Probabilistic Graphical Models & Probabilistic AI

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Lecture 6: Exact Inference

February 6, 2025

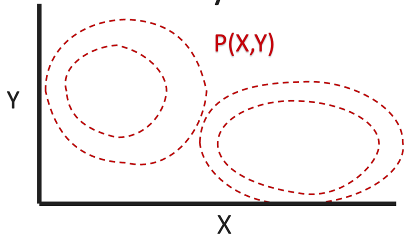
Reading: See course homepage

Logistics Reminders

- No class Tuesday, Feb 11
- HW2 due Tuesday, Feb 11 on Canvas
- Quiz in-class Thursday, Feb 13

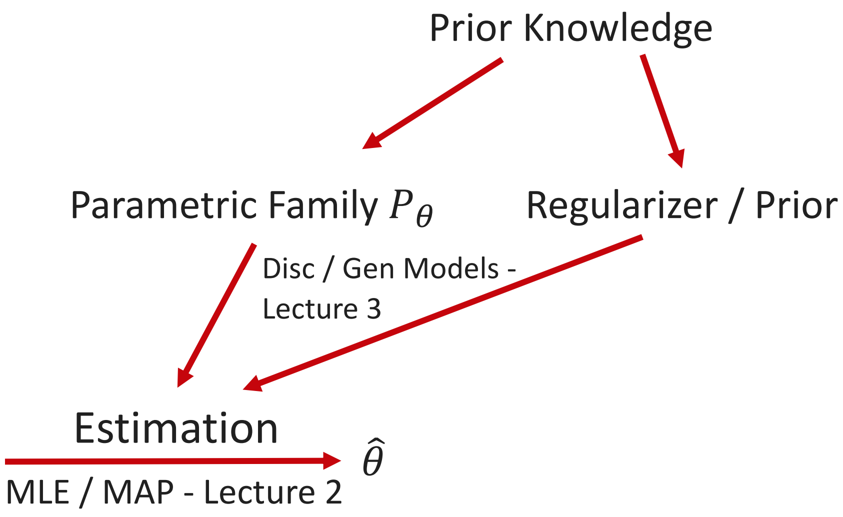
A Brief Recap of our Roadmap

Probability Distribution



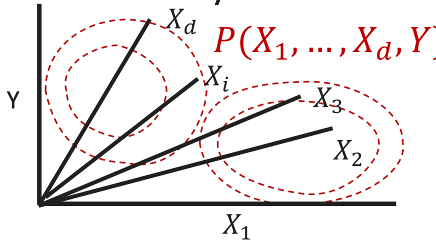
Observations

X	Y
0	0
0.1	1
0.2	1



A Brief Recap of our Roadmap

Probability Distribution



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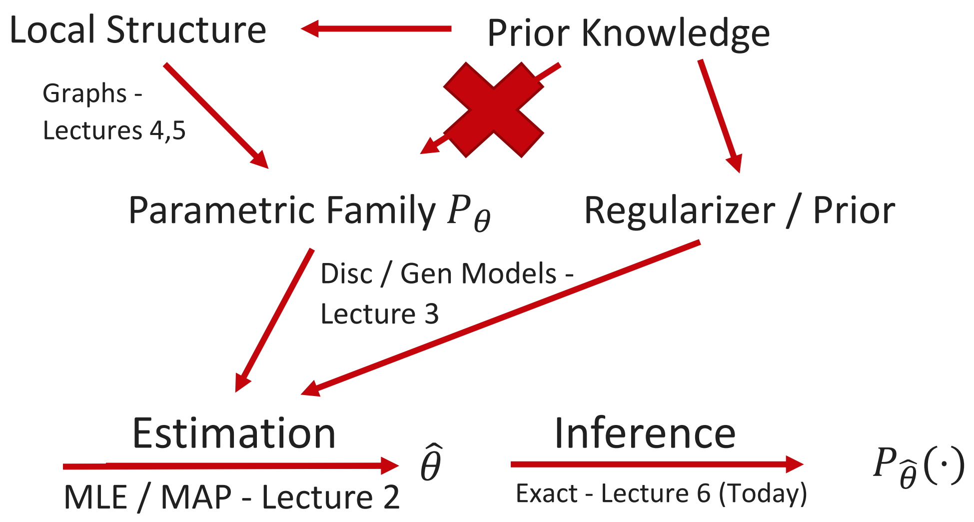
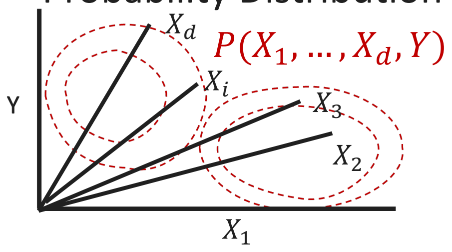


A Brief Recap of our Roadmap



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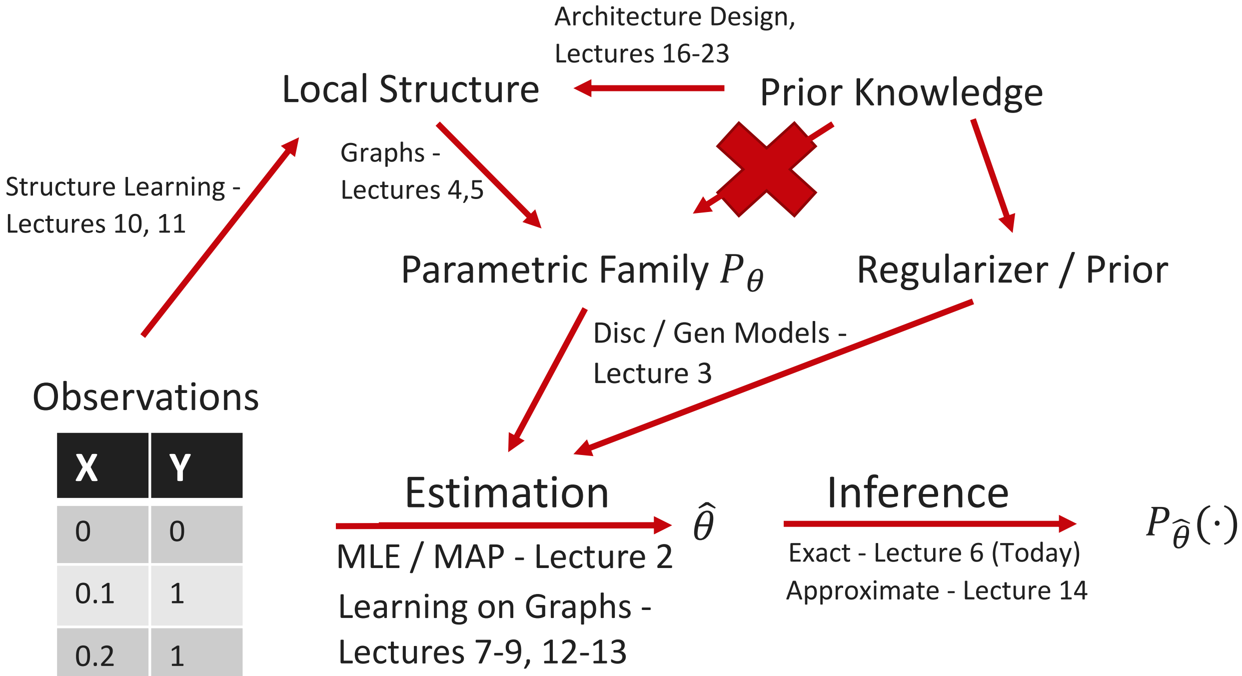


Today

- Exact Inference
  - Variable Elimination

Exact Inference

Probabilistic Inference and Learning

- We now have compact representations of probability distributions: Graphical Models (GMs)
- A GM M describes a probability distribution P_M.
- Typical tasks:
  - Task 1 (**Inference**): How do we answer queries about P_M - e.g. $P_M(X \mid Y)$?
  - Task 2 (**Learning**): How do we estimate a plausible model M from data D?

When could "learning" be seen as a form of inference?

Bayesian Perspective:
Seeks $P_{prior}(M|D)$

Missing Data: Must impute missing data
$P(M|D) = \int_{D_{missing}} P\big(D \mid D_{present} \big) P(M|D)$

Example Query 1: Likelihood

- Many queries involve **evidence**
  - Evidence $\boldsymbol{e}$ is an assignment of values to a set $\boldsymbol{E}$ of variables
- Example: compute the probability of evidence $\boldsymbol{e}$

$$P(e) = \sum_{X_1} \cdots \sum_{X_k} P(X_1, \ldots, X_k, e)$$

- aka compute the likelihood of $\boldsymbol{e}$

Example Query 2: Conditional Probability

- Often we are interested in the **conditional probability distribution** of a variable given the evidence

$$P(X \mid e) = \frac{P(X, e)}{P(e)} = \frac{P(X, e)}{\sum_x P(X = x, e)}$$

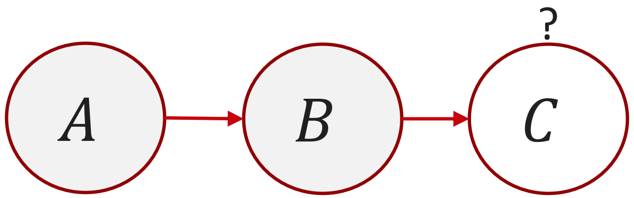
  - aka compute the ***a posteriori belief*** in X given evidence e
- We usually query a subset Y of all domain variables $X = \{Y, Z\}$ and don't care about the remaining Z:

$$P(Y \mid e) = \sum_z P(Y, Z = z \mid e)$$

  - aka ***maginalization***.

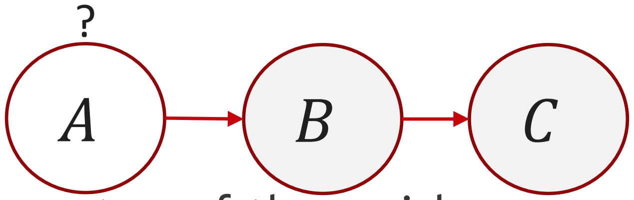
Examples of a Posteriori Belief

- **Prediction:** What's the probability of an outcome given the starting condition?



  - Query node is a descendent of the evidence

- **Diagnosis:** What's the probability of an underlying disease/fault given observed symptoms?



  - Query node is an ancestor of the evidence

Probabilistic inference combines evidence from all parts of the network, not just following the directionality of the edges in a GM.

Example Query 3: Most Probable Assignment

- What's the most probable assignment (MPA) for some variables of interest?
- Usually performed under some evidence e and marginalized over other variables Z:

$$MPA(Y \mid e) = \text{argmax}_y P(Y = y \mid e)$$
$$= \text{argmax}_y \sum_z P(Y = y, Z = z \mid e)$$

- Examples:
  - Classification: $\hat{Y} = MPA(Y \mid e)$
  - Explanation: What is the most likely scenario given the evidence?

A cautionary note on MPA

- The MPA of a variable depends on the query “context” – the set of variables being jointly queried.
- Example:
  - MPA of Y_1?
  - MPA of (Y_1, Y_2)?

Y_1	Y_2	$P(Y_2, Y_2)$
0	0	0.35
0	1	0.05
1	0	0.3
1	1	0.3

Complexity of inference

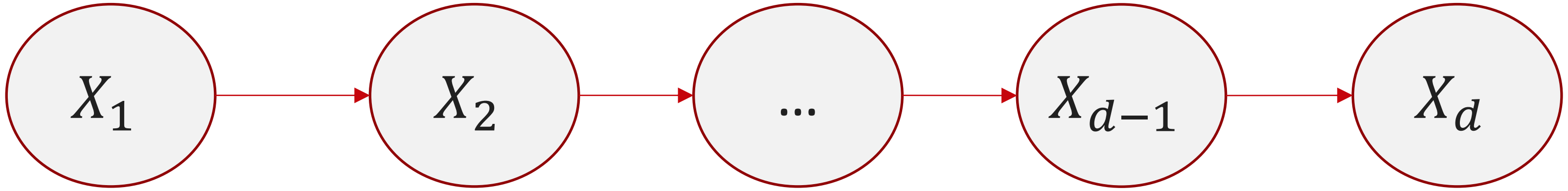
- Computing $P(X = x \mid e)$ in a GM is **NP-hard**

What does this mean for us?

- ➢ Inference cannot be solved in polynomial time unless P=NP.
- ➢ No general procedure that works efficiently for arbitrary GMs.
  - ➢ For families of GMs, we can have provably efficient procedures.
- ➢ Exponential worst-case performance for exact inference.
  - ➢ Motivates approximate inference.

Elimination on Chains

- Consider the following GM:



- What is the likelihood that X_d is true?

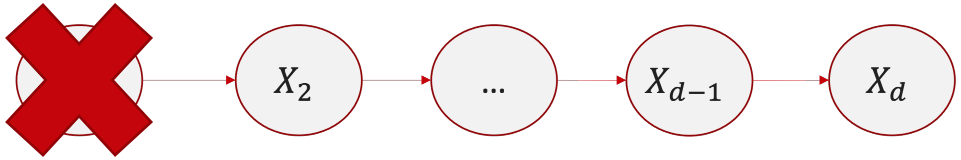
$$P(e) = \sum_{x_1} \sum_{x_2} \cdots \sum_{x_{d-1}} P(X_1 = x_1, X_2 = x_2, \ldots, X_d = x_d)$$

Exponential # of terms

- Leverage chain structure:

$$P(e) = \sum_{x_1} \sum_{x_2} \cdots \sum_{x_{d-1}} P(X_1 = x_1) \prod_{i=2}^{d} P(X_i = x_i \mid X_{i-1} = x_{i-1})$$

Elimination on Chains



- Leverage chain structure:

$$P(e) = \sum_{x_1} \sum_{x_2} \cdots \sum_{x_{d-1}} P(X_1 = x_1) \prod_{i=2}^{d} P(X_i = x_i \mid X_{i-1} = x_{i-1})$$

- Reorder terms:

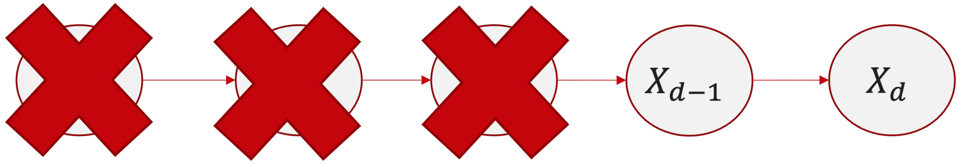
$$P(e) = \sum_{x_2} \cdots \sum_{x_{d-1}} \prod_{i=3}^{d} P(X_i \mid X_{i-1}) \sum_{x_1} P(X_1) P(X_2 \mid X_1)$$

- Substitute:

$$P(e) = \sum_{x_2} \cdots \sum_{x_{d-1}} \prod_{i=3}^{d} P(X_i \mid X_{i-1}) P(X_2)$$

Eliminates one variable from our summation at a **local cost.**

Elimination on Chains



- Continue eliminating variables:

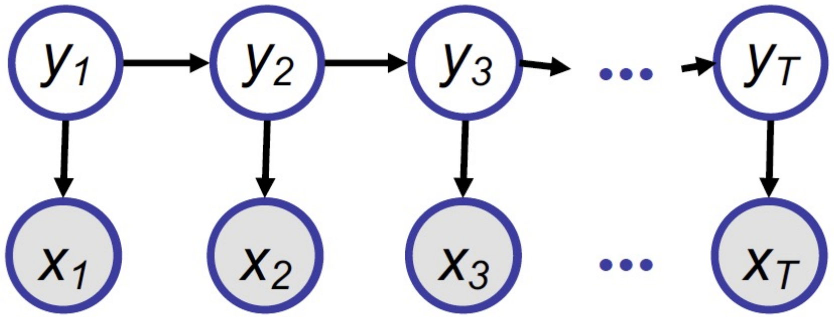
$$P(e) = \sum_{x_3} \cdots \sum_{x_{d-1}} \prod_{i=4}^{d} P(X_i \mid X_{i-1})\, P(X_3)$$

- Eliminate nodes one-by-one all the way to the end

$$P(e) = \sum_{x_{d-1}} P(X_d \mid X_{d-1})\, P(X_{d-1})$$

- Complexity of this calculation:
  - d steps, Each step takes $\approx |Dom(X_i)| * |Dom(X_{i-1})|$ operations
  - ➔ $\mathcal{O}(dn^2)$ where $n = \max_i |Dom(X_i)|$
  - Compare to naïve $\mathcal{O}(d^n)$

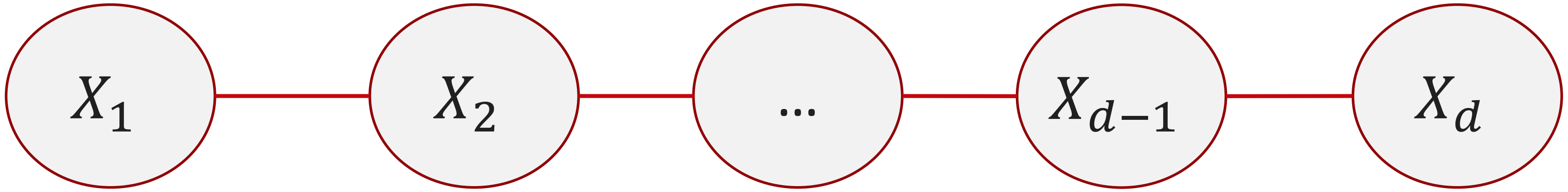
Example: HMMs



$$p(\mathbf{x}, \mathbf{y}) = p(x_1 \ldots\ldots x_T, y_1, \ldots\ldots, y_T)$$
$$= p(y_1)\, p(x_1 \mid y_1)\, p(y_2 \mid y_1)\, p(x_2 \mid y_2) \ldots p(y_T \mid y_{T-1})\, p(x_T \mid y_T)$$

$$p(y_i | x_1, \ldots, x_T) = \sum_{y_1} \cdots \sum_{y_{i-1}} \sum_{y_{i+1}} \cdots \sum_{y_T} p(y_i, \ldots, y_T, x_1, \ldots, x_T)$$
$$= \sum_{y_1} \cdots \sum_{y_{i-1}} \sum_{y_{i+1}} \cdots \sum_{y_T} p(y_1)p(x_1|y_1) \ldots p(y_T|y_{T-1})p(x_T|y_T)$$

Elimination on Undirected Chains

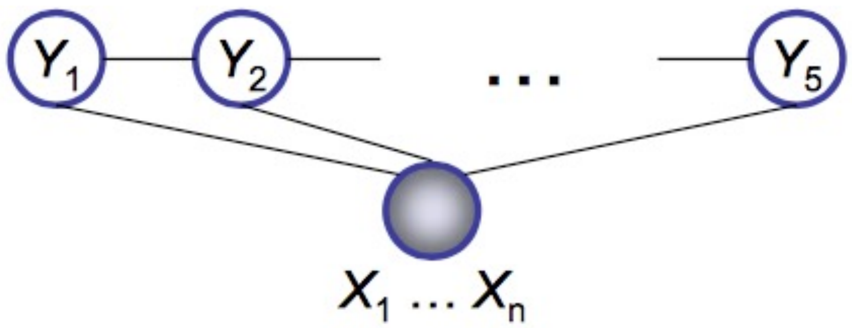


$$P(e) = \sum_{X_1}\sum_{X_2}\cdots\sum_{X_d}\frac{1}{Z}\prod_{i=2}^{d}\phi(X_i, X_{i-1})$$

$$= \frac{1}{Z}\sum_{X_d}\cdots\sum_{X_2}\prod_{i=3}^{d}\phi(X_i, X_{i-1})\sum_{X_1}\phi(X_2, X_1)$$

$$= \cdots$$

Example: Conditional Random Fields



$$
\begin{aligned}
& p(y_1, \ldots, y_T | \mathbf{x}) \\
\propto \quad & \exp\Big(w_{1,2}\phi(y_1, y_2|\mathbf{x}) + w_{2,3}\phi(y_2, y_3|\mathbf{x}) + \ldots + w_{T-1,T}\phi(y_{T-1}, y_T|\mathbf{x}) \\
& + u_1\phi(y_1|\mathbf{x}) + u_2\phi(y_2|\mathbf{x}) + \ldots + u_T\phi(y_T|\mathbf{x})\Big) \\
= \quad & \Phi(y_1, y_2)\Phi(y_2, y_3)\ldots\Phi(y_{T-1}, y_T)
\end{aligned}
$$

The Sum-Product Operation

- In general, we want to compute the value of an expression of the form:

$$\sum_{z} \prod_{\phi \in F} \phi$$

where F is a set of factors

- We call this task the **sum-product inference task**.

Variable Elimination: General form

- Write query in the form

$$P(X_1, e) = \sum_{x_d} \cdots \sum_{x_3} \sum_{x_2} \prod_i P(x_i \mid pa_i)$$

- Then iteratively:
  - Move all irrelevant terms outside of innermost sum.
  - Perform innermost sum, getting a new term.
  - Insert the new term into the product.

Outcome of elimination

- Let X be some set of variables
- Let F be a set of factors such that for each $\phi \in F, Scope[\phi] \in X$
- Let $Y \subset X$ be a set of query variables and $Z = X - Y$ be the variable to be eliminated.
- The result of eliminating Z is a factor

$$\tau(Y) = \sum_{z} \prod_{\phi \in F} \phi$$

- This doesn't necessarily correspond to any probability or conditional probability.

Evidence and Sum-Product

- Evidence potential $\delta(E_i, \bar{e}_i) = \begin{cases} 1 & \text{if } E_i \equiv \bar{e}_i \\ 0 & \text{if } E_i \neq \bar{e}_i \end{cases}$
- Total evidence potential $\delta(\mathbf{E}, \bar{\mathbf{e}}) = \prod_{i \in I_{\mathbf{E}}} \delta(E_i, \bar{e}_i)$
- Introducing evidence-restricted factors:

$$\tau(Y, \bar{e}) = \sum_{z,e} \prod_{\phi \in F} \phi \cdot \delta(E, \bar{e})$$

Variable Elimination Algorithm

Procedure **Elimination**(

G, // the GM

E, // evidence

Z, // set of variables to be eliminated

X, // query variable(s)

)

1. Initialize (G)
2. Evidence (E)
3. Sum-product-Elimination (F, Z)
4. Normalization (F)

Variable Elimination Algorithm

Procedure Initialize (G, Z)

1. Let $Z_1, \ldots, Z_k$ be an ordering of Z such that $Z_i \prec Z_j$ iff $i < j$
2. Initialize F with the full the set of factors

Procedure Evidence $(\mathbf{E})$

1. for each $i \in I_E$,

   $F = F \cup \delta(E_i, e_i)$

Procedure Sum-Product-Variable-Elimination $(F, Z, \prec)$

1. for $i = 1, \ldots, k$

   $F \leftarrow$ Sum-Product-Eliminate-Var(F, Z_i)
2. $\phi^* \leftarrow \prod_{\phi \in F} \phi$
3. return ϕ^*
4. Normalization (ϕ^*)

Procedure Normalization (ϕ^*)

1. $P(X|\mathbf{E}) = \phi^*(X) / \sum_x \phi^*(X)$

Procedure Sum-Product-Eliminate-Var (

F, // Set of factors

Z // Variable to be eliminated

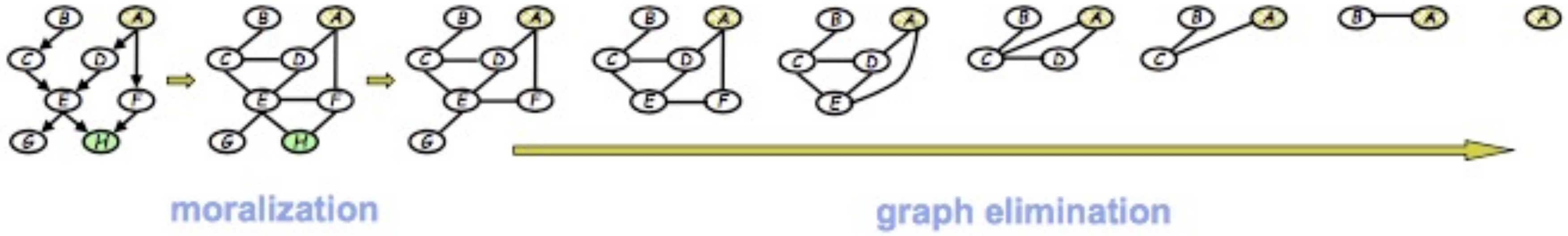
)

1. $F' \leftarrow \{\phi \in F : Z \in Scope[\phi]\}$
2. $F'' \leftarrow F - F'$
3. $\psi \leftarrow \prod_{\phi \in F'} \phi$
4. $\tau \leftarrow \sum_Z \psi$
5. return $F'' \cup \{\tau\}$

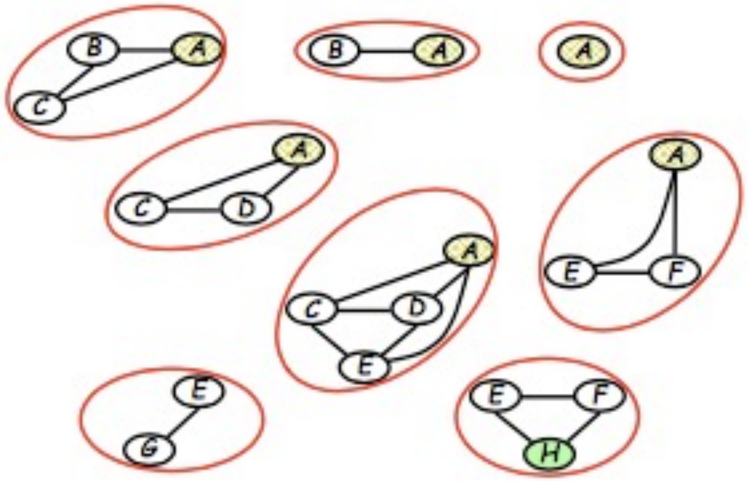
Complexity is **exponential** in number of variables in the **intermediate factor**

Understanding Variable Elimination

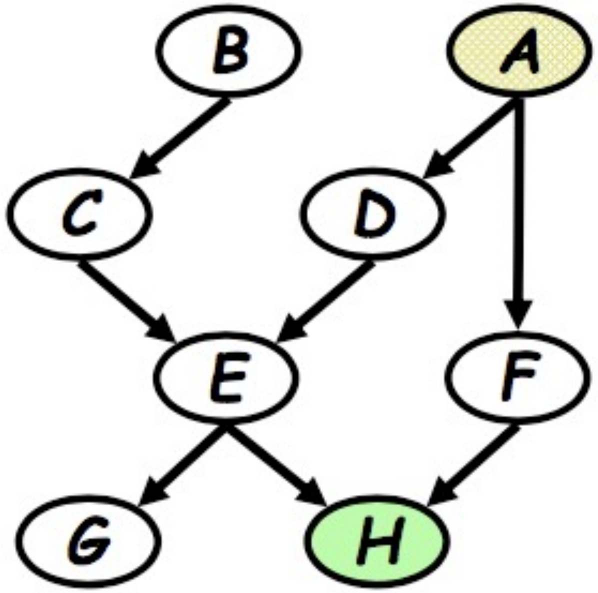
- A graph elimination algorithm



- Intermediate terms correspond to the **cliques** resulted from elimination



Variable Elimination: Example



Query: P(A|h)

- Need to eliminate: B, C, D, E, F, G, H

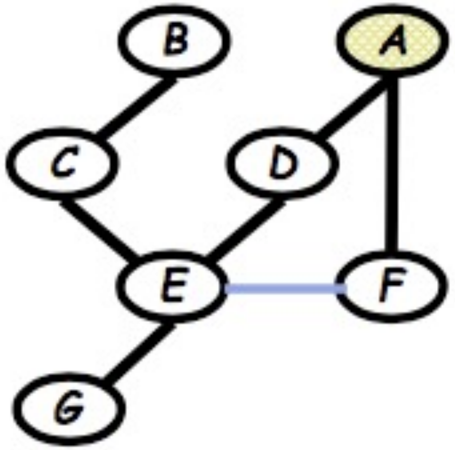
Initial factors:

P(A)P(B)P(C|B)P(D|A)P(E|C,D)P(F|A)P(G|E)P(H|E,F)

Step 1:

- **Conditioning** on evidence (fix H to h)

$$p_H(E,F) = P(H=h|E,F)$$



Same as a marginalization step

$$p_H(E,F) = \sum_{h'} P(H=h|E,F)\delta(h'=h)$$

Variable Elimination: Example, p2

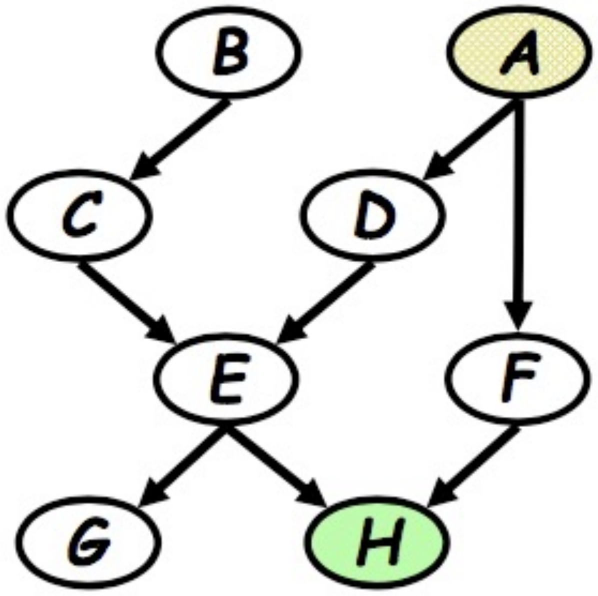
Query: P(A|h)

- Need to eliminate: B, C, D, E, F, G, H

Initial factors:

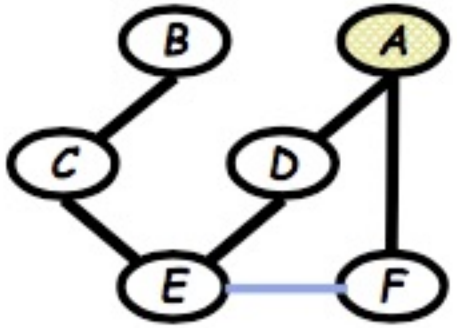
P(A)P(B)P(C|B)P(D|A)P(E|C,D)P(F|A)P(G|E)P(H|E,F)

=> P(A)P(B)P(C|B)P(D|A)P(E|C,D)P(F|A)P(G|E)p_H(E,F)



Step 2: Eliminate G

$$p_G(E) = \sum_g P(G = g|E) = 1$$



=> P(A)P(B)P(C|B)P(D|A)P(E|C,D)P(F|A)P(G|E)p(E,F)

=> P(A)P(B)P(C|B)P(D|A)P(E|C,D)P(F|A) p_H(E,F)

Variable Elimination: Example, p3

Query: P(A|h)

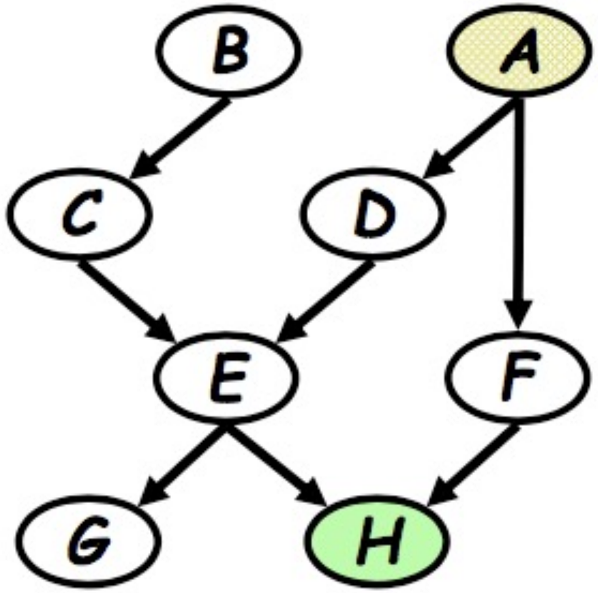
- Need to eliminate: B, C, D, E, F, G, H

Initial factors:

P(A)P(B)P(C|B)P(D|A)P(E|C,D)P(F|A)P(G|E)P(H|E,F)

=> P(A)P(B)P(C|B)P(D|A)P(E|C,D)P(F|A)P(G|E)p_H(E,F)

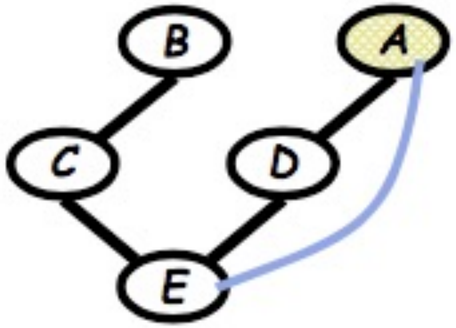
=> P(A)P(B)P(C|B)P(D|A)P(E|C,D)P(F|A) p_H(E,F)



Step 3: Eliminate F

$$p_H(E,A) = \sum_f P(F=f|A) p_H(E,F)$$

=> P(A)P(B)P(C|B)P(D|A)P(E|C,D) p_F(A,E)



Variable Elimination: Example, p4

Query: P(A|h)

- Need to eliminate: B, C, D, E, F, G, H

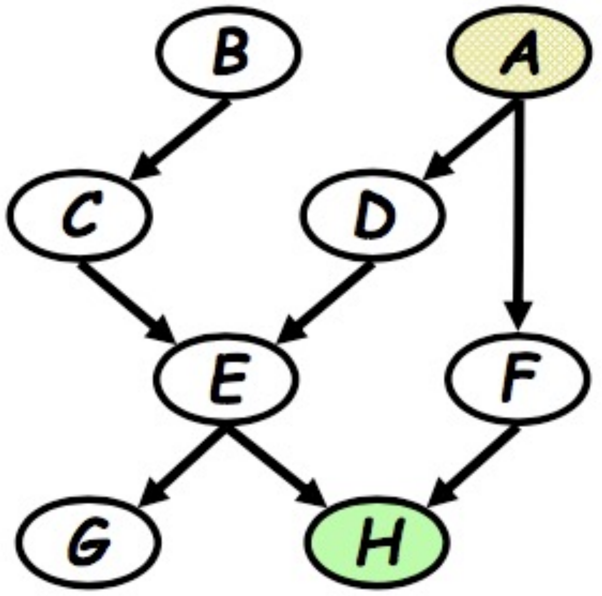
Initial factors:

P(A)P(B)P(C|B)P(D|A)P(E|C,D)P(F|A)P(G|E)P(H|E,F)

=> P(A)P(B)P(C|B)P(D|A)P(E|C,D)P(F|A)P(G|E)p_H(E,F)

=> P(A)P(B)P(C|B)P(D|A)P(E|C,D)P(F|A) p_H(E,F)

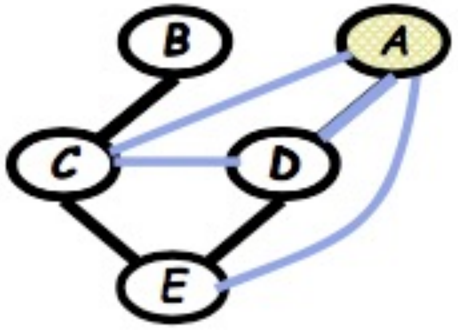
=> P(A)P(B)P(C|B)P(D|A)P(E|C,D) p_F(A,E)



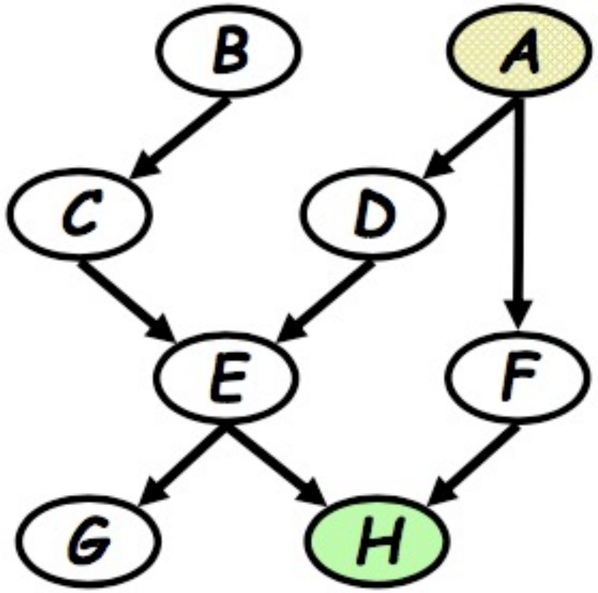
Step 4: Eliminate E

$$p_E(A, C, D) = \sum_e P(E = e|C, D) p_F(A, E)$$

=> P(A)P(B)P(C|B)P(D|A)p_E(A,C,D)



Variable Elimination: Example, p5



Query: P(A|h)

- Need to eliminate: B, C, D, E, F, G, H

Initial factors:

P(A)P(B)P(C|B)P(D|A)P(E|C,D)P(F|A)P(G|E)P(H|E,F)

=> P(A)P(B)P(C|B)P(D|A)P(E|C,D)P(F|A)P(G|E)p_H(E,F)

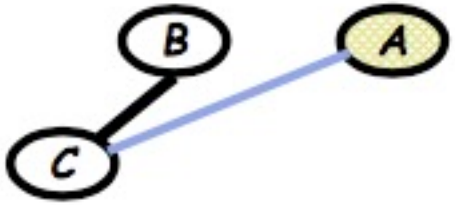
=> P(A)P(B)P(C|B)P(D|A)P(E|C,D)P(F|A) p_H(E,F)

=> P(A)P(B)P(C|B)P(D|A)P(E|C,D) p_F(A,E)

=> P(A)P(B)P(C|B)P(D|A)p_E(A,C,D)

Step 5: Eliminate D

$$p_D(A, C) = \sum_d P(D = d|A) p_E(A, C, D)$$



=> P(A)P(B)P(C|B) p_D(A,C)

Variable Elimination: Example, p6

Query: P(A|h)

- Need to eliminate: B, C, D, E, F, G, H

Initial factors:

P(A)P(B)P(C|B)P(D|A)P(E|C,D)P(F|A)P(G|E)P(H|E,F)

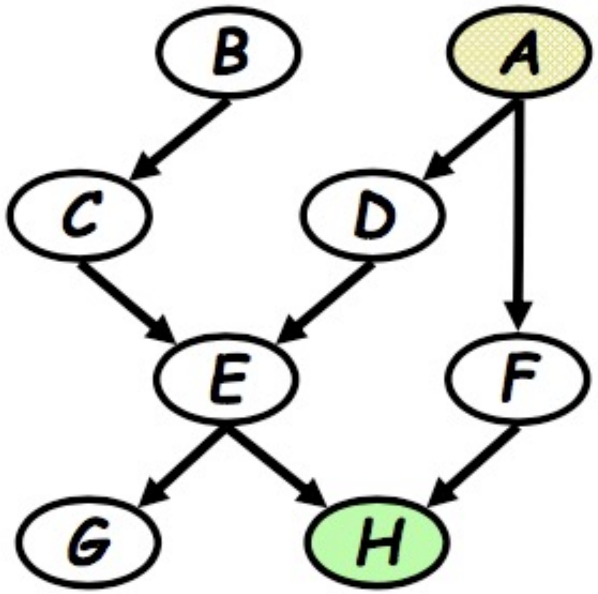
=> P(A)P(B)P(C|B)P(D|A)P(E|C,D)P(F|A)P(G|E)p_H(E,F)

=> P(A)P(B)P(C|B)P(D|A)P(E|C,D)P(F|A) p_H(E,F)

=> P(A)P(B)P(C|B)P(D|A)P(E|C,D) p_F(A,E)

=> P(A)P(B)P(C|B)P(D|A)p_E(A,C,D)

=> P(A)P(B)P(C|B) p_D(A,C)

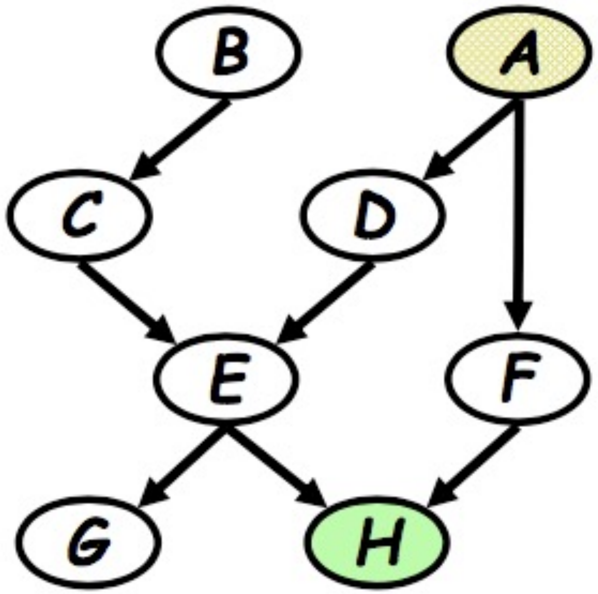


Step 6: Eliminate C

$$p_C(A,B) = \sum_c P(C=c|B)p_D(A,C)$$

=> P(A)P(B)P(C|B) p_C(A,B)

Variable Elimination: Example, p7



Query: P(A|h)

- Need to eliminate: B, C, D, E, F, G, H

Initial factors:

P(A)P(B)P(C|B)P(D|A)P(E|C,D)P(F|A)P(G|E)P(H|E,F)

=> P(A)P(B)P(C|B)P(D|A)P(E|C,D)P(F|A)P(G|E)p_H(E,F)

=> P(A)P(B)P(C|B)P(D|A)P(E|C,D)P(F|A) p_H(E,F)

=> P(A)P(B)P(C|B)P(D|A)P(E|C,D) p_F(A,E)

=> P(A)P(B)P(C|B)P(D|A)p_E(A,C,D)

=> P(A)P(B)P(C|B) p_D(A,C)

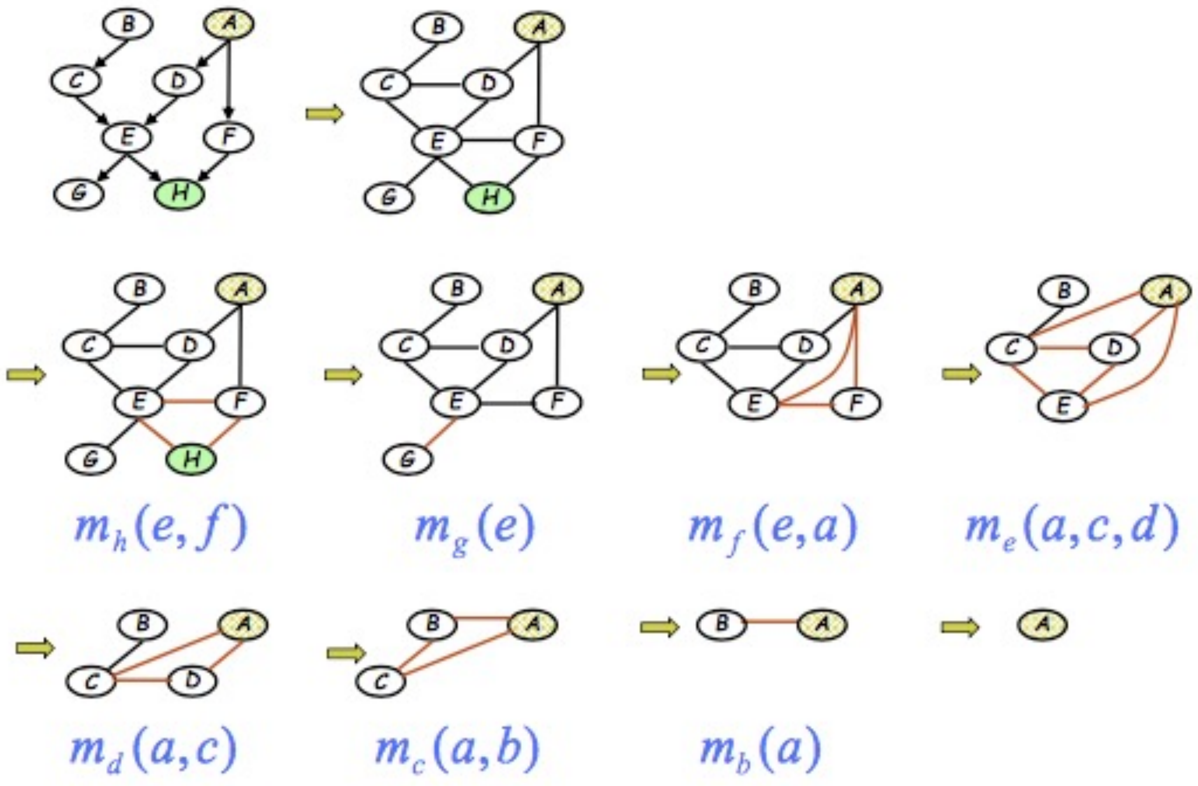
=> P(A)P(B)p_C(A,B)

Step 7: Eliminate B

$$p_B(A) = \sum_b P(B=b|A) p_C(A,B)$$

=> P(A)p_B(A)

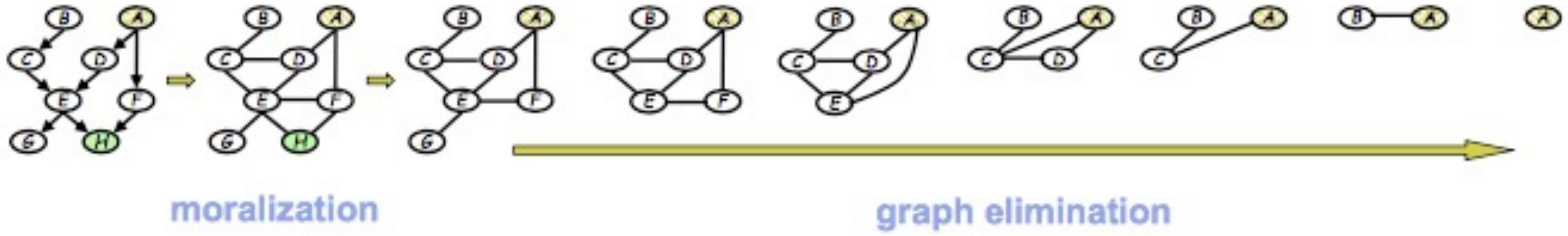
Elimination Cliques



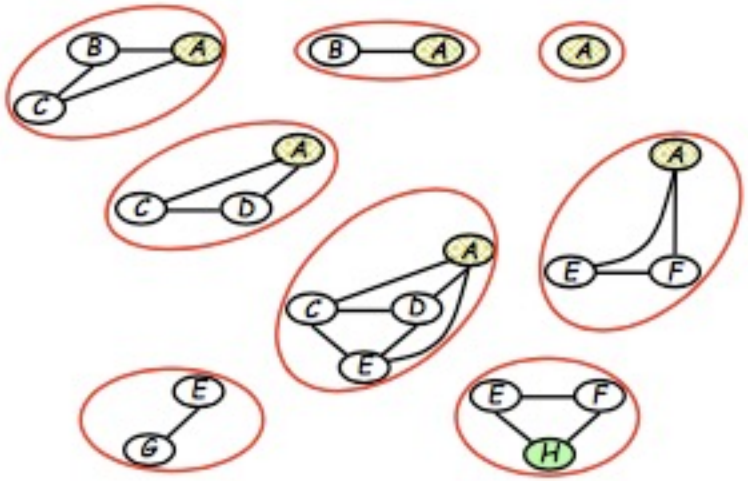
Algebraic elimination = Graphical Elimination

Understanding Variable Elimination

- A graph elimination algorithm



- Intermediate terms correspond to the **cliques** resulted from elimination



Questions?

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