Readings:
K&F: 8.4, 12.1, 12.2, 9

Complexity of Var. Elim
MPE Inference
Junction Trees

Graphical Models – 10708
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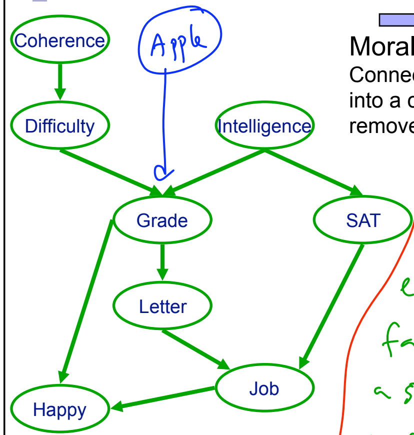
What's next

- Thus far: Variable elimination
  - (Often) Efficient algorithm for inference in graphical models
- Next: Understanding complexity of variable elimination
  - Will lead to cool junction tree algorithm later

Complexity of variable elimination – Graphs with loops



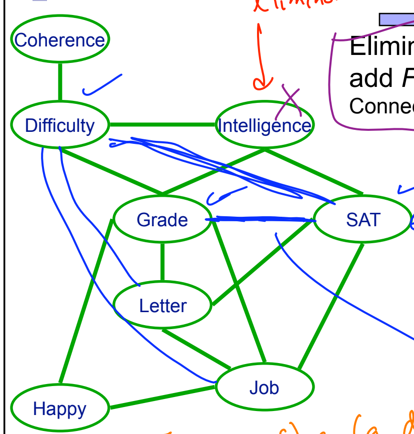
Moralize graph:
Connect parents into a clique and remove edge directions

initial factors $f_i = P(X_i | Pa_{X_i})$

every initial factor f_i is a subset of a maximal clique in moralized graph

Connect nodes that appear together in an initial factor

Eliminating a node – Fill edges



Eliminate variable add *Fill Edges*:
Connect neighbors

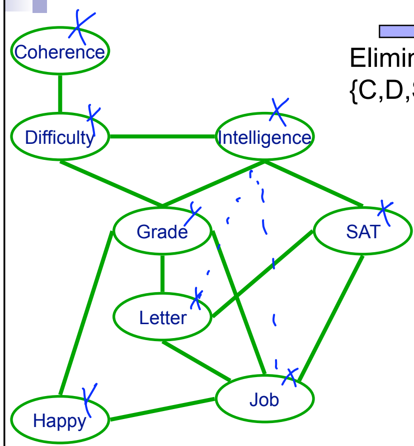
not a subset of a maximal clique ⇒ add fill edges

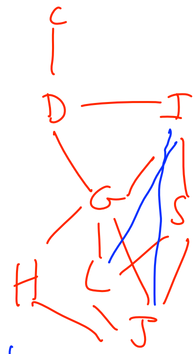
Induced graph

The induced graph $I_{F\lhd}$ for elimination order $\lhd$ has an edge $X_i - X_j$ if X_i and X_j appear together in a factor generated by VE for elimination order $\lhd$ on factors F

$\lhd \equiv$ {

Elimination order:
{C,D,S,I,L,H,J,G}



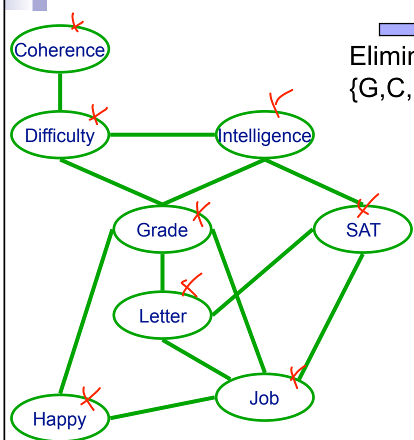


each VE factor subset of maximal clique

largest clique: {G,I,L,J} => VE exp. in 4

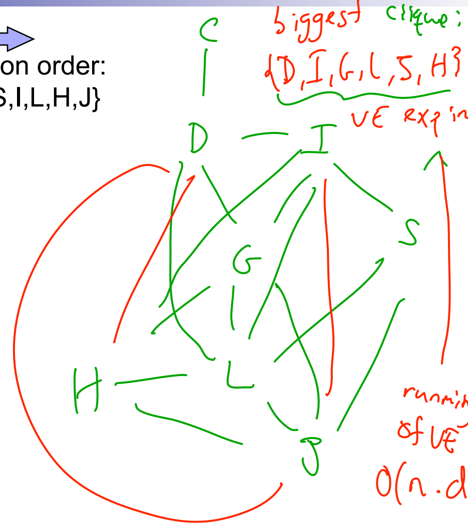
Different elimination order can lead to different induced graph

Elimination order:
{G,C,D,S,I,L,H,J}



biggest clique: {D,I,G,L,S,H}

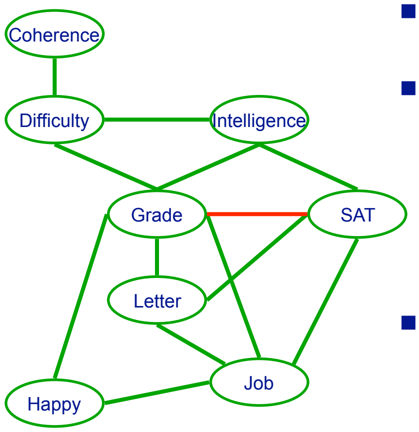
VE exp in 6



running of VE $O(n \cdot d^6)$

Induced graph and complexity of VE

Read complexity from cliques in induced graph



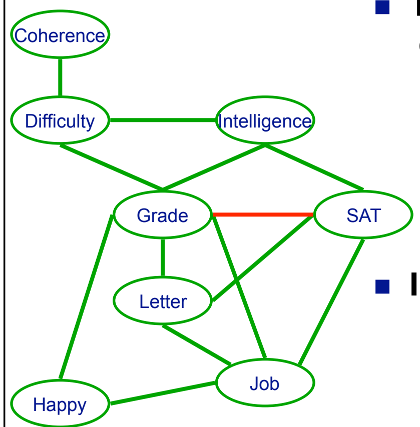
Elimination order:
{C,D,I,S,L,H,J,G}

- Structure of induced graph encodes complexity of VE!!!
- **Theorem**:
  - Every factor generated by VE subset of a maximal clique in $I_{F\triangleleft}$
  - For every maximal clique in $I_{F\triangleleft}$ corresponds to a factor generated by VE
- **Induced width** (or treewidth)
  - Size of largest clique in $I_{F\triangleleft}$ minus 1
  - *Minimal induced width* – induced width of best order ·

Example: Large induced-width with small number of parents

Compact representation $\not\Rightarrow$ Easy inference ☹

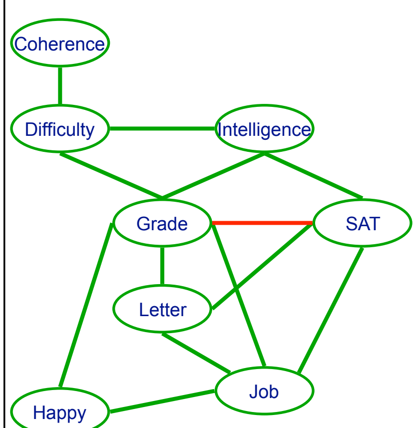
Finding optimal elimination order



Elimination order:
{C,D,I,S,L,H,J,G}

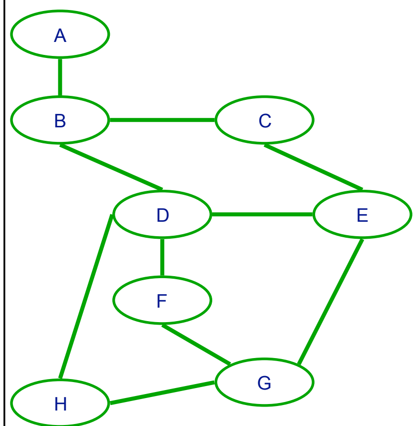
- **Theorem**: Finding best elimination order is NP-complete:
  - Decision problem: Given a graph, determine if there exists an elimination order that achieves induced width ≤ K
- **Interpretation**:
  - Hardness of finding elimination order in addition to hardness of inference
  - Actually, can find elimination order in time exponential in size of largest clique – same complexity as inference

Induced graphs and chordal graphs



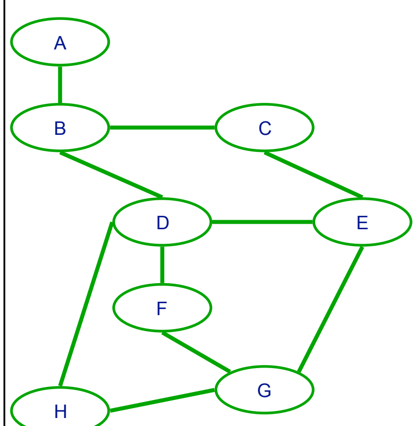
- **Chordal graph**:
  - Every cycle $X_1 – X_2 – \ldots – X_k – X_1$ with $k \geq 3$ has a chord
    - Edge $X_i – X_j$ for non-consecutive i & j
- **Theorem**:
  - Every induced graph is chordal
- "Optimal" elimination order easily obtained for chordal graph

Chordal graphs and triangulation



- **Triangulation**: turning graph into chordal graph
- **Max Cardinality Search**:
  - Simple heuristic
- Initialize unobserved nodes **X** as unmarked
- For k = |**X**| to 1
  - X ← unmarked var with most **marked** neighbors
  - ◁(X) ← k
  - Mark X
- **Theorem**: Obtains optimal order for chordal graphs
- Often, not so good in other graphs!

Minimum fill/size/weight heuristics

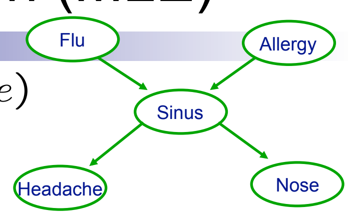


- Many more effective heuristics
  - see reading
- **Min (weighted) fill heuristic**
  - Often very effective
- Initialize unobserved nodes **X** as unmarked
- For k = 1 to |**X**|
  - X ← unmarked var whose elimination adds fewest edges
  - ◁(X) ← k
  - Mark X
  - Add fill edges introduced by eliminating X
- Weighted version:
  - Consider size of factor rather than number of edges

Choosing an elimination order

- Choosing best order is NP-complete
  - Reduction from MAX-Clique
- Many good heuristics (some with guarantees)
- Ultimately, can't beat NP-hardness of inference
  - Even optimal order can lead to exponential variable elimination computation
- In practice
  - Variable elimination often very effective
  - Many (many many) approximate inference approaches available when variable elimination too expensive
  - Most approximate inference approaches build on ideas from variable elimination

Most likely explanation (MLE)



- Query: $\operatorname{argmax}_{x_1,\ldots,x_n} P(x_1,\ldots,x_n \mid e)$
- Using defn of conditional probs:

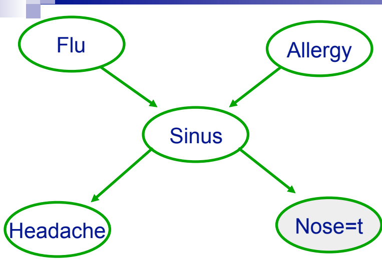
$$\operatorname{argmax}_{x_1,\ldots,x_n} P(x_1,\ldots,x_n \mid e) = \operatorname{argmax}_{x_1,\ldots,x_n} \frac{P(x_1,\ldots,x_n,e)}{P(e)}$$

- Normalization irrelevant:

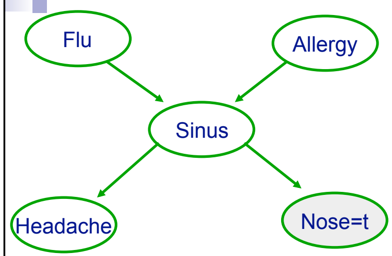
$$\operatorname{argmax}_{x_1,\ldots,x_n} P(x_1,\ldots,x_n \mid e) = \operatorname{argmax}_{x_1,\ldots,x_n} P(x_1,\ldots,x_n,e)$$

Max-marginalization

Example of variable elimination for MLE – Forward pass



Example of variable elimination for MLE – Backward pass



MLE Variable elimination algorithm – Forward pass

- Given a BN and a MLE query $\max_{x_1,\ldots,x_n} P(x_1,\ldots,x_n,\mathbf{e})$
- Instantiate evidence **E**=**e**
- Choose an ordering on variables, e.g., $X_1, \ldots, X_n$
- For i = 1 to n, If $X_i \notin \mathbf{E}$
  - Collect factors $f_1,\ldots,f_k$ that include X_i
  - Generate a new factor by eliminating X_i from these factors

$$g = \max_{x_i} \prod_{j=1}^{k} f_j$$

  - Variable X_i has been eliminated!

MLE Variable elimination algorithm – Backward pass

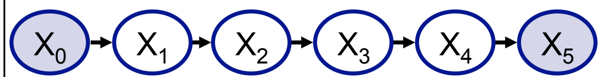
- $\{x_1^*, \ldots, x_n^*\}$ will store maximizing assignment
- For i = n to 1, If $X_i \notin \mathbf{E}$
  - Take factors $f_1, \ldots, f_k$ used when X_i was eliminated
  - Instantiate $f_1, \ldots, f_k$, with $\{x_{i+1}^*, \ldots, x_n^*\}$
    - Now each f_j depends only on X_i
  - Generate maximizing assignment for X_i:

$$x_i^* \in \operatorname*{argmax}_{x_i} \prod_{j=1}^{k} f_j$$

What you need to know about VE

- Variable elimination algorithm
  - Eliminate a variable:
    - Combine factors that include this var into single factor
    - Marginalize var from new factor
  - Cliques in induced graph correspond to factors generated by algorithm
  - Efficient algorithm ("only" exponential in induced-width, not number of variables)
    - If you hear: "Exact inference only efficient in tree graphical models"
    - You say: "No!!! Any graph with low induced width"
    - And then you say: "And even some with very large induced-width" (special recitation)
- Elimination order is important!
  - NP-complete problem
  - Many good heuristics
- Variable elimination for MLE
  - Only difference between probabilistic inference and MLE is "sum" versus "max"

What if I want to compute $P(X_i|x_0,x_{n+1})$ for each i?

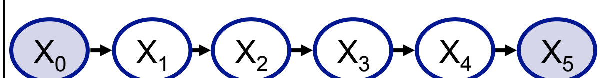


Compute:
$$P(X_i \mid x_0, x_{n+1})$$

Variable elimination for each i?

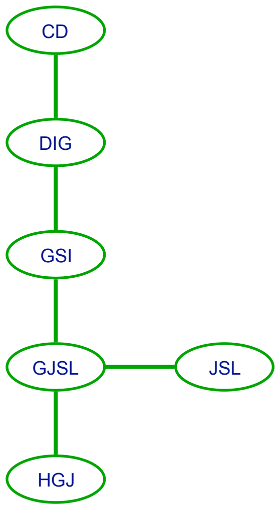
Variable elimination for every i, what's the complexity?

Reusing computation

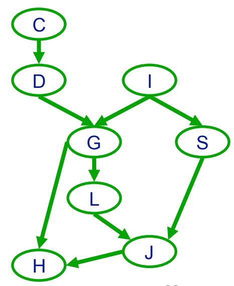


Compute:
$$P(X_i \mid x_0, x_{n+1})$$

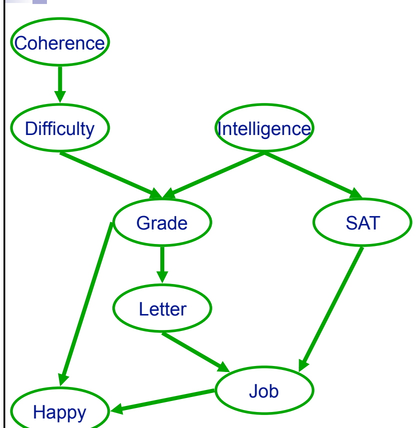
Cluster graph



- **Cluster graph**: For set of factors *F*
  - Undirected graph
  - Each node i associated with a cluster $\mathbf{C}_i$
  - *Family preserving*: for each factor $f_j \in F$, $\exists$ node i such that scope[f_j] $\subseteq \mathbf{C}_i$
  - Each edge i – j is associated with a separator $\mathbf{S}_{ij} = \mathbf{C}_i \cap \mathbf{C}_j$

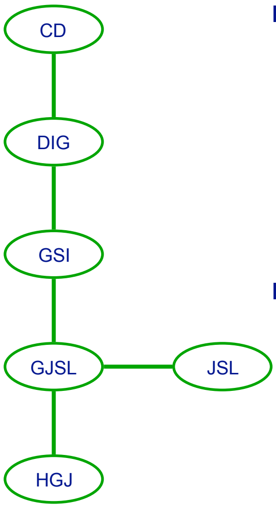


Factors generated by VE



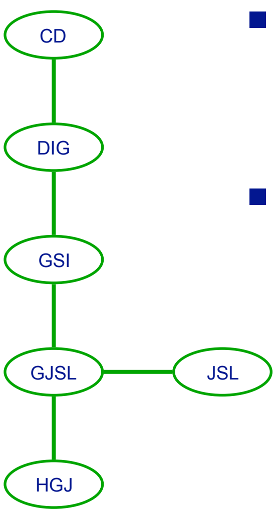
Elimination order:
{C,D,I,S,L,H,J,G}

Cluster graph for VE



- **VE generates cluster tree!**
  - One clique for each factor used/generated
  - Edge i – j, if f_i used to generate f_j
  - "Message" from i to j generated when marginalizing a variable from f_i
  - Tree because factors only used once
- **Proposition**:
  - "Message" δ_{ij} from i to j
  - Scope[δ_{ij}] $\subseteq$ $\mathbf{S}_{ij}$

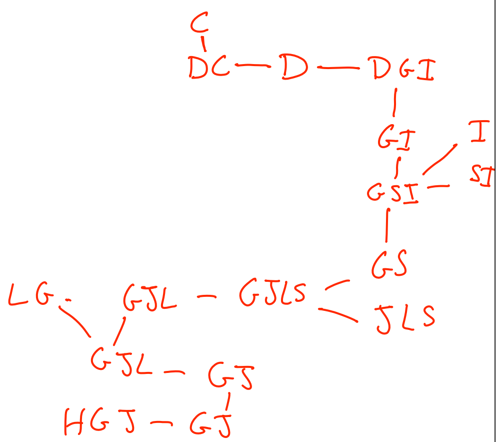
Running intersection property



- **Running intersection property (RIP)**
  - Cluster tree satisfies RIP if whenever $X \in \mathbf{C}_i$ and $X \in \mathbf{C}_j$ then X is in every cluster in the (unique) path from $\mathbf{C}_i$ to $\mathbf{C}_j$
- **Theorem**:
  - Cluster tree generated by VE satisfies RIP

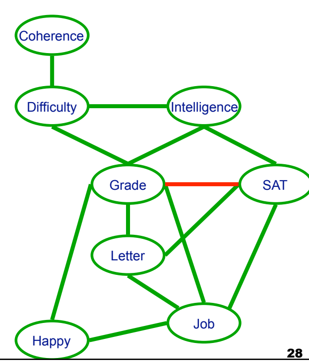
Constructing a clique tree from VE

- Select elimination order ◁
- Connect factors that would be generated if you run VE with order ◁
- Simplify!
  - Eliminate factor that is subset of neighbor

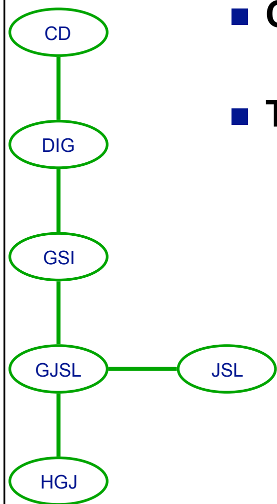


Find clique tree from chordal graph

- Triangulate moralized graph to obtain chordal graph
- Find maximal cliques
  - NP-complete in general
  - Easy for chordal graphs
  - Max-cardinality search
- Maximum spanning tree finds clique tree satisfying RIP!!!
  - Generate weighted graph over cliques
  - Edge weights (i,j) is separator size – $|C_i \cap C_j|$

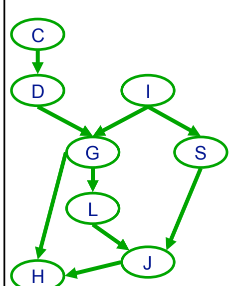


Clique tree & Independencies



- **Clique tree (or Junction tree)**
  - A cluster tree that satisfies the RIP
- **Theorem**:
  - Given some BN with structure *G* and factors *F*
  - For a clique tree *T* for *F* consider $\mathbf{C}_i - \mathbf{C}_j$ with separator $\mathbf{S}_{ij}$:
    - **X** – any set of vars in $\mathbf{C}_i$ side of the tree
    - **Y** – any set of vars in $\mathbf{C}_j$ side of the tree
  - Then, $(\mathbf{X} \perp \mathbf{Y} \mid \mathbf{S}_{ij})$ in BN
  - Furthermore, $I(T) \subseteq I(G)$

Variable elimination in a clique tree 1

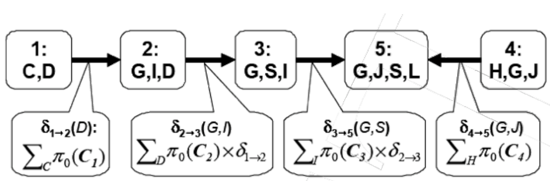


- **Clique tree for a BN**
  - Each CPT assigned to a clique
  - Initial potential $\pi_0(\mathbf{C}_i)$ is product of CPTs

Variable elimination in a clique tree 2

- **VE in clique tree to compute $P(X_i)$**
  - Pick a root (any node containing X_i)
  - Send messages recursively from leaves to root
    - Multiply incoming messages with initial potential
    - Marginalize vars that are not in separator
  - Clique *ready* if received messages from all neighbors

Belief from message

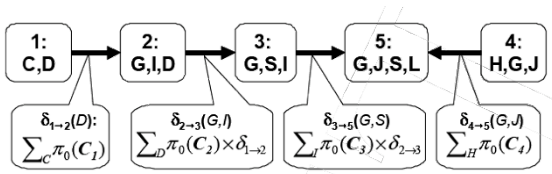


- **Theorem**: When **clique C_i is ready**
  - Received messages from all neighbors
  - Belief $\pi_i(\mathbf{C}_i)$ is product of initial factor with messages:

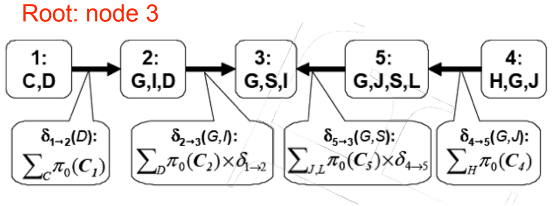
Choice of root

- **Message does not depend on root!!!**

Root: node 5

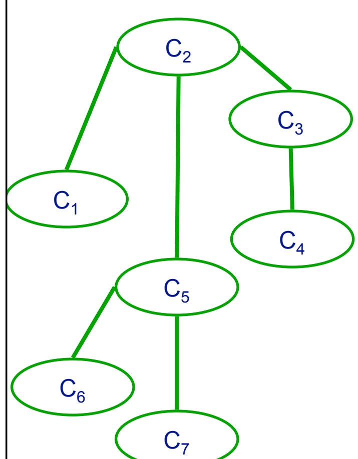


Root: node 3



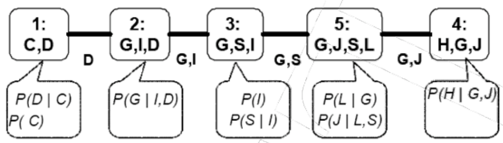
"Cache" computation: Obtain belief for all roots in linear time!!

Shafer-Shenoy Algorithm (a.k.a. VE in clique tree for all roots)



- Clique $\mathbf{C}_i$ *ready to transmit* to neighbor $\mathbf{C}_j$ if received messages from all neighbors but j
  - Leaves are always ready to transmit
- While $\exists$ $\mathbf{C}_i$ ready to transmit to $\mathbf{C}_j$
  - Send message $\delta_{i\to j}$
- Complexity: Linear in # cliques
  - One message sent each direction in each edge
- **Corollary**: At convergence
  - Every clique has correct belief

Calibrated Clique tree



- Initially, neighboring nodes don't agree on "distribution" over separators
- **Calibrated clique tree**:
  - At convergence, tree is *calibrated*
  - Neighboring nodes agree on distribution over separator

Answering queries with clique trees

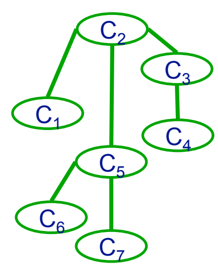
- Query within clique
- Incremental updates – Observing evidence Z=z
  - Multiply some clique by indicator **1**(Z=z)
- Query outside clique
  - Use variable elimination!

Message passing with division

- Computing messages by multiplication:
- Computing messages by division:

Lauritzen-Spiegelhalter Algorithm (a.k.a. belief propagation)

Simplified description see reading for details



- Initialize all separator potentials to 1
  - $\mu_{ij} \leftarrow 1$
- All messages ready to transmit
- While $\exists\ \delta_{i\rightarrow j}$ ready to transmit
  - $\mu_{ij}' \leftarrow$
  - If $\mu_{ij}' \neq \mu_{ij}$
    - $\delta_{i\rightarrow j} \leftarrow$
    - $\pi_j \leftarrow \pi_j \times \delta_{i\rightarrow j}$
    - $\mu_{ij} \leftarrow \mu_{ij}'$
    - $\forall$ neighbors k of j, $k \neq i$, $\delta_{j\rightarrow k}$ ready to transmit
- Complexity: Linear in # cliques
  - for the “right” schedule over edges (leaves to root, then root to leaves)
- **Corollary**: At convergence, every clique has correct belief

VE versus BP in clique trees

- VE messages (the one that multiplies)
- BP messages (the one that divides)

Clique tree invariant

- **Clique tree potential**:
  - Product of clique potentials divided by separators potentials
- Clique tree **invariant**:
  - P(**X**) = π_T(**X**)

Belief propagation and clique tree invariant

- **Theorem**: Invariant is maintained by BP algorithm!
- BP reparameterizes clique potentials and separator potentials
  - At convergence, potentials and messages are marginal distributions

Subtree correctness

- **Informed message** from i to j, if all messages into i (other than from j) are informed
  - Recursive definition (leaves always send informed messages)
- **Informed subtree**:
  - All incoming messages informed
- **Theorem**:
  - Potential of connected informed subtree *T'* is marginal over scope[*T'*]
- **Corollary**:
  - At convergence, clique tree is *calibrated*
    - π_i = P(scope[π_i])
    - μ_{ij} = P(scope[μ_{ij}])

Clique trees versus VE

- Clique tree advantages
  - Multi-query settings
  - Incremental updates
  - Pre-computation makes complexity explicit

- Clique tree disadvantages
  - Space requirements – no factors are "deleted"
  - Slower for single query
  - Local structure in factors may be lost when they are multiplied together into initial clique potential

Clique tree summary

- Solve marginal queries for all variables in only twice the cost of query for one variable
- Cliques correspond to maximal cliques in induced graph
- Two message passing approaches
  - VE (the one that multiplies messages)
  - BP (the one that divides by old message)
- Clique tree invariant
  - Clique tree potential is always the same
  - We are only reparameterizing clique potentials
- Constructing clique tree for a BN
  - from elimination order
  - from triangulated (chordal) graph
- Running time (only) exponential in size of largest clique
  - Solve **exactly** problems with thousands (or millions, or more) of variables, and cliques with tens of nodes (or less)