CSCI E-82a
Probabilistic Programming and AI
Lecture 3
Exact Inference for Graphical Models

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Agenda

- Exact Inference for Graphical Models
- The Variable Elimination Algorithm
- Factors in Graphical Models
- Factor Example
- Variable Elimination in Undirected Graphs
- Queries with Evidence
- Problems with Variable Elimination
- The Belief Propagation Algorithm
- Background for Junction Tree Algorithm
- Junction Tree Algorithm
- Relationship between Junction Tree and Variable Elimination

Inference for Graphical Models

Inference is the process of making **queries** on models to receive posterior distributions or marginal distributions of selected variables

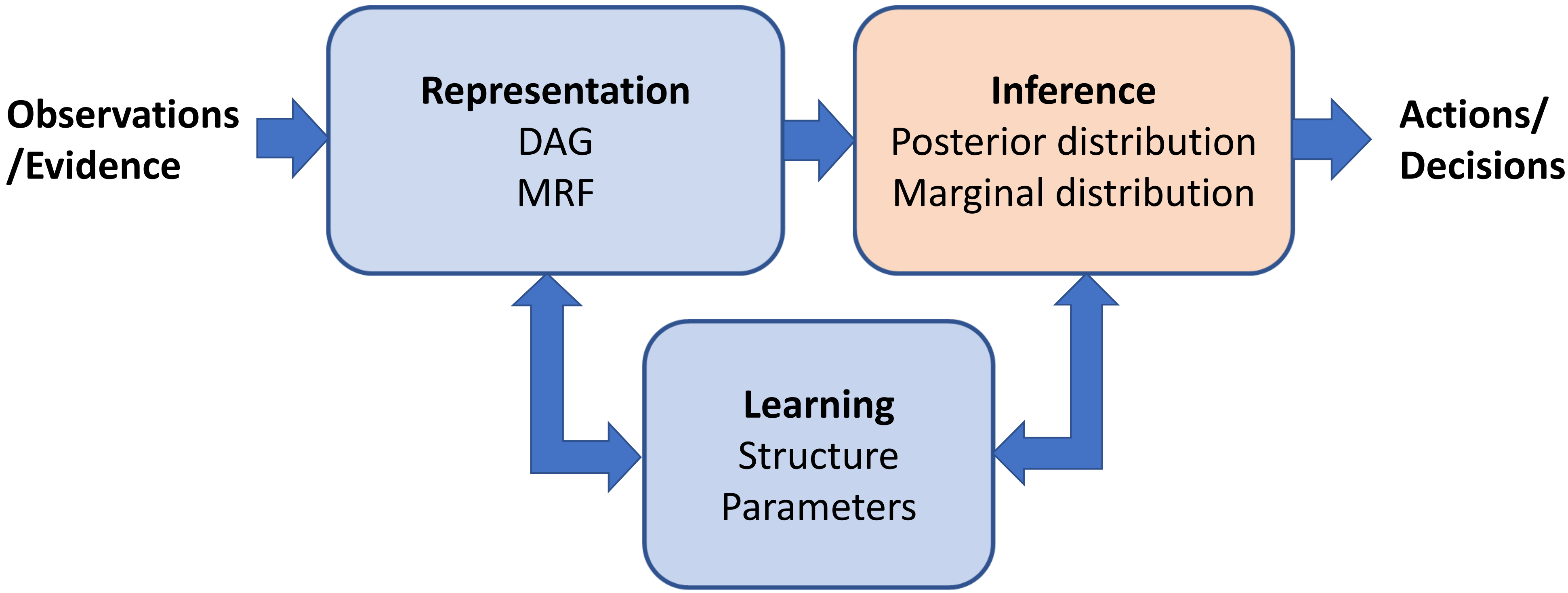
- In other words, inference is the process of getting useful answers from a model!
- **Evidence** (observations) is typically a component of a query
- Query can be on one or more variables

Inference for Graphical Models

In the past 2 lessons our focus was on **representation**

- Representation allows us to define or represent a model
- We have investigated two representations:
  - Bayes networks or directed acyclic graphs (DAGs)
  - Undirected graphical networks, Markov random fields (MRF)
- **Efficient representation**
  - Represent independences
  - Potentials for cliques
- A good representation is required to perform inference

Focus on Inference for Graphical Models



Schematic of intelligent agent using directed graphical model

Inference for Graphical Models

Inference is a **computationally difficult** problem

- Direct tabular solutions can be **computationally infeasible**
- Computational complexity is NP, or $O(n^k)$
- But, we can work with **distributions factored on a graph by independencies**

Inference for Graphical Models

Two major classes of inference algorithms

- In this lecture we focus on **exact inference algorithms**
  - Generally computationally efficient for problems with limited numbers of variables and states
  - Algorithms provide a basis for understanding other methods
- Take up **approximate methods** in later lesson
  - Highly scalable to high dimensional problems
  - Accommodate continuous variables

Inference for Graphical Models

There are no exact algorithms which have guaranteed low computational complexity

- In practice, a number of algorithms work well most of the time
- But, computational complexity can change radically with ordering of variables

Inference for Graphical Models

We focus on the 3 most widely used algorithms

- Variable elimination
- Message passing or belief propagation
    - Generalizes variable elimination on trees
- Junction tree
    - Generalizes belief propagation to complex graphs
- There are many other variations and research continues

The Variable Elimination Algorithm

Variable elimination works by marginalizing out variables one by one

- Variables are ordered
- Working in order, the variables are marginalized out, **eliminated**
- The result is the marginal distribution of the variable queried
- Finding the most efficient elimination order is an NP hard problem
- Different ordering of the variables changes computational complexity a lot!

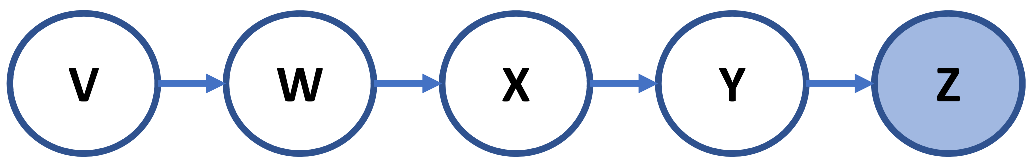
The Variable Elimination Algorithm

Example of variable elimination on a **chain graph**

- The joint distribution factors a follows:

$$P(V, W, X, Y, Z) = P(V)\ P(W \mid V)\ P(X \mid W)\ P(Y \mid X)\ P(Z \mid Y)$$

- The DAG is a chain:

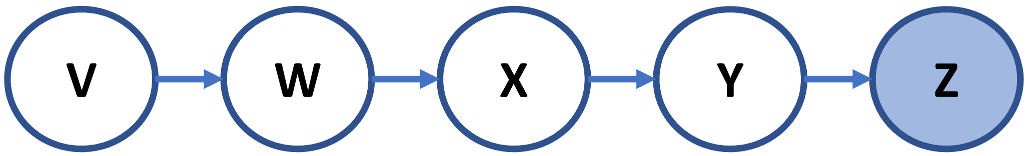


- The query is to find the marginal distribution of Z

The Variable Elimination Algorithm

Example of variable elimination on a chain graph

- Starting with the DAG chain:



- The query is to find the marginal distribution of Z:

$$P(Z) = \sum_V \sum_W \sum_X \sum_Y P(V, W, X, Y, Z)$$

- Or for the factorized distribution:

$$P(Z) = \sum_V \sum_W \sum_X \sum_Y P(V)\, P(W \mid V)\, P(X \mid W)\, P(Y \mid X)\, P(Z \mid Y)$$

The Variable Elimination Algorithm

Example of variable elimination on a chain graph

- First, eliminate the variable V
- Start with the factorized distribution:

$$P(Z) = \sum_V \sum_W \sum_X \sum_Y P(V)\, P(W \mid V)\, P(X \mid W)\, P(Y \mid X)\, P(Z \mid Y)$$

- Rearrange terms and the summation:

$$P(Z) = \sum_W \sum_X \sum_Y P(X \mid W)\, P(Y \mid X)\, P(Z \mid Y) \sum_V P(V)\, P(W \mid V)$$

The Variable Elimination Algorithm

Example of variable elimination on a chain graph

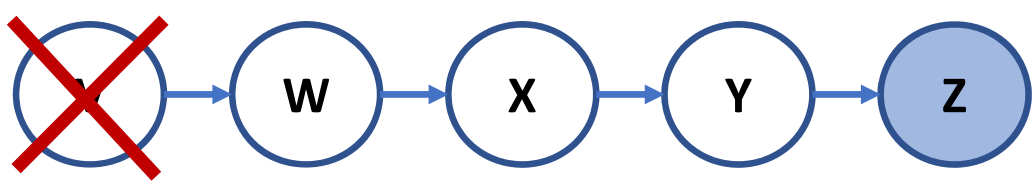
- The marginal of the variable W is:

$$p(W) = \sum_{V} P(V)\, P(W \mid V)$$

- The expression of the marginal distribution of Z is:

$$P(Z) = \sum_{W} \sum_{X} \sum_{Y} P(X \mid W)\, P(Y \mid X)\, P(Z \mid Y) p(W)$$

- The variable V is eliminated and the DAG is now:



The Variable Elimination Algorithm

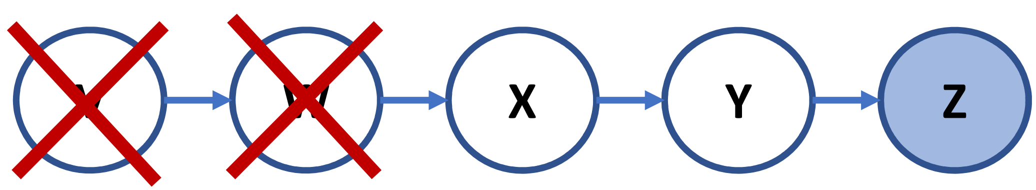
Example of variable elimination on a chain graph

- Now eliminate W, making the marginal of Z:

$$P(Z) = \sum_{X} \sum_{Y} P(Y \mid X)\, P(Z \mid Y) \sum_{W} p(W)\, P(X \mid W)$$

$$= \sum_{X} \sum_{Y} P(Y \mid X)\, P(Z \mid Y)\, p(X)$$

- The variable W is eliminated and the DAG is now:



The Variable Elimination Algorithm

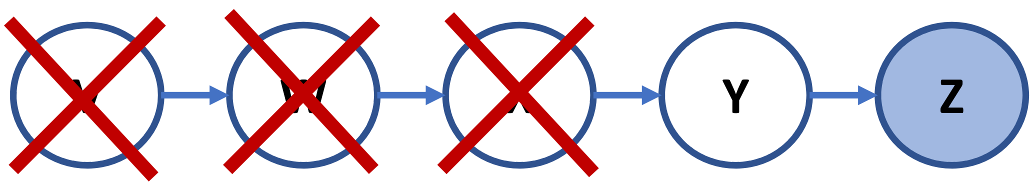
Example of variable elimination on a chain graph

- Now eliminate X, making the marginal of Z:

$$P(Z) = \sum_{Y} P(Z \mid Y) \sum_{X} p(X)\, P(Y \mid X)$$

$$= \sum_{Y} P(Z \mid Y)\, p(Y)$$

- The variable X is eliminated and the DAG is now:



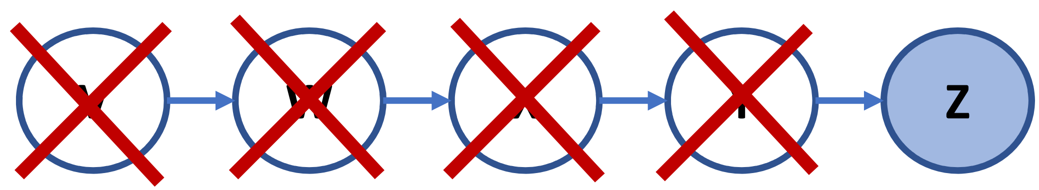
The Variable Elimination Algorithm

Example of variable elimination on a chain graph

- Finally, eliminate Y, and the marginal of Z is:

$$P(Z) = \sum_{Y} p(Z)\ P(Z \mid Y)$$

- The DAG now just has one variable Z:

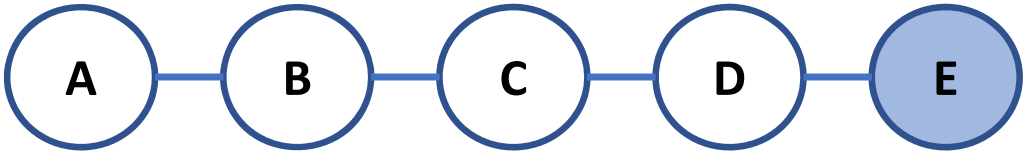


- The variable elimination process is now complete

Variable Elimination for Undirected Graphs

The same principle of variable elimination can be applied to the potentials of an undirected graph

- Start with the undirected chain graph:



- The marginal distribution is represented by the sum over the variables of the product of the 4 potentials:

$$P(E) = \sum_A \sum_B \sum_C \sum_D \frac{1}{Z} \phi(A, B)\, \phi(B, C)\, \phi(C, D)\, \phi(D, E)$$

Factors in Graphical Models

Factors are a generalized formulation

- A factor is a multidimensional table which assigns a value to a set of variables
- CPTs are factors for DAGS
- Potentials are factors for MRFs
- A joint distribution can be computed using general factors:

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

- There are two essential operations on factors
  - Computing a product
  - Marginalization

Factor example

Taking the product of two factors with a common variable

$$\phi(A, B, C) := \phi(A, B) \times \phi(B, C)$$

Computationally is an outer product

A	B	
-a	-b	0.1
-a	+b	0.2
+a	-b	0.8
+a	+b	0.9

$\phi(A, B)$

X

B	C	
-b	-c	0.3
-b	+c	0.2
+b	-c	0.7
+b	+c	0.8

$\phi(B, C)$

A	B	C	
-a	-b	+c	0.02
-a	+b	+c	0.16
+a	-b	+c	0.16
+a	+b	+c	0.72
-a	-b	-c	0.03
-a	+b	-c	0.14
+a	-b	-c	0.24
+a	+b	-c	0.63

$\phi(A, B, C)$

Factor example

Computing the (unnormalized) marginal factor

Compute factor $\tau(C)$ by marginalizing $\phi(A, B, C)$

A	B	C	
-a	-b	+c	0.02
-a	+b	+c	0.16
+a	-b	+c	0.16
+a	+b	+c	0.72
-a	-b	-c	0.03
-a	+b	-c	0.14
+a	-b	-c	0.24
+a	+b	-c	0.63

$\phi(A, B, C)$

$$\sum_A \phi(A, B, C)$$

B	C	
-b	-c	0.27
-b	+c	0.18
+b	-c	0.77
+b	+c	0.88

$\tau(B, C)$

$$\sum_B \tau(B, C)$$

C	
+c	1.06
-c	1.04

$\tau(C)$

Variable Elimination for Undirected Graphs

The same principle of variable elimination can be applied to the factors of an undirected graph

- Distribution is factorized by the potentials:

$$P(E) = \sum_A \sum_B \sum_C \sum_D \frac{1}{Z} \phi(A,B)\, \phi(B,C)\, \phi(C,D)\, \phi(D,E)$$

- As with the DAG example, start by eliminating the first variable in the chain, A:

$$\begin{aligned} P(E) &= \frac{1}{Z} \sum_B \sum_C \sum_D \phi(B,C)\, \phi(C,D)\, \phi(D,E) \underbrace{\sum_A \phi(A,B)} \\ &= \frac{1}{Z} \sum_B \sum_C \sum_D \phi(B,C)\, \phi(C,D)\, \phi(D,E)\, \tau(B) \end{aligned}$$

Variable Elimination for Undirected Graphs

The same principle of variable elimination can be applied to the factors of an undirected graph

- Continuing with the variable elimination:

$$
\begin{aligned}
P(E) &= \frac{1}{Z} \sum_{C} \sum_{D} \phi(C, D)\, \phi(D, E) \underbrace{\sum_{B} \phi(B, C)\, \tau(B)} \\
&= \frac{1}{Z} \sum_{D} \phi(D, E) \underbrace{\sum_{C} \phi(C, D)\, \tau(C)} \\
&= \frac{1}{Z} \sum_{D} \phi(D, E)\, \tau(D) \\
&= \frac{1}{Z} \tau(E)
\end{aligned}
$$

Queries with Evidence

How do we incorporate evidence into a query?

- Need to compute the conditional distribution:

$$p(Y \mid E = e) = \frac{p(Y, E = e)}{p(E = e)}$$

- $P(X, Y, E)$ is the distribution of query variables Y, evidence variables E and unobserved variables X
- To compute $p(Y \mid E = e)$, sum every factor $\phi(X, Y, E)$ where E is in scope of Y and is set to e
- Variable elimination is used to compute $p(E = e)$
- In other words, adding evidence reduces the number of states of the evidence variable

Problems with Variable Elimination

Why is variable elimination not sufficient for all inference problems?

- Computational complexity depends on order of elimination
- Finding optimal elimination order is NP hard!
- Each query requires a new series of elimination
  - Inefficient for multiple queries

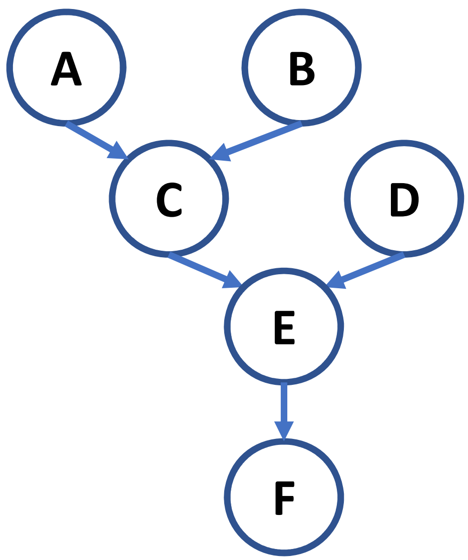
The Message Passing Algorithm

Message passing algorithm enables multiple queries from a single set of messages

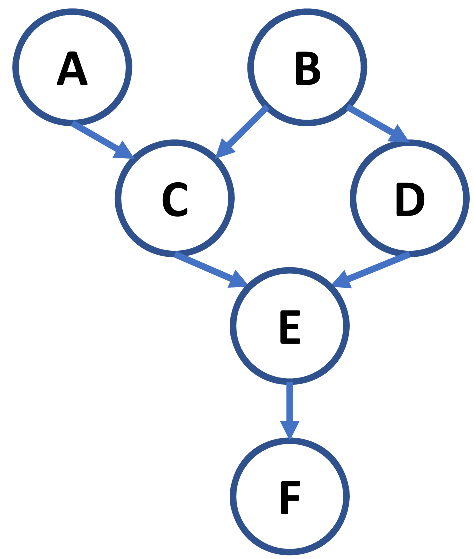
- Also know as the **belief propagation algorithm**
- Message passing algorithm works on **tree graphs**
- The values passed along the tree are **factors**
    - Factors are functions of potentials
    - Factors are not probabilities!
- Intermediate results are saved for future queries in the form of **messages**

The Message Passing Algorithm

Definition: A tree graph is a undirected acyclic graph, in which any pair of nodes are connected by exactly one path.



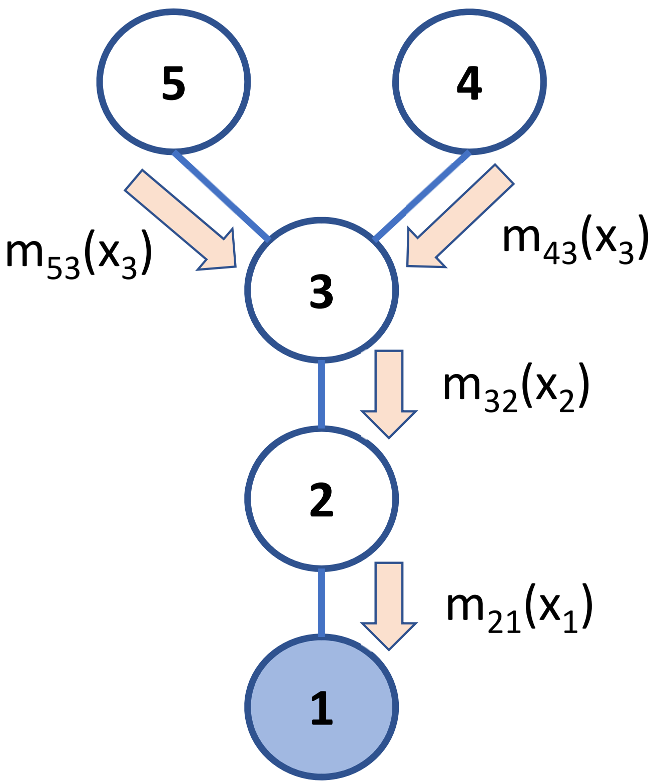
Example of a **tree graph**



This is **not a tree graph!**

The Message Passing Algorithm

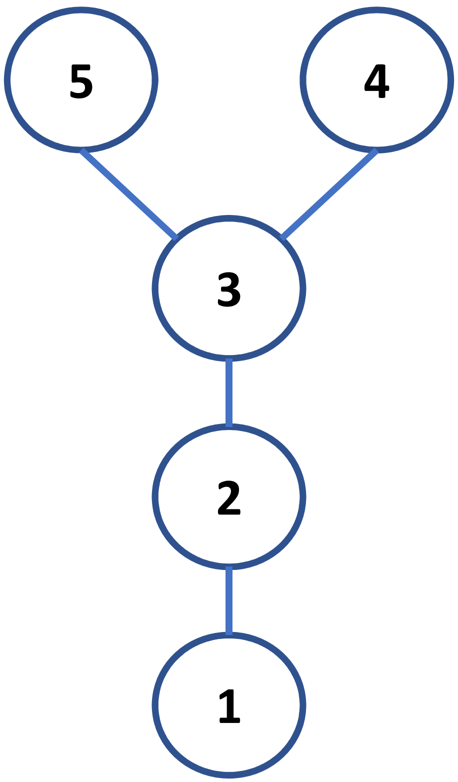
Example: query variable 1 in tree graph

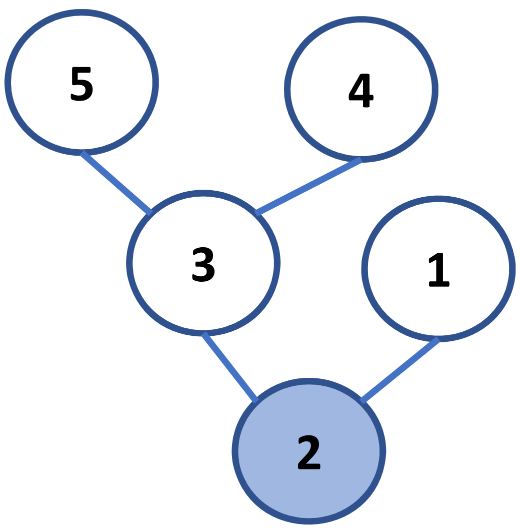


- Variable 1 at root of tree
- Start from the leaf nodes passing messages down the tree
- Messages **propagate belief**
- When each node receives messages from all 'upstream' neighbors, then emits a message down
- Final message is to the root or query node
- Executes in **linear time!**

The Message Passing Algorithm

What happens if we want to query node 2?





- Node 2 becomes the root
- The result is still a tree
- But, we **must pass new messages!**

The Belief Propagation Algorithm

Is there an approach that only requires **passing messages one time?**

- **Yes!**
- **Pass messages in both directions**
- **Cache** messages
- Add **evidence**
- Then, any **query is computed using save messages**

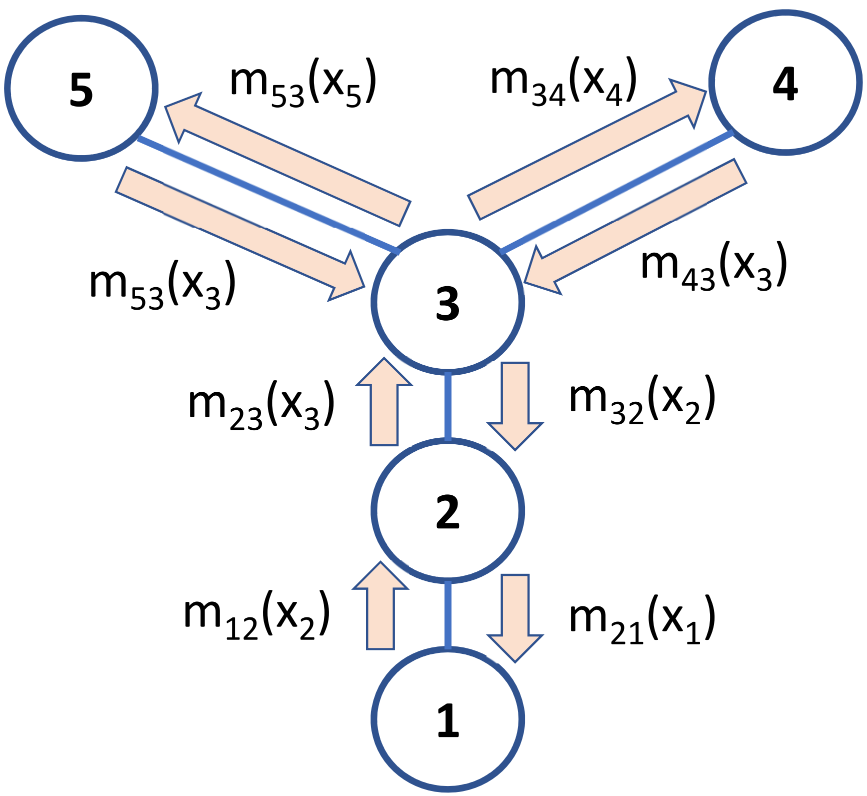
The Belief Propagation Algorithm

Steps of the two-step message passing algorithm:

1. CPTs are updated with evidence
2. Nodes **collect** messages emitted by their neighbors.
   - **Leaf nodes** emit messages at the start of the collection step.
3. Once a node has collected messages from neighbors it **distributes** or **emits** messages to its neighbors.
   - In the distribution phase, a node may only emit a message once it has collected messages from all other neighbors.

The Belief Propagation Algorithm

Messages are passed both directions



- 'Up' the tree from the leaves
- 'Down' the tree from the root
- Caching complete set of messages allows query on any node
- **Message m_{ij} propagates a belief** from one node to a neighbor
- Pass all messages **in 2*node count time!**

The Belief Propagation Algorithm

Upward pass:

- Each leaf in the junction tree sends a message to its parent
  - Message is the marginal of its table; the sum of variables not in the separator.
- When a parent receives a message from a child,
  it multiplies its table by the message table to update its table
- When a parent receives messages from all its children, it acts as the next leaf
- Process continues until the root receives messages from all children

The Belief Propagation Algorithm

Downward pass:

- Reverse of upward pass, starting at root
- Root sends a message to each child
- Root divides current table by the message received from the child
  - Marginalize out variables not in the separator
  - Send result to the child
- Each child multiplies its table by its parent's table
- Child then acts as the root until leaves are reached
- Find marginal of variables by summing out variables as needed
- Done!

The Message Passing Algorithm

Message passing as **variable elimination**

- We can formulate **variable elimination** in terms of **factors**

$$\tau_{jk}(x_k) = \sum_{x_j} \phi(x_k, x_j)\tau_j(x_j)$$

- Sum-product of messages passes from one variable, i, to the next , j:

$$m_{ji}(x_i) = \sum_{x_j} \phi(x_j)\, \phi(x_i, x_j) \prod_{f \in Pa(j)\backslash i} m_{fj}(x_j)$$

Where,

$\phi(x_j) = edge\ factor$; or junction factor

$\phi(x_i, x_j) = clique\ factor$; includes the nodes

And, $f \in Pa(j)\backslash i$ indicates all the parents of x_j except i

The Belief Propagation Algorithm

Add evidence to a query:

- Factor is update using evidence with the relationship:

$$\phi^E(x_i) = \phi(x_i)\ \delta(x_i, \bar{x}_j)$$

Where

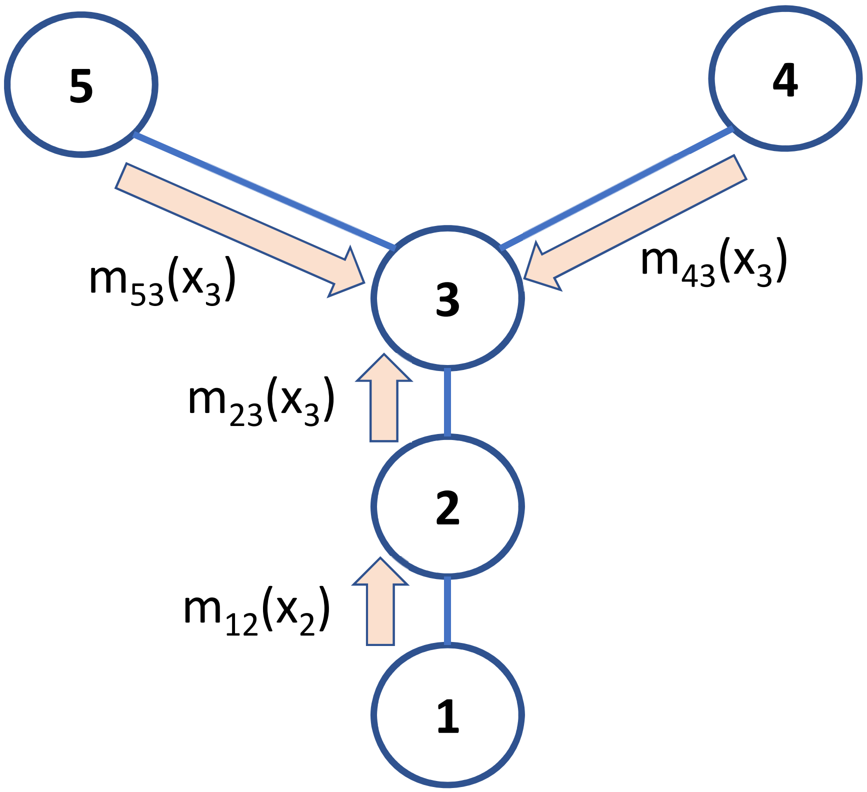
$$\delta(x_i, \bar{x}_j) = 1\ if\ i = j$$

$$\delta(x_i, \bar{x}_j) = 0\ otherwise$$

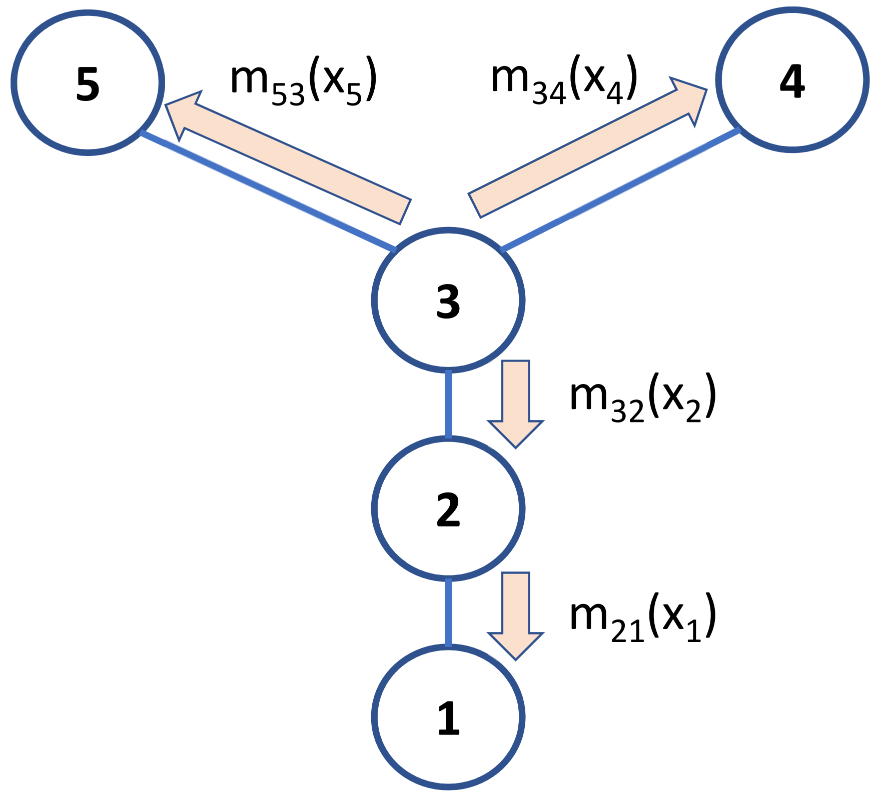
- Evidence reduces the number of states of variables

The Belief Propagation Algorithm

Two message phases for each node



Collect phase: node receives messages from neighbors



Emit phase: The node emits messages to its neighbors

The Belief Propagation Algorithm

The marginal distributions are computed

$$p(x_i) \propto \phi^E(x_i) \prod_{j \in N(i)} m_{ji}(x_i)$$

Where

$m_{ji}(x_i)$ is the message from the jth neighbor

$\phi(x_i)$ is the potential of the node

This is a form of **variable elimination!**

Background for Junction Tree Algorithm

We need some machinery to understand the junction tree algorithm

- Factor graphs are used to form the junction tree
- Running intersection property is used to construct the junction tree
- Sum product algorithm used for belief propagation on junction tree
  - Or, get MAP value with max product algorithm
- Triangulation used to break cycles to form tree

Factor Graphs

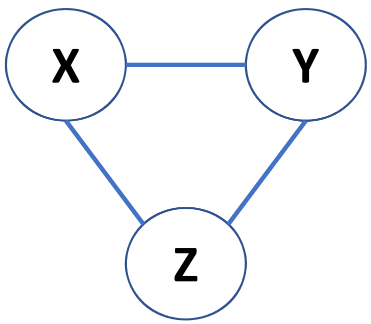
Factor graphs are another representation of graphical models

- A factor is a representation of an unnormalized conditional distribution
- Potentials are a specific case of factor
- Factor graphs are the basis of **message passing algorithms**
- Factor graphs include **variables and (intersection) factors**
- Constructing factor graphs relies on the **running intersection property:**

  For each pair of cliques *U*, *V* with intersection *S*, all cliques on the path between *U* and *V* contain *S*.

Factor Graphs

The factor graph decomposition is **not unique**



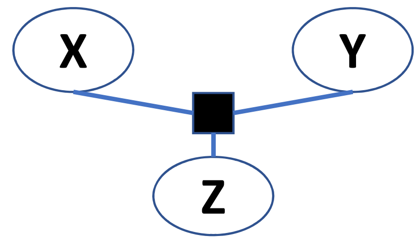
Markov Network

Can use a single potential

$$p(X,Y,Z) = \phi(X,Y,Z)$$

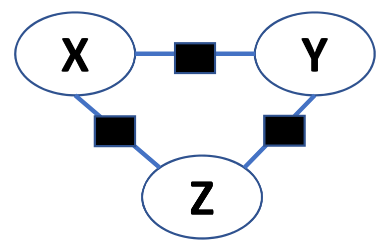
Or, 3 cliques

$$p(X,Y,Z) = \phi(X,Y)\phi(X,Z)\phi(Z,Y)$$



Factor Network

Single factor



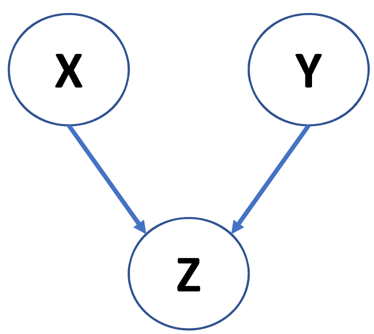
Factor Network

Three intersection factors

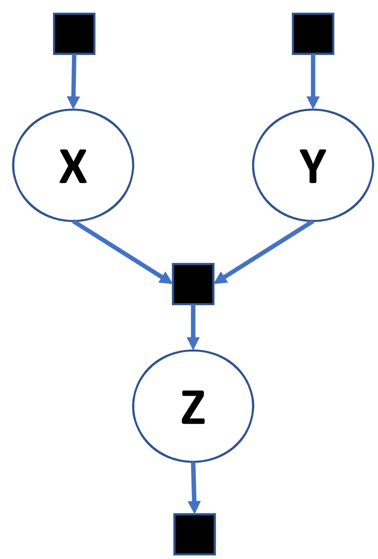
Factor Graphs

Turn a DAG into a factor graph:

- Start with a DAG
- There is one factor for the nodes
- Leaf nodes have factors
- Root node has a terminal factor



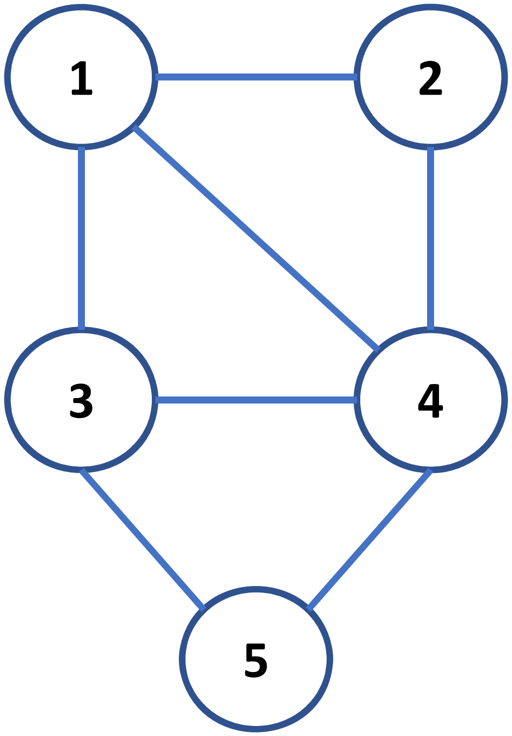
Directed Graph



Factor Graph

Running Intersection Property

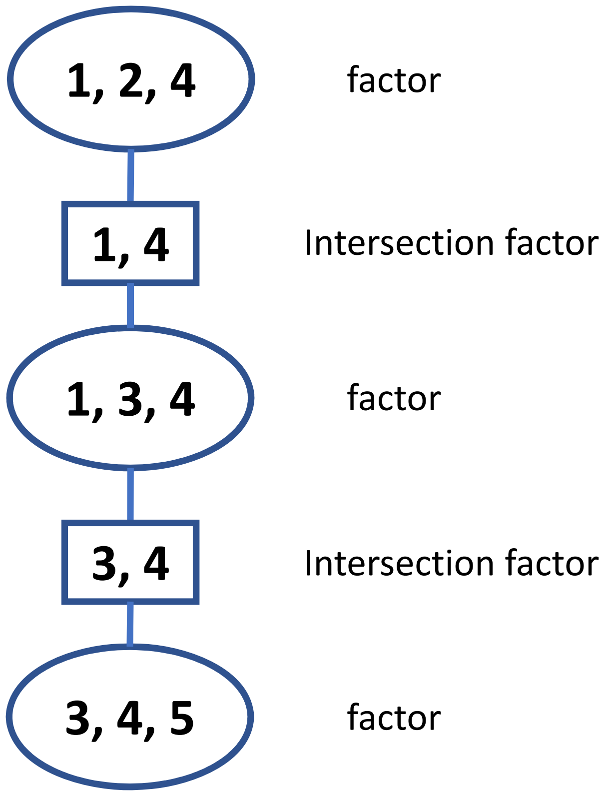
Example of running intersection property



- There are three maximal cliques:
  {1,3,4}, {1,2,4}, and {3,4,5}
- With intersections:
  {1,4} between {1,3,4} and {1,2,4}
  {3,4} between {1,2,4} and {3,4,5}
- In summary:
  node 4 is in 4 cliques and both intersections
  node 1 is in 2 cliques and one intersection
  node 3 is in 2 cliques and one intersection

Running Intersection Property

Example of running intersection property



- Start with factor {1, 2, 4}
- Add factor {1, 3, 4}
- Intersection is factor {1,4}
- Add factor {3, 4, 5}
- Intersection is factor {3, 4}

Sum-Product Algorithm

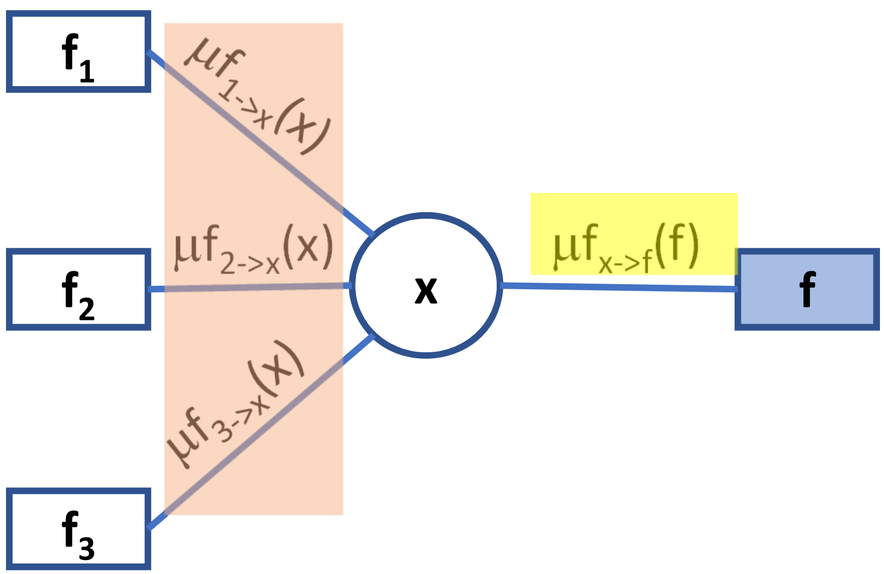
There are **two types of messages** in factor graphs

- The sum-product algorithm is constructed from these messages
- Compute the values for two types of messages
- Variable to factor message
- Factor to variable message

Sum-Product Algorithm

Variable to factor message

$\mu f_{x\to f}(f)$



- Start with variable x
- Variable receives messages from factors
- Variable emits a message to factor
- The value of the message is the product of the messages from neighbor (na) factors

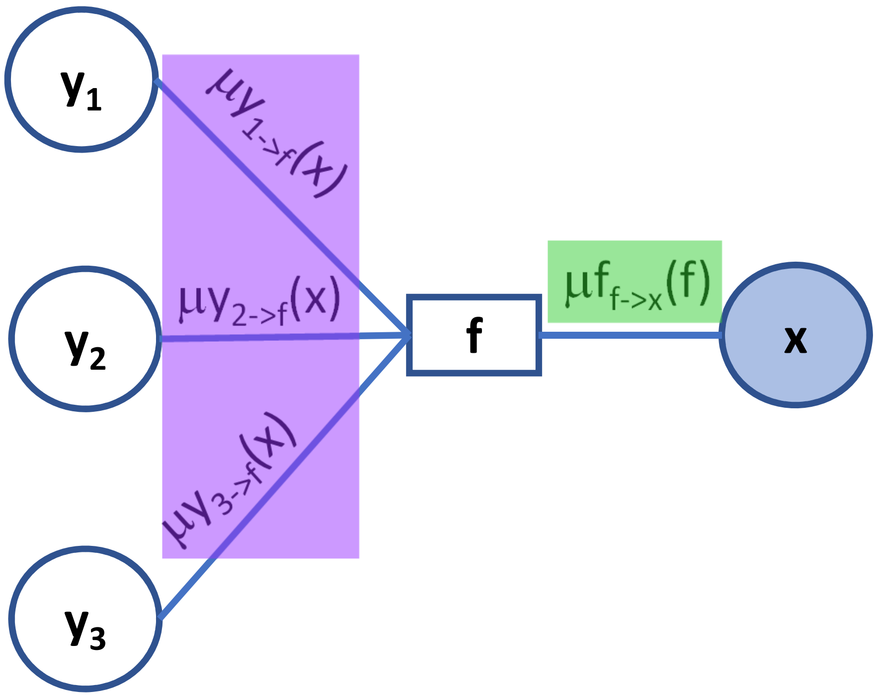
$$u_{x\to f}(x) = \prod_{h \in na(x)\backslash f} u_{h\to x}(x)$$

Where the notation $\backslash f$ excludes the factor f

Sum-Product Algorithm

Factor to variable message

$\mu f_{f\text{->}x}(f)$



- Start with factor f
- Factor receives messages from variables
- The factor emits a message to the variable
- The value of the message is the sum of product of the messages

$$u_{f\to x}(x) = \sum_{\chi_f \setminus x} \psi_f(\chi_f) \prod_{y \in na(f)\setminus x} u_{y\to f}(y)$$

Where the notation $\setminus x$ excludes the current variable

And $\sum_{\chi_f \setminus x} \psi_f(\chi_f)$ is the sum over all states of the variables $\chi_f \setminus x$

Max-Product Algorithm

Sometimes we just want the maximum or most probable value

- Use the **max-product algorithm**
- Max-product algorithm replaces the sum with a max operation
- The **maximum a postiriori (MAP)** value is found with argmax operation

Max-Product Algorithm

Formulation of the max-product algorithm

- Variable to factor message remains unchanged – no sum

$$u_{x\to f}(x) = \prod_{h\in na(x)\backslash f} u_{h\to x}(x)$$

- The factor to variable message is then:

$$u_{f\to x}(x) = argmax_{\chi_f\backslash x}\, \phi_f(\chi_f) \prod_{y\in na(f)\backslash x} u_{y\to f}(y)$$

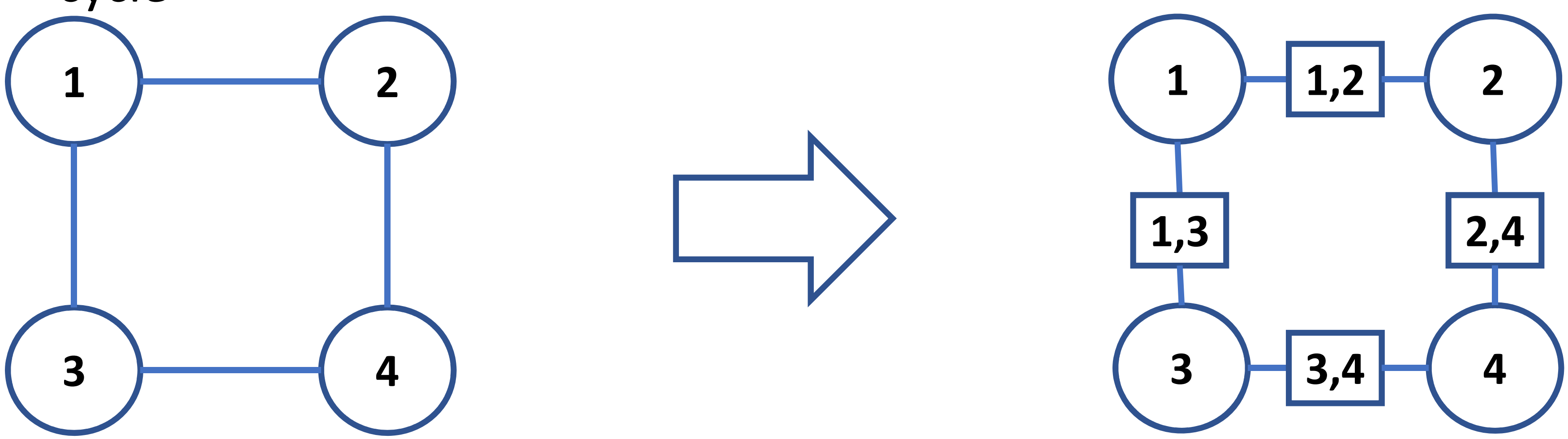
- Algorithm is a form of **linear programming**

See sections 13.1, 13.2 and 13.3 of Koller and Friedman for details

Triangulation

Triangulation is a process of breaking cycles in an undirected graph

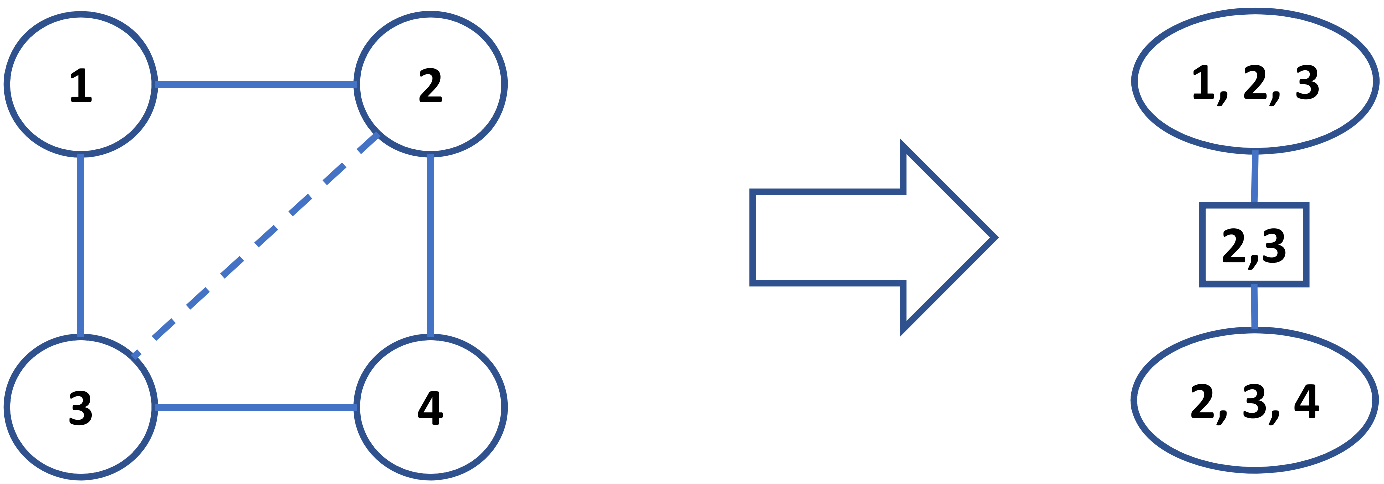
- The Markov network has a **cycle**
- Cycle has 4 or more nodes
- Trees cannot have cycles
- Turn Markov network into factor graph: the factor graph also has a cycle



Triangulation

Triangulation is a process of breaking cycles in an undirected graph

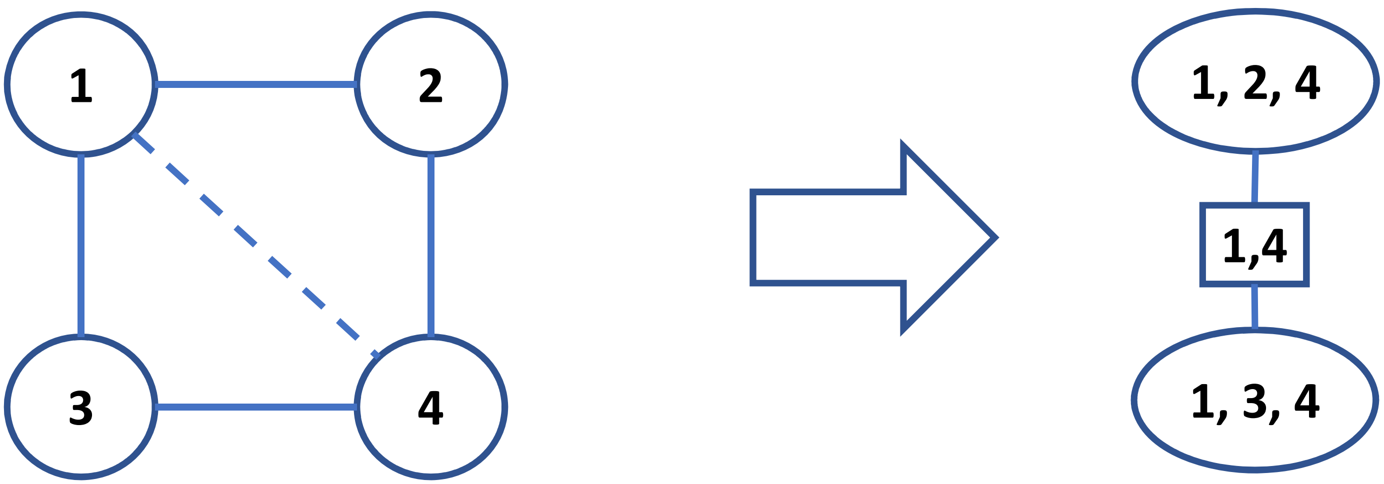
- How to break the cycle of the Markov network?
- Add an **edge to triangulate the graph**
- Turn Markov network into factor graph: **the factor graph is now a tree**!



Triangulation

Triangulation is a process of breaking cycles in an undirected graph

- Or, add a **different edge** to triangulate the graph
- The factor graph is again a **tree**!
- The triangulation and factor graph are **not unique!**



Junction Tree Algorithm

Steps of the Junction Tree algorithm

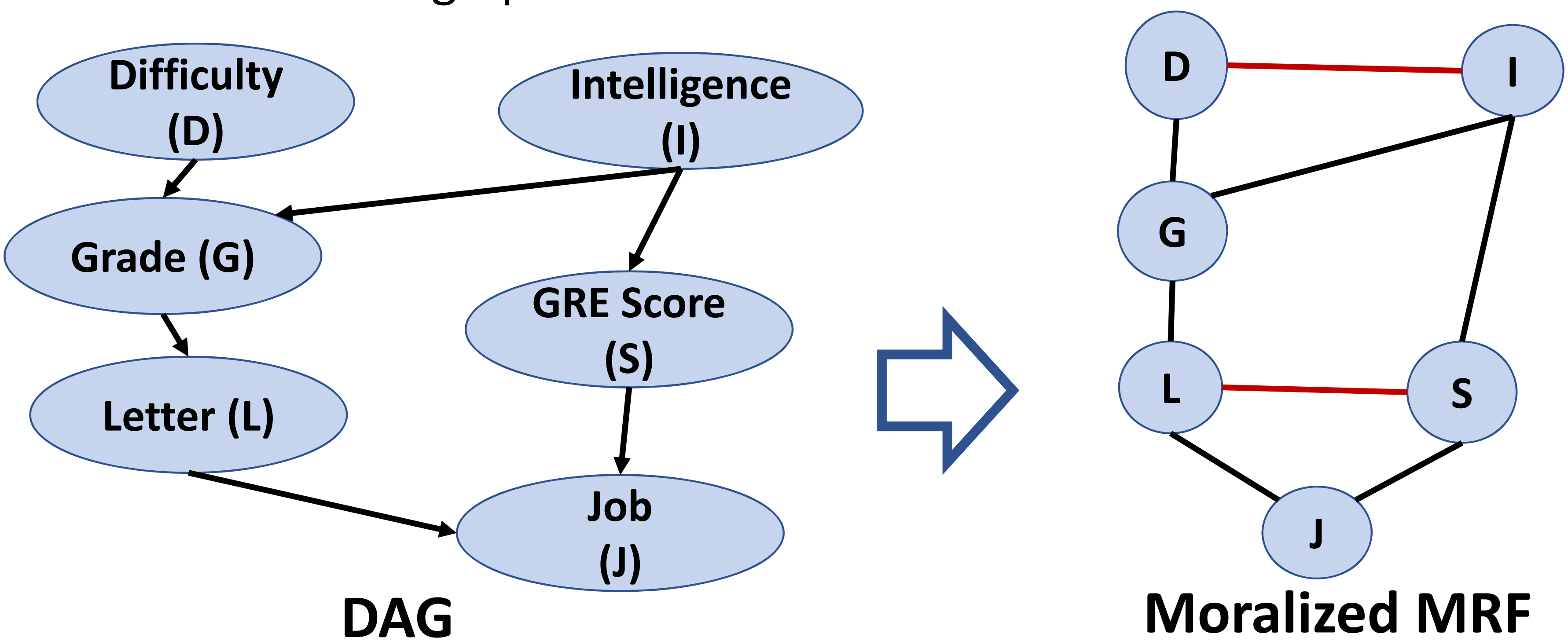
1. If Bayes network, moralize
2. If Bayes network, remove directional arrows
3. Triangulate the undirected graph if cycles
4. Build a clique tree
5. Build a junction tree, a factor graph
6. Choose a root
7. Populate the cliques
8. Perform belief propagation with sum-product algorithm

Junction Tree Example

Start with the familiar student example

Remove direction from arrows

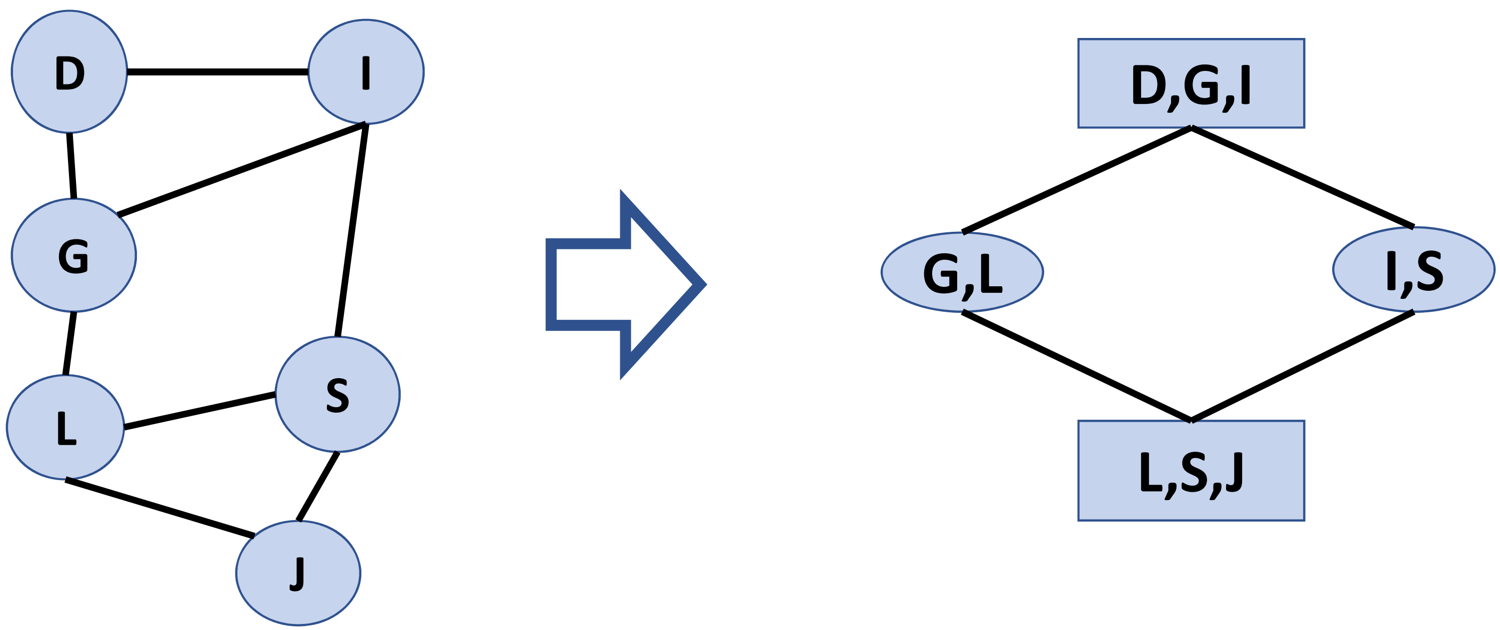
Moralize the graph



Junction Tree Example

Try to build a clique tree

- Wait! This is **not a tree**!
- It has a cycle
- Must triangulate

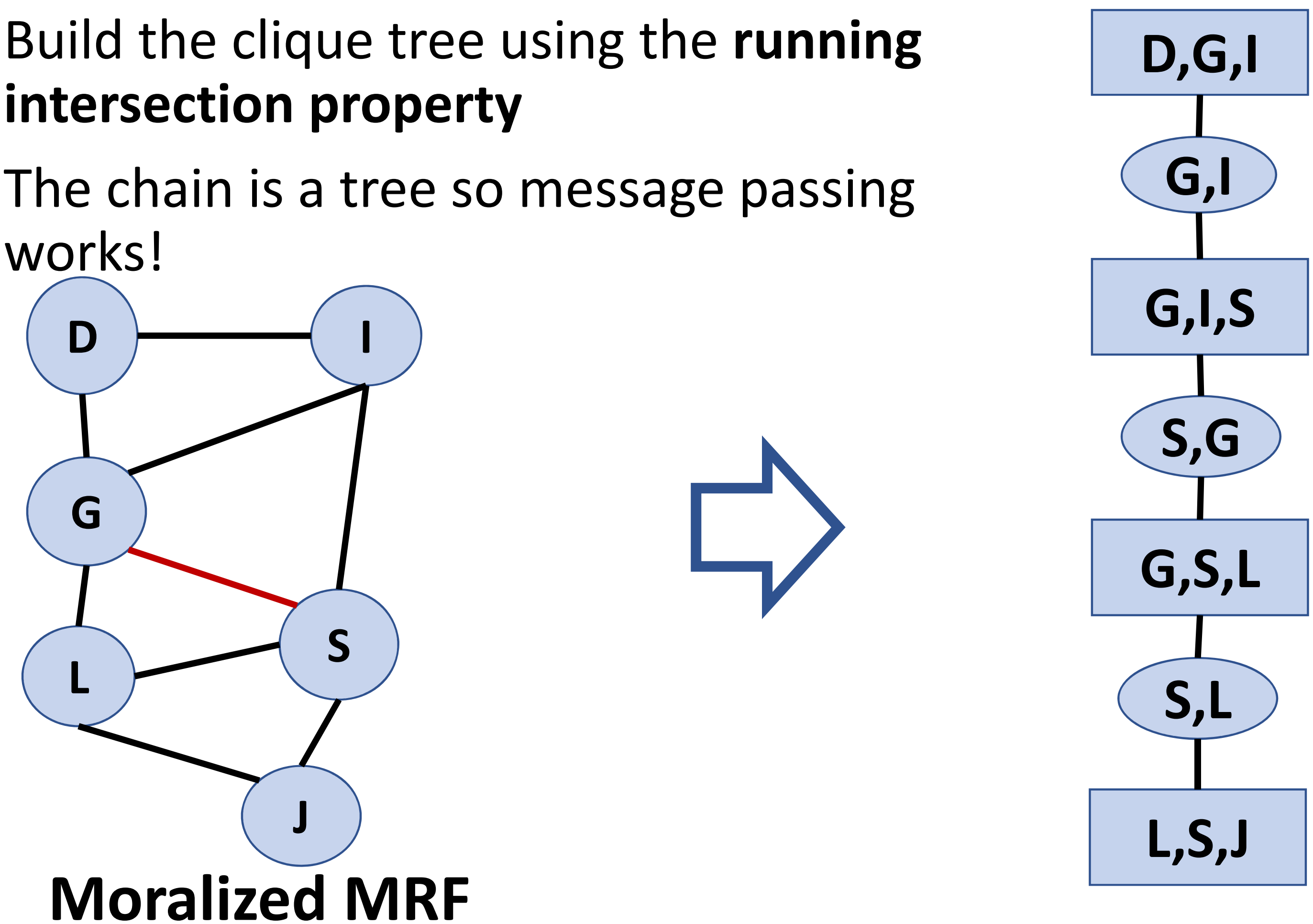


Moralized MRF

Junction Tree Example

Triangulate

- Build the clique tree using the **running intersection property**
- The chain is a tree so message passing works!



Relationship Between Junction Tree and Variable Elimination

There is a strong relationship between the Junction tree and variable elimination algorithms

- Combining all remaining tables containing a variable eliminates it
- A node in the junction tree corresponds to the variable in variable elimination
- An arc in the junction tree shows the flow of data for the elimination computation

Vocabulary

- **Exact inference algorithms** = methods to get a marginal distribution
- **Variable Elimination Algorithm** = marginalize variables one-by-one in order, to solve for a marginal distribution of 1 variable
- **Factor** = multidimensional table which assigns a value to a set of variables; representation of an unnormalized conditional distribution
- **Message Passing Algorithm** or **Belief Propagation Algorithm** = cascading queries that pass factors through a tree graph, to solve for a marginal distribution of 1 variable
- **Tree graph** = undirected acyclic graph, in which any pair of nodes are connected by exactly one path.

Vocabulary

- **Message** $m_{ji}(x_i)$ = the message from node j to node i
- **Running Intersection Property** = for each pair of cliques U, V with intersection S, all cliques on the path between U and V contain S.
- **Triangulation** = a process of breaking cycles in an undirected graph
- **Cycle** has 4 or more nodes

Key Points

- Faster computation is achievable by using distributions factored on a graph by independencies
- Categories of Inference on Graphical Models: exact inference, approximate
- 3 most common exact inference algorithms: variable elimination, message passing, junction tree
- Variable elimination algorithm: eliminate variables one by one; choice of variable order determines computational complexity
- Message passing algorithm: factors (not probabilities!) are passed along a tree graph; factors can be stored for speeding up later queries; messages "propagate belief"; linear time complexity

Key Points

- Belief propagation algorithm: (similar to message-passing) leaf nodes emit messages, each node collects all neighbors' messages then emits messages to all its neighbors
- Factor graphs: another graphical model representation; the basis of message passing algorithms; have variables, factors, intersections
- Factor graph message types: variable to factor, factor to variable
- Junction tree algorithm: convert to Markov, triangulate, build clique tree, build factor graph, choose root, populate cliques, use sum-product algorithm to calculate marginal distribution