in Statistical Machine Learning

A Bighine Int Propagation

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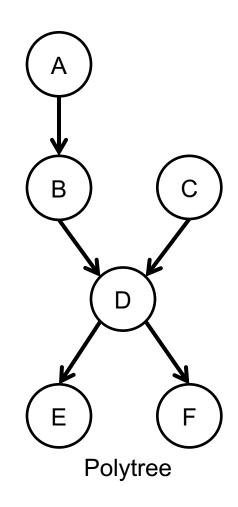
#### Introduction

- 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.
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- 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
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    A polytree is a network with only one undirected path
    between any two nodes <a href="https://tutorcs.com">https://tutorcs.com</a>
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   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

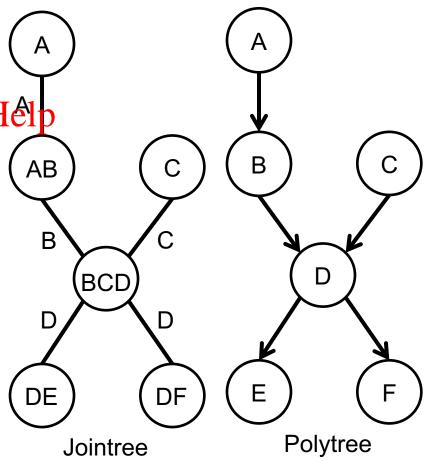
In this case, we can create a "special" jointree has Help the same structure as the polytree

• A node i in the jointree habite X where U are the parents of X

where U are the parents of XWe Chat: cstutores • 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

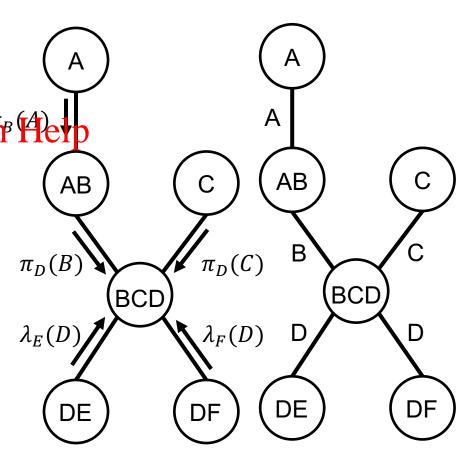
• Message from node U to chasignmente Project Example (causal support)

• Messages from node Y to parent X denoted  $X_Y$  (diagnostic support)

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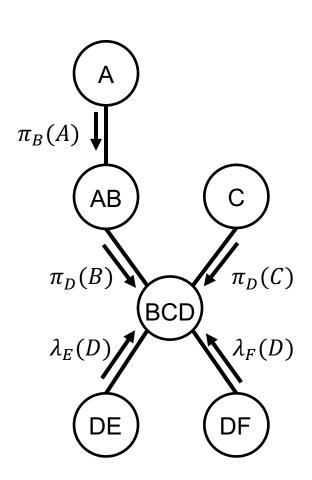
• The joint marginal for the family of variable X with parents  $U_i$  and children  $Y_i$  is given by

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



- 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 pyidence eand reconsistent with the pyidence eand reconsistent with the pyidence eand reconsistent with the pyidence example of the pyidence of
  - We can rewrite the joint material that the second of variable X with parents  $U_i$ , children  $Y_i$  and evidence e as WeChat: cstutorcs

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



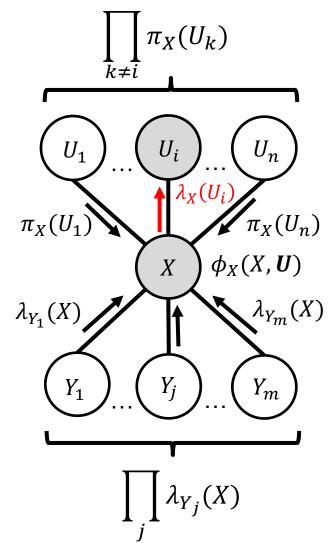
Using this notation, diagnostic messages can be defined as

$$\lambda_X(U_i) = \sum_{X \mathbf{U} \setminus \{U_i\}} \lambda_e(X) \, \phi_X(X, \mathbf{U}) \prod_{k \neq i} \pi_X(U_k) \prod_j \lambda_{Y_j}(X)$$
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And causal messages as <a href="https://tutorcs.com">https://tutorcs.com</a>

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

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



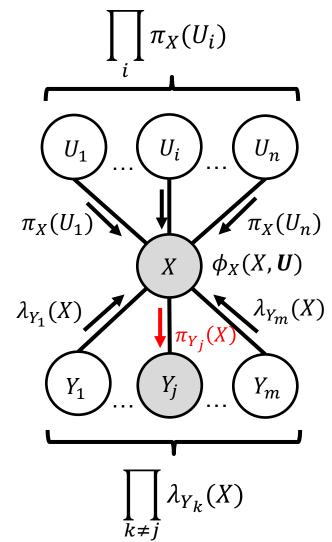
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$$\pi_{Y_j}(X) = \sum_{\boldsymbol{U}} \lambda_e(X) \, \phi_X(X, \boldsymbol{U}) \, \prod_{i} \pi_{\boldsymbol{X}}(U_i) \, \prod_{k \neq j} \lambda_{\boldsymbol{X}}(X)$$

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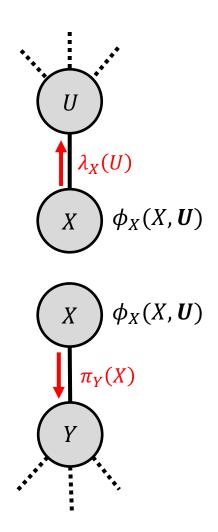
- When a node has a single neighbour, it can immediately send a message to that neighbour
  - This includes a leaf node X with a single parent U

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$$\lambda_X(U) = \sum_{X \in X} \lambda_e(X) \, \phi_X(X, U)$$

• And a root node X with a single child Y

$$\pi_Y(X) = \lambda_Y(X)\phi_X(X,U)$$
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- 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

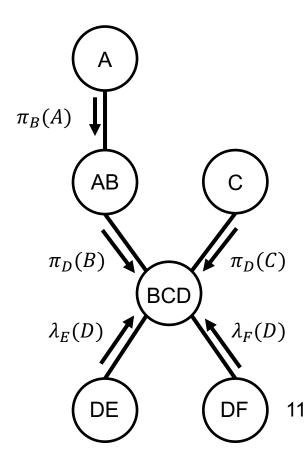
- We can use P(B, C, D, e) to compute marginals for the variables B, C and D. For instance
  - We can also compute the joint marginal for C once we compute the message from D to C
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  - To compute conditional marginals, we simply normalize joint marginals
- Another approach is to use a constant \( \eta\) that normalizes the factor to sum to one
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$$P(X\boldsymbol{U}|\boldsymbol{e}) = \eta \ \lambda_{\boldsymbol{e}}(X) \ \phi_{X}(X,\boldsymbol{U}) \prod_{i} \pi_{X}(U_{i}) \prod_{j} \lambda_{Y_{j}}(X)$$

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

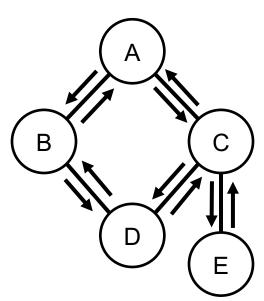
$$\pi_{Y_{j}}(X) = \eta \sum_{X\boldsymbol{U}\setminus\{U_{i}\}} \lambda_{\boldsymbol{e}}(X) \ \phi_{X}(X,\boldsymbol{U}) \prod_{i} \pi_{X}(U_{i}) \prod_{i\neq i} \lambda_{Y_{k}}(X)$$

$$egin{array}{c|c} C & P(C, e) \\ \hline c & .0009 \\ \hline ar{c} & .3067 \\ \hline \end{array}$$



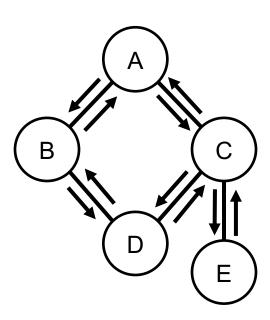
# Belief Propagation in Connected Networks

- 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
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     The correctness of belief propagation depends on the underlying polytree
- The results can be incorrect if the toconnected 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



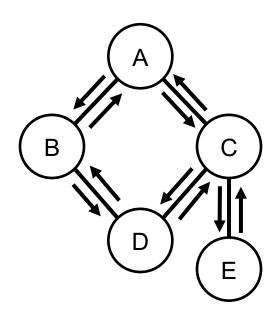
# Iterative Belief Propagation (IBP)

- 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
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  - At each iteration t, every node X send a message to its neighbours using the messages received from 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
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     Sequential schedule: messages are propagates as soon as they are computed WeChat: cstutorcs
- 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 project Exam Help
                  for each parent U_i do \lambda_X^t(U_i) \leftarrow \eta \sum_{X \boldsymbol{U} \setminus \{U_i\}} \lambda_e(X) \phi_X(X, \boldsymbol{U}) \prod_{k \neq i} \pi_X^{t-1}(U_k) \prod_j \lambda_{Y_j}^{t-1}(X)
                  for each child we Chat: cstutorcs
                             \pi_{Y_i}^t(X) \leftarrow \eta \sum_{\boldsymbol{U}} \lambda_e(X) \, \phi_X(X, \boldsymbol{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

$$KL(P'(X|e), P(X|e)) \stackrel{\text{def}}{=} \sum_{e \in E} P'(x|e) \log \frac{P'(x|e)}{\text{Help}}$$
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- 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 WeChat: cstutorcs
  - 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 Assignment Project Exam Help parameters
- The Iterative Belief Propagation algorithm presented before assumes that the approximate distribution P'(X) factors as  $P'(X|e) = \prod_{u \in U} \frac{P'(X|u|e)}{\prod_{u \in U} P'(u|e)}$

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

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

# Optimizing KL Divergence

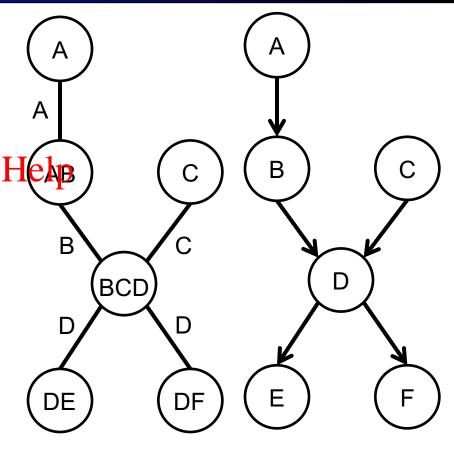
The approximate distribution P'(X) factors as

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

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

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- Some observations about this assumption
  - This choice of P'(X|e) is expressive the region to describe to the content of distributions induced by polytree networks
  - If the network N is a polytree then P(X|e) factors 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 oject Exam Help
  - When IBP performs well, it often has fixed points that are minima of the KL divergence
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  - 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 separateignment Project Exam Help
- If we base our factorization in a jointree https://tutorcs.com
  - Solving the previous optimization problem yields the same update equations of the jointree algorithme Chat: cstutorcs
- 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

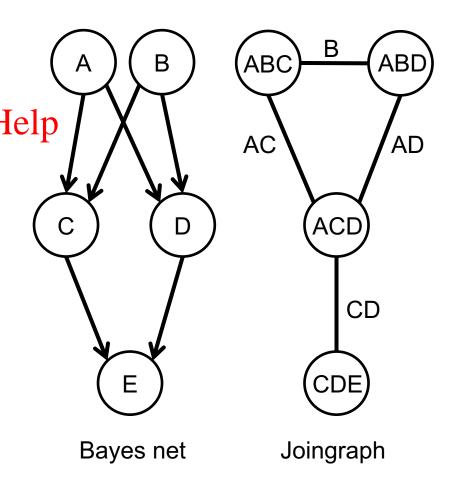
- There is a spectrum of factorizations that fall in between these two extremes
  - This allows a trade-off quality and efficiency Exam Help
  - The notion of joingraph is one way to obtain such a spectrum https://tutorcs.com
- Joingraphs are generaliza Worshot: jointuteess
  - They can be used to obtain 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 like 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  $S_i$  Exam Help Moreover, G satisfies the following properties

• Clusters  $C_i$  and separators  $S_{ij}$  are sets of nodes from N WeChat: cstutores

- lacktriangle Each factor in N must appear in some cluster  $oldsymbol{\mathcal{C}}_i$
- 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,  $S_{ij} \subseteq C_i \cap C_j$



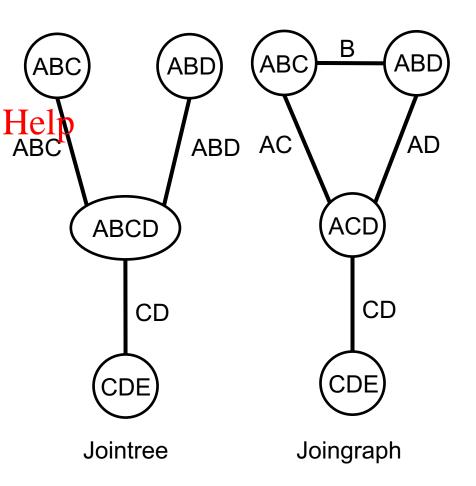
# Jointrees and Joingraphs

 We can think of a jointgraph as a way of relaxing some constraints of jointrees

In a jointree, if two clusters  $C_i$  and  $C_i$  share a set  $C_i$  of variables X then every cluster and separator on the path connecting  $C_i$  and  $C_i$  are  $C_i$  and  $C_i$  are  $C_i$  and  $C_i$  are  $C_i$  are  $C_i$  and  $C_i$  are  $C_i$  are  $C_i$  and  $C_i$  are  $C_i$  are  $C_i$  are  $C_i$  and  $C_i$  are  $C_i$  a

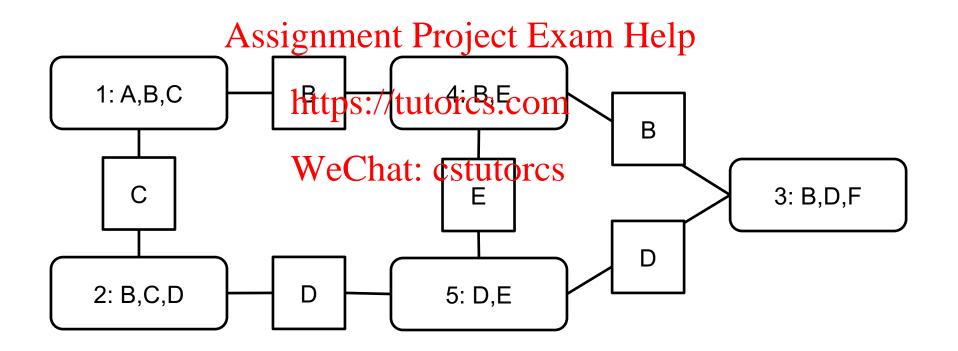
• In a joingraph, we assert each variable  $X \in X$  be contained in clusters and separators of some path connecting  $C_i$  and  $C_j$ 

• We do not require separators  $S_{ij}$  to be precisely the intersection of  $C_i$  and  $C_j$ , as in the case of jointrees



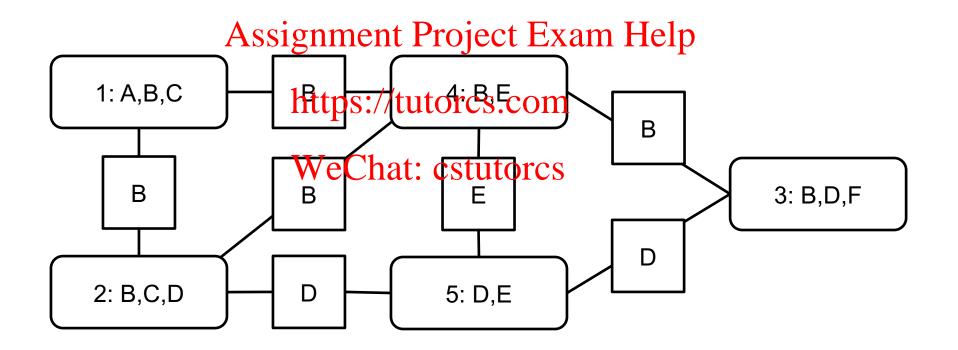
# Valid Joingraph?

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



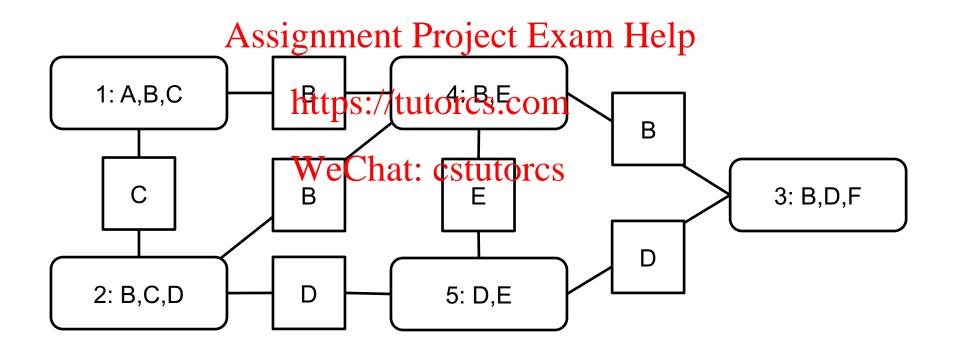
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# Valid Joingraph?

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

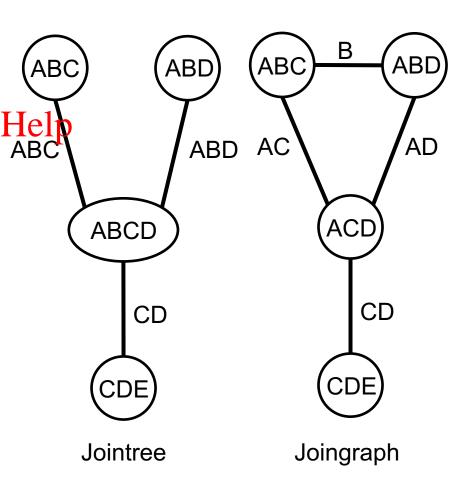


# Joingraph Factorization

A joingraph induces an approximate factorization

$$P'(X|e) = \frac{\prod_{i} P'(C_i|e)}{\prod_{ij} P'(S_{ij}|e)}$$
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When the joingraph corresponds: testilointree,
 the factorization is exact



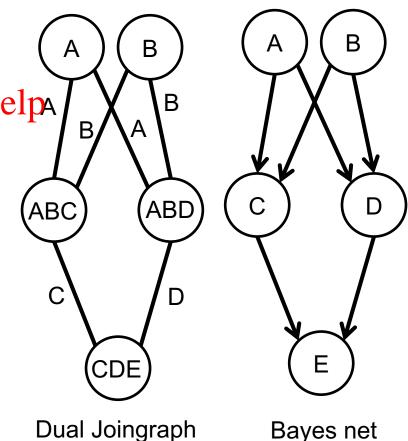
#### **Dual Joingraph**

 A dual joingraph is a special joingraph whose factorization reduces to the one used by IBP

 A dual joingraph G fox singstwent Project Exam Helps obtained as follows

• G has the same undirected structure as N

- For each family XU in N, the collappoint 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  $\mathbf{S}_{ij} = U$



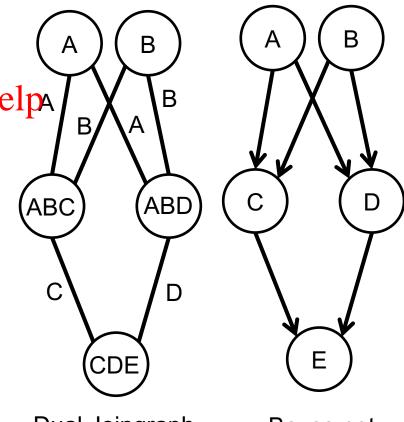
Dual jointgraph (approximate, same as IBP)

 $P'(\boldsymbol{X}|\boldsymbol{e}) = \frac{P'(A|\boldsymbol{e})P'(B|\boldsymbol{e})P'(A,B,C|\boldsymbol{e})P'(A,B,D|\boldsymbol{e})P'(C,D,E|\boldsymbol{e})}{P'(A|\boldsymbol{e})^2P'(B|\boldsymbol{e})^2P'(C|\boldsymbol{e})P'(D|\boldsymbol{e})}$ 

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**Dual Joingraph** 

Bayes net

Dual jointgraph (approximate, same as IBP)

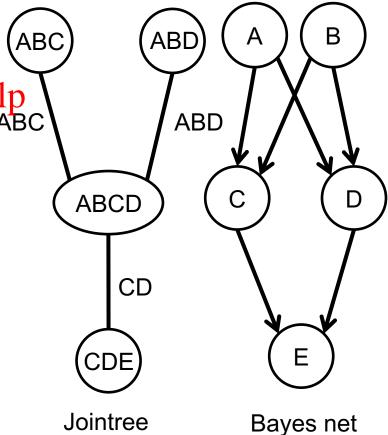
$$P'(\boldsymbol{X}|\boldsymbol{e}) = \frac{P'(A|\boldsymbol{e})P'(B|\boldsymbol{e})P'(A,B,C|\boldsymbol{e})P'(A,B,D|\boldsymbol{e})P'(C,D,E|\boldsymbol{e})}{P'(A|\boldsymbol{e})^2P'(B|\boldsymbol{e})^2P'(C|\boldsymbol{e})P'(D|\boldsymbol{e})}$$

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Jointree (exact)

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

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Dual jointgraph (approximate, same as IBP)

$$P'(\boldsymbol{X}|\boldsymbol{e}) = \frac{P'(A|\boldsymbol{e})P'(B|\boldsymbol{e})P'(A,B,C|\boldsymbol{e})P'(A,B,D|\boldsymbol{e})P'(C,D,E|\boldsymbol{e})}{P'(A|\boldsymbol{e})^2P'(B|\boldsymbol{e})^2P'(C|\boldsymbol{e})P'(D|\boldsymbol{e})}$$

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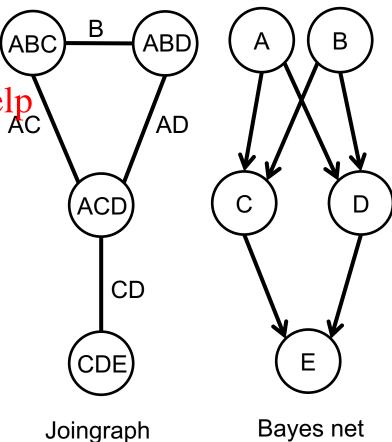
Jointree (exact)

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

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Joingraph (trade complexity and quality)

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



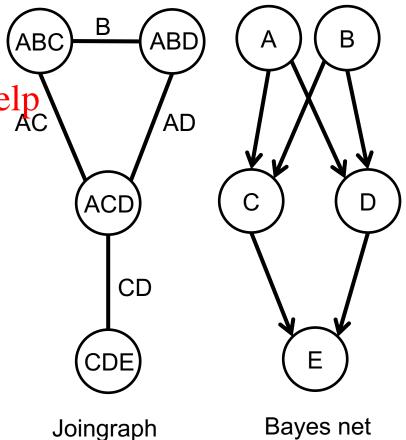
Joingraph (trade complexity and quality)

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

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# 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 the sign magnitude of the separator marginals  $P'(S_{ij}|e)$  that minimize the KL divergence between P(X|e) and the state of the separator of the se
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   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  $\phi$  and evidence indicator  $\lambda_e$  to some cluster  $C_i$  that contains variables in  $\phi$ 
  - All factors are associated to so ignustrated (Renject a Examps Help
  - No factor is present in more than one cluster (no overcounting of information)

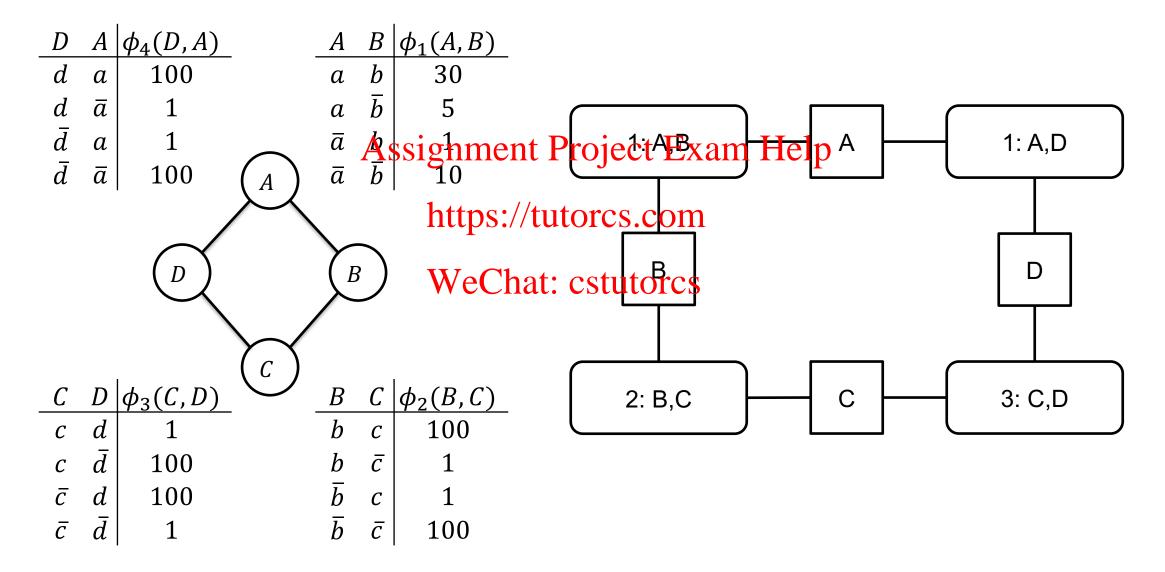
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- It propagates messages with the equations
  - $M_{ij} = \eta \sum_{C_i \setminus S_{ij}} \psi_i \prod_{k \neq j} M_{ki}$
  - where  $\psi_i$  is the product of all CPTs and evidence indicators assigned to cluster  $m{C}_i$
  - $M_{ii}$  is the message sent from cluster i to cluster j

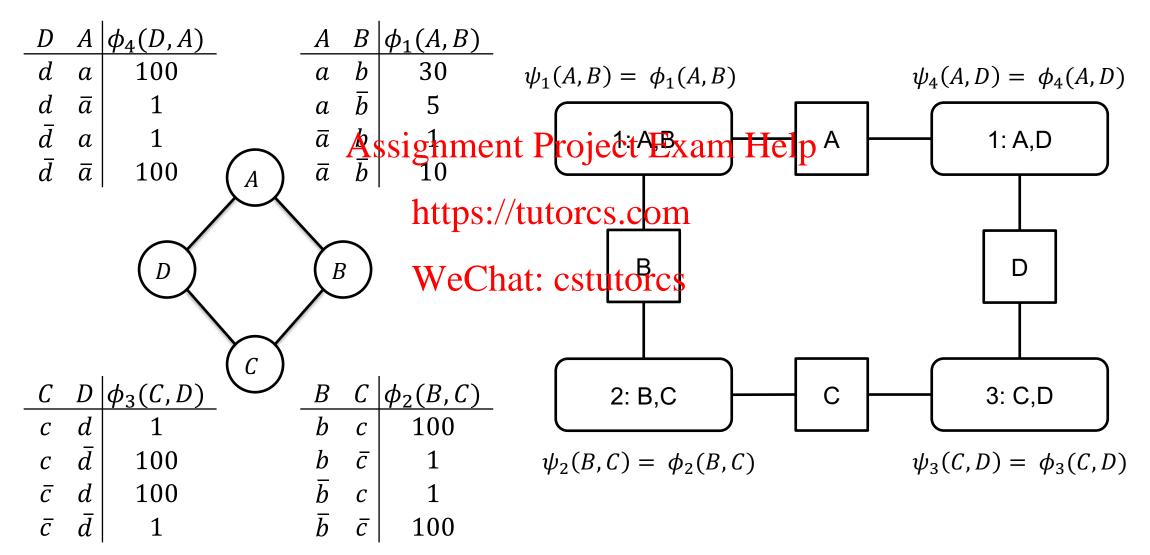
# Parallel Iterative Joingraph Propagation

```
initialize all messages  \begin{array}{l} \textbf{while} \text{ messages have not converged do} \\ \hline & t \leftarrow t \\ \hline & Assignment \\ & For each joingraph edge \\ & t \leftarrow t \\ \hline & Signment \\ & t \leftarrow t \\ \hline & Signment \\ & t \leftarrow t \\ \hline & Signment \\ & t \leftarrow t \\ \hline & Signment \\ & t \leftarrow t \\ \hline & Signment \\ & t \leftarrow t \\ \hline & Signment \\ & t \leftarrow t \\ \hline & Signment \\ & t \leftarrow t \\ \hline & Toject \\ & Exam \\ & Help \\ & t \rightarrow t \\ \hline & t
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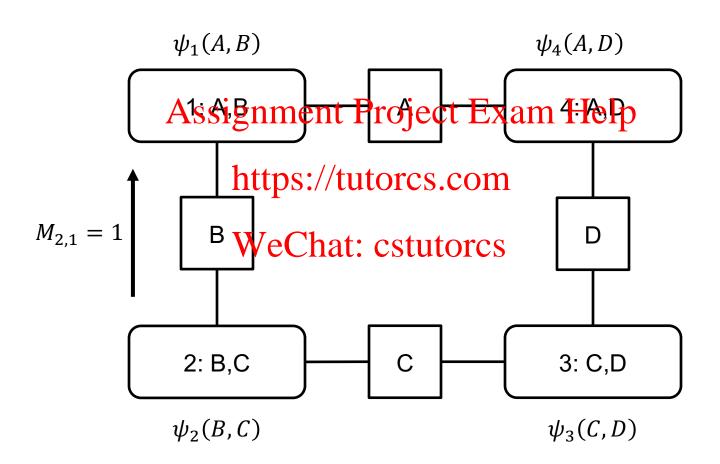
# Joingraph Example with Markov Nets



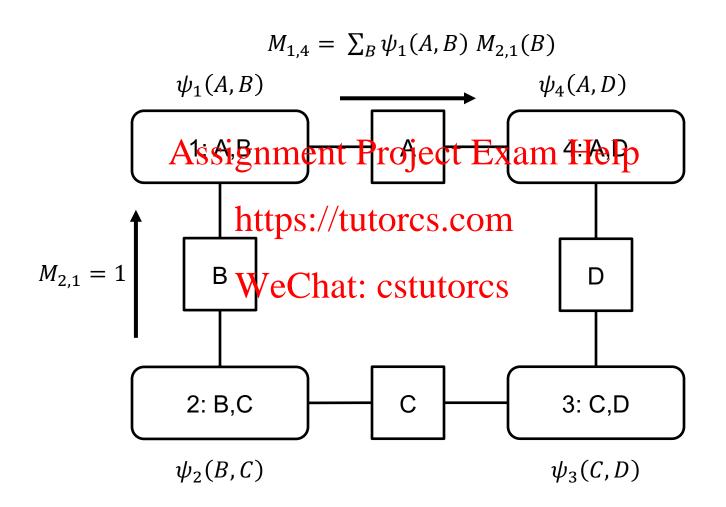
### Joingraph Example with Markov Nets



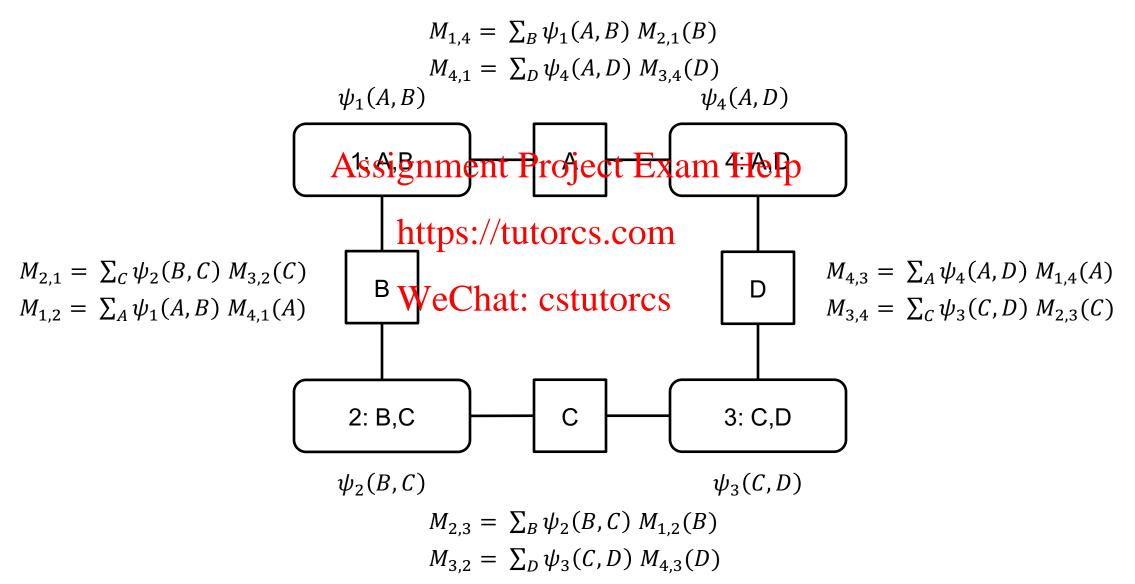
### Joingraph Example with Markov Nets



# Message Passing with Markov Nets



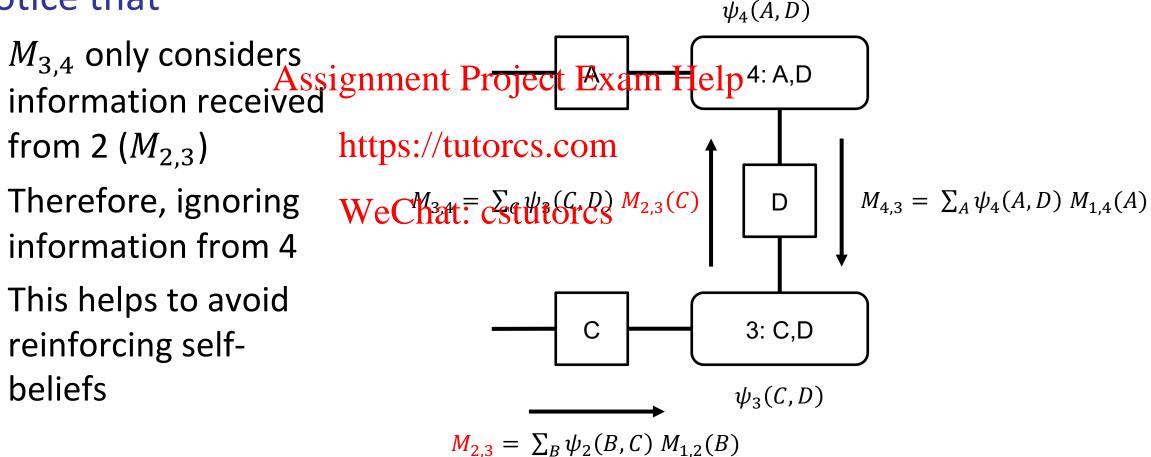
### Message Passing with Markov Nets



### Message Passing: Avoid Self-Beliefs

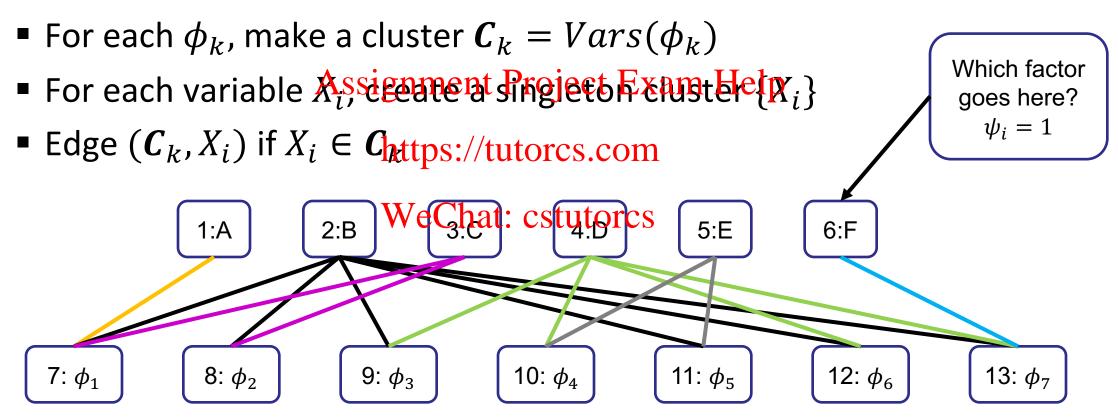
### Notice that

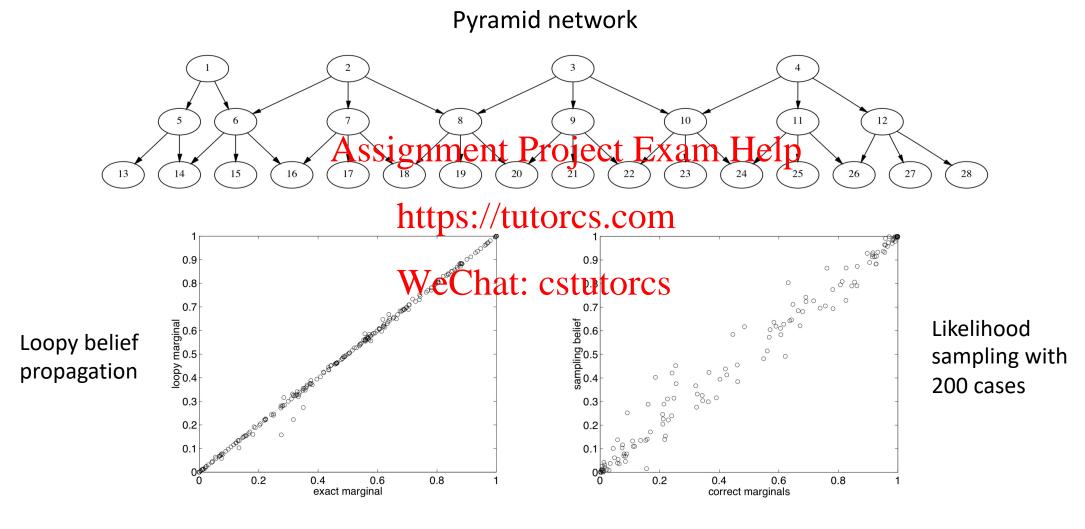
- $M_{3,4}$  only considers from 2 ( $M_{2.3}$ )
- Therefore, ignoring information from 4
- This helps to avoid reinforcing selfbeliefs



### Bethe Graph

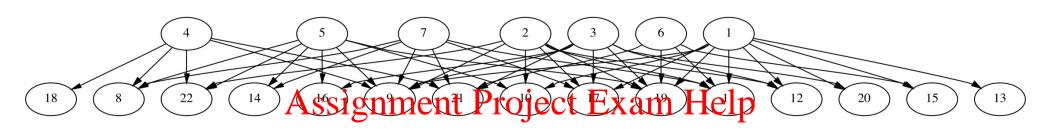
A simple way to generate a valid joingraph

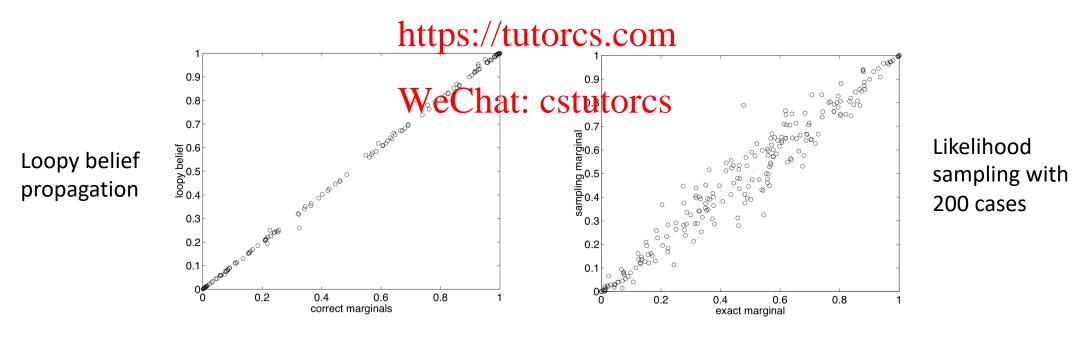




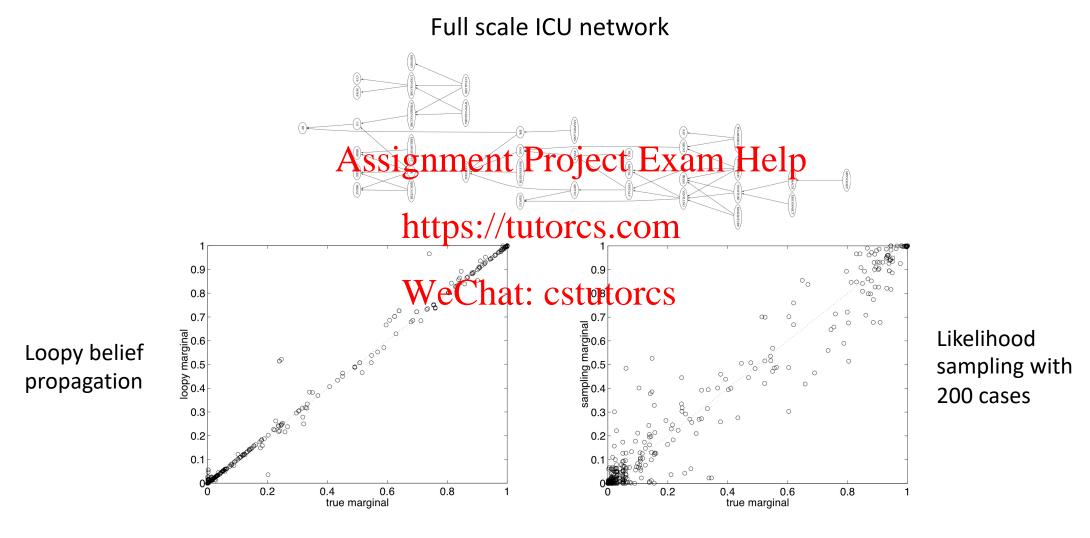
Murphy, K., Weiss, Y., & Jordan, M. I. (2013). Loopy belief propagation for approximate inference: An empirical study. *arXiv* preprint *arXiv*:1301.6725.

#### toyQMR network



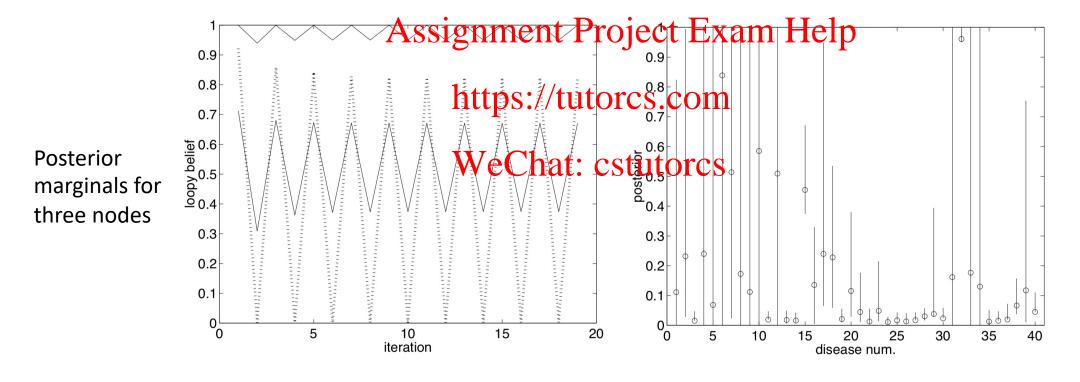


Murphy, K., Weiss, Y., & Jordan, M. I. (2013). Loopy belief propagation for approximate inference: An empirical study. *arXiv* preprint *arXiv*:1301.6725.



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

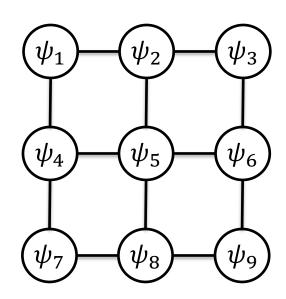


Exact marginals (circles) and error bars

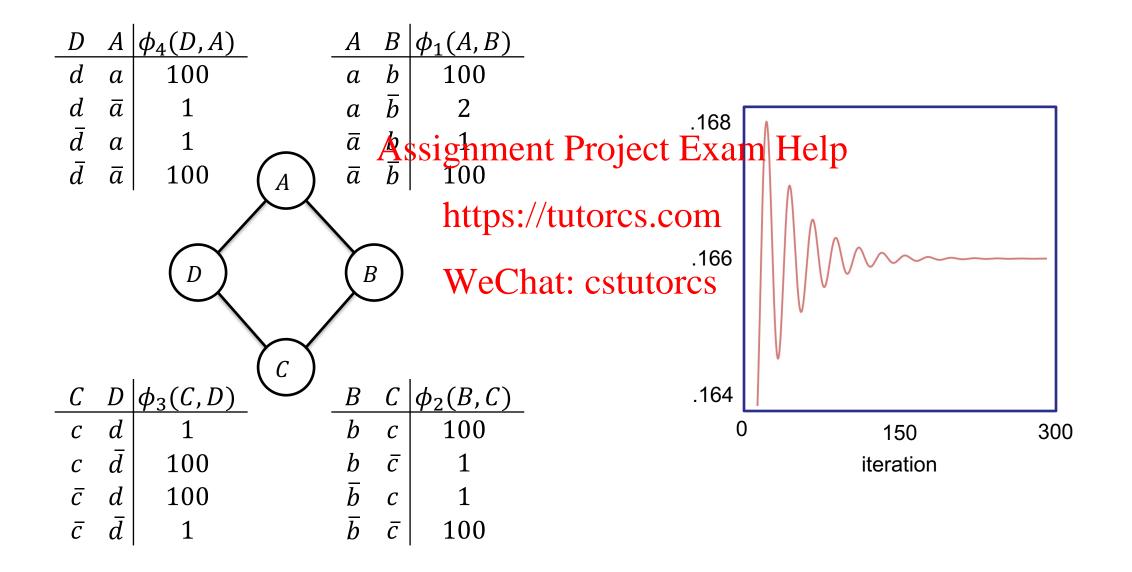
Murphy, K., Weiss, Y., & Jordan, M. I. (2013). Loopy belief propagation for approximate inference: An empirical study. *arXiv* preprint *arXiv*:1301.6725.

### Convergence and Message Schedule

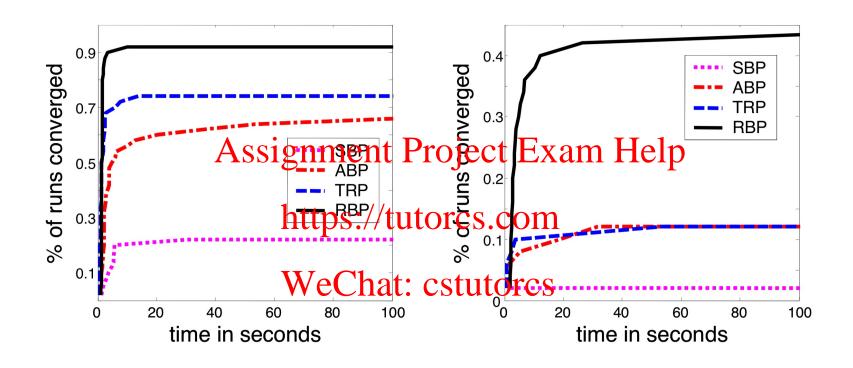
- In their analysis, Murphy, Weiss & Jordan used synchronous (parallel) message passaging
  - However, convergence can be improved with asynchronous approaches
     Assignment Project Exam Help
- Some approaches for asynchronous message scheduling https://tutorcs.com
   Tree reparameterization (TRP): Choose a tree (spanning tree is a good
  - 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



### Convergence and Message Schedule



50 random grids of size  $11 \times 11$  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 Apprigath them to Principes the Kladive I ger pe between
    - The factorization induced by the network
    - The factorization induced by thetique raptutores.com
- IJGP messages convergence
  - Guaranteed in a single iteration if the folingraph is a tree (foint ee)
  - 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)