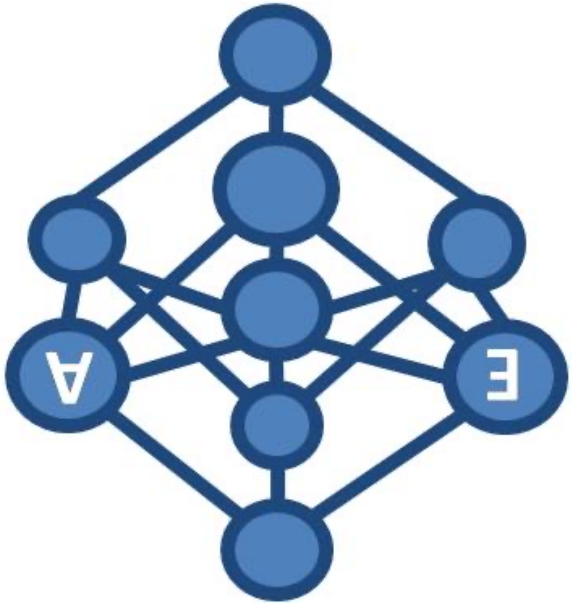
Probabilistic Graphical Models*

Bayesian Networks - Inference



*Thanks to Bert Huang, Carlos Guestrin, Pedro Domingos and many others for making their slides publically available

What’s next

- So far, variable elimination for “efficient” inference on conditional probabilitiy queries.
- Now:
  - Other types of inference
  - Hardness result of inference

So far: A-Posteriori Belief

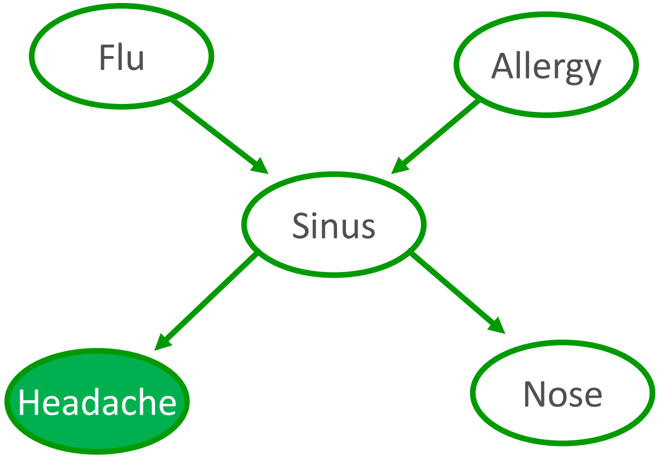
This query is useful in many cases:

- **Prediction**: what is the probability of an outcome given the starting condition
  - Target is a descendent of the evidence
- **Diagnosis**: what is the probability of disease/fault given symptoms
  - Target is an ancestor of the evidence
- So, the direction between variables does not restrict the directions of the queries. Probabilistic inference can combine evidence form all parts of the network

Abductive Inference in BNs

So far, we have considered inference problems where the goal is to obtain **posterior probabilities for variables given evidence**.

In abductive inference it is to find the **configuration of a set of variables (hypothesis) which will best explain the evidence**.



What would count as the best explanation of an headache (H=t)?

A configuration of all the other variables?

A subset of them?

Abductive Inference in BNs

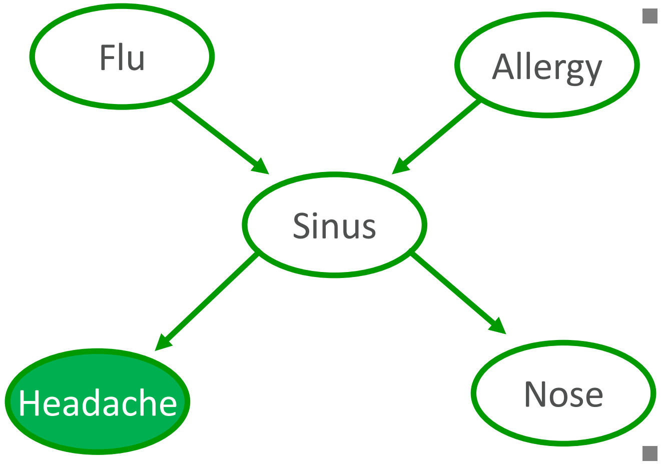
There are two types of abductive inference in BNs:

- **MPE (Most Probable Explanation)** - the most probable configuration of ***all variables*** in the BN given evidence
- **MAP (Maximum A Posteriori)** - the most probable configuration of ***a subset of variables*** in the BN given evidence

Note 1: In general the MPE cannot be found by taking the most probable configuration of nodes individually!

Note 2: And the MAP cannot be found by taking the projection of the MPE onto the explanation set!

Abductive Inference in BNs



sometimes called maximum a posteriori (MAP)

- **Most probable explanation (MPE)**
  - Most likely assignment to all hidden vars given evidence

$$\max_{f,a,s,n} P\left(F=f, A=a, S=s, N=n \mid H=t\right)$$

- **Maximum a posteriori (MAP)**
  - Most likely assignment to some var(s) given evidence

$$\max_{a} P\left(A=a \mid H=t\right)$$

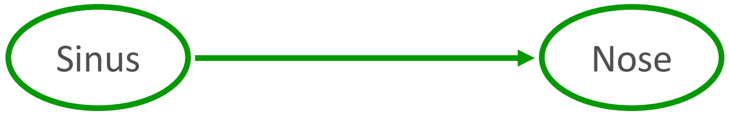
$$=\max_{a} \sum_{s,f,b} P\left(F=f, a, s, n \mid H=t\right)$$

Why MPE and MAP?

We can use MPE and MAP for

- **Classification**
  - find most likely label, given the evidence
- **Explanation**
  - What is the most likely scenario, given the evidence

Are MPE and MAP Consistent?



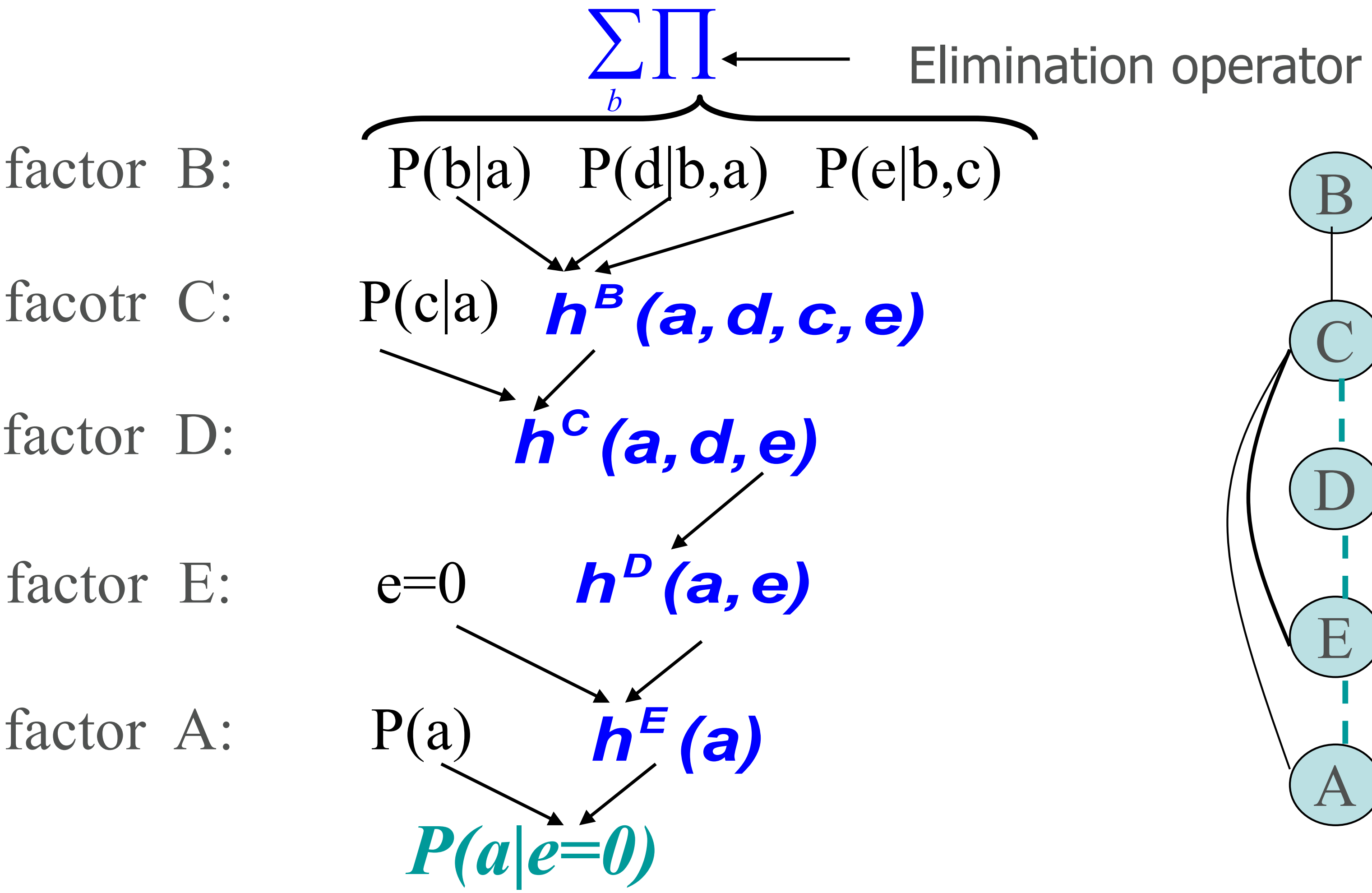
P(S=t)=0.4
P(S=f)=0.6

P(N|S)	N=t	N=f
S=t	0.9	0.1
S=f	0.5	0.5

- **Most probable explanation (MPE)**
  - □ Most likely assignment to all hidden variables given evidence
  - □ S=t, N=t: 0.4*0.9 = 0.36
  - □ S=f, N=t: 0.6*0.5 = 0.2
  - □ So, we should assume to have a sinus and a running nose
- **Maximum a posteriori (MAP)**
  - □ Most likely assignment to some var(s) given evidence
  - □ According to the numbers, P(S=f) is higher, so apriori we do **not** have a sinus.

MPE and MAP are not consistent!!

Finding MPE



$\sum_b \prod$ ← Elimination operator

factor B: $P(b|a)$ $P(d|b,a)$ $P(e|b,c)$

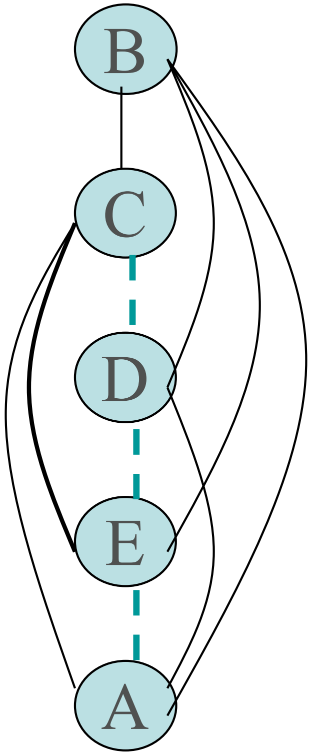
facotr C: $P(c|a)$ $h^B(a,d,c,e)$

factor D: $h^C(a,d,e)$

factor E: $e=0$ $h^D(a,e)$

factor A: $P(a)$ $h^E(a)$

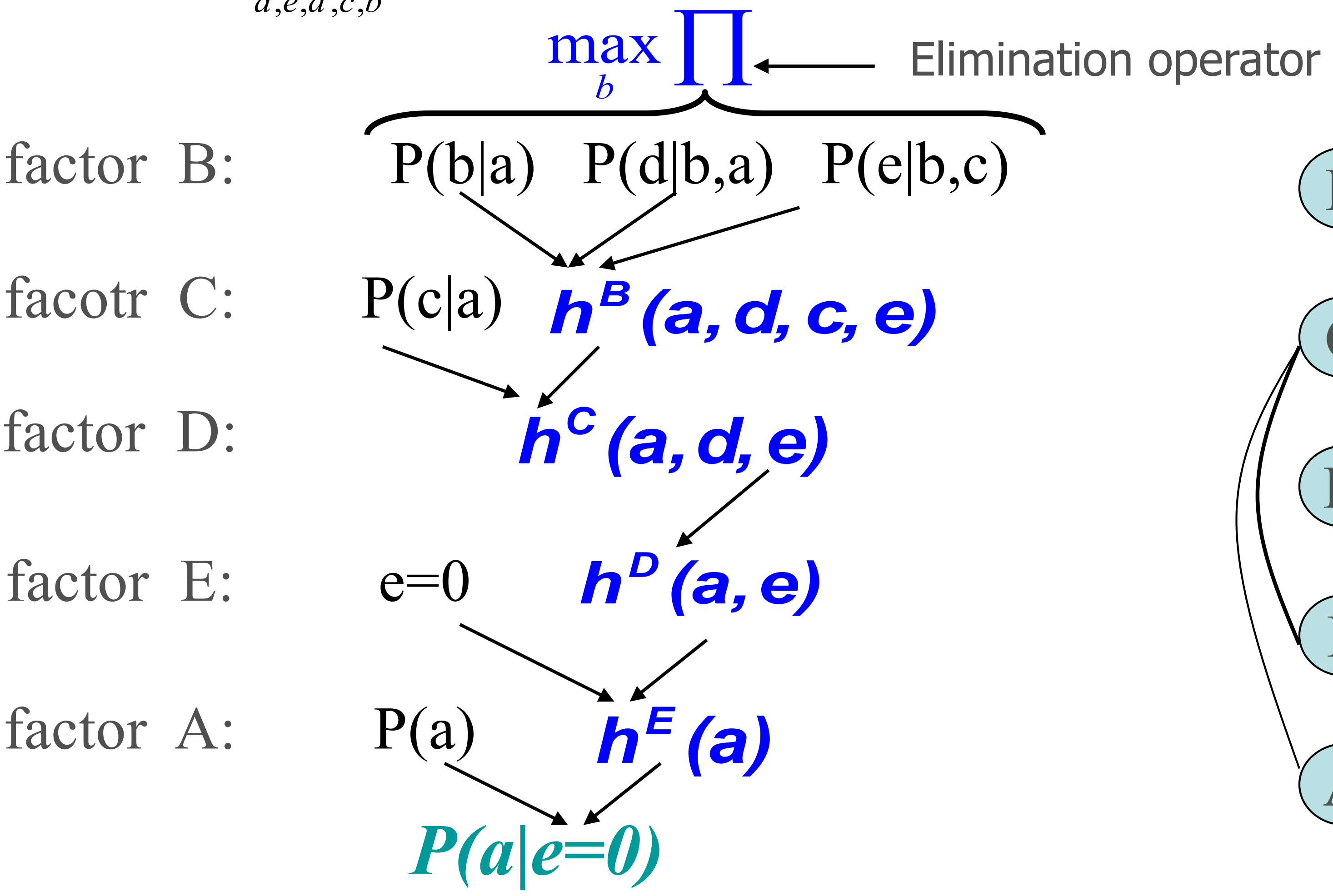
$P(a|e=0)$



Finding MPE

$\sum$ is replaced by ***max*** :

$$MPE = \max_{a,e,d,c,b} P(a)P(c\,|\,a)P(b\,|\,a)P(d\,|\,a,b)P(e\,|\,b,c)$$



$\max_{b} \prod$ ← Elimination operator

factor B: $\underbrace{P(b|a) \quad P(d|b,a) \quad P(e|b,c)}$

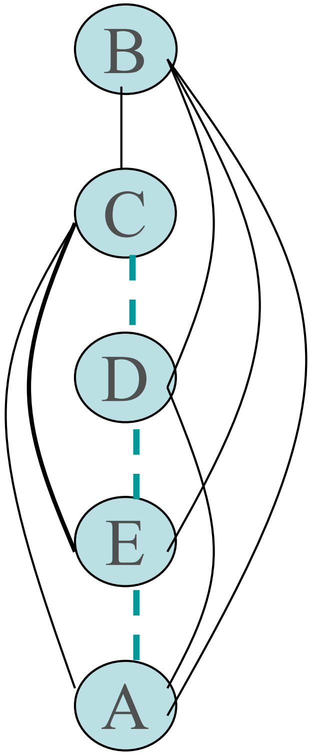
facotr C: P(c|a) $h^B(a,d,c,e)$

factor D: $h^C(a,d,e)$

factor E: e=0 $h^D(a,e)$

factor A: P(a) $h^E(a)$

$P(a|e=0)$



Generating the MPE-tuple

Two passes algorithm:
(Top-Down) Max Probs (Bottom-Up) Max Configuration

5. $b' = \arg\max_{b} P(b \mid a') \times P(d' \mid b, a') \times P(e' \mid b, c')$

4. $c' = \arg\max_{c} P(c \mid a') \times h^{B}(a', d', c, e')$

3. $d' = \arg\max_{d} h^{C}(a', d, e')$

2. $e' = 0$

1. $a' = \arg\max_{a} P(a) \cdot h^{E}(a)$

B:	$P(b \mid a)$	$P(d \mid b,a)$	$P(e \mid b,c)$
C:	$P(c \mid a)$	$h^{B}(a,d,c,e)$	
D:		$h^{C}(a,d,e)$	
E:	$e=0$	$h^{D}(a,e)$	
A:	$P(a)$	$h^{E}(a)$	

Return (a', b', c', d', e')

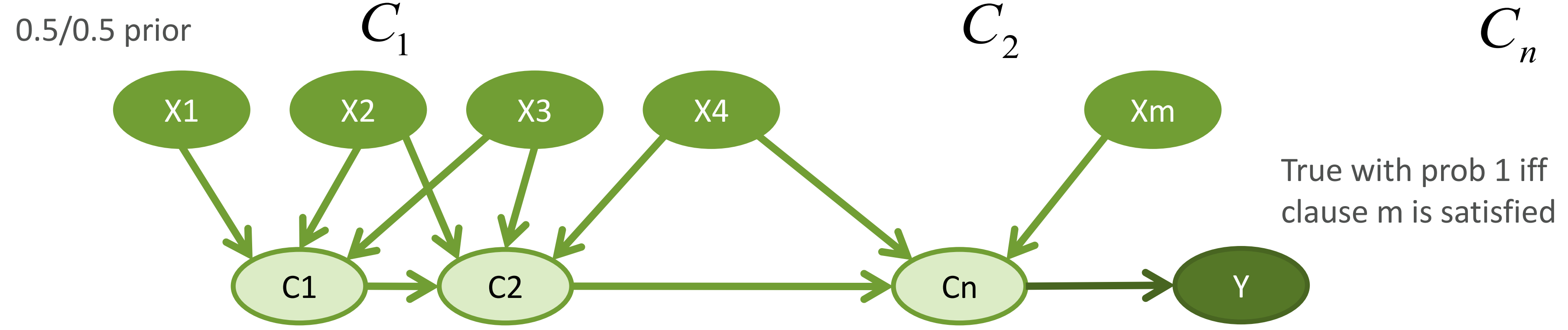
So far

- Variable elimination for “efficient” inference on conditional probabilitiy queries.
- Now, general hardness result of inference

Complexity of conditional probability queries

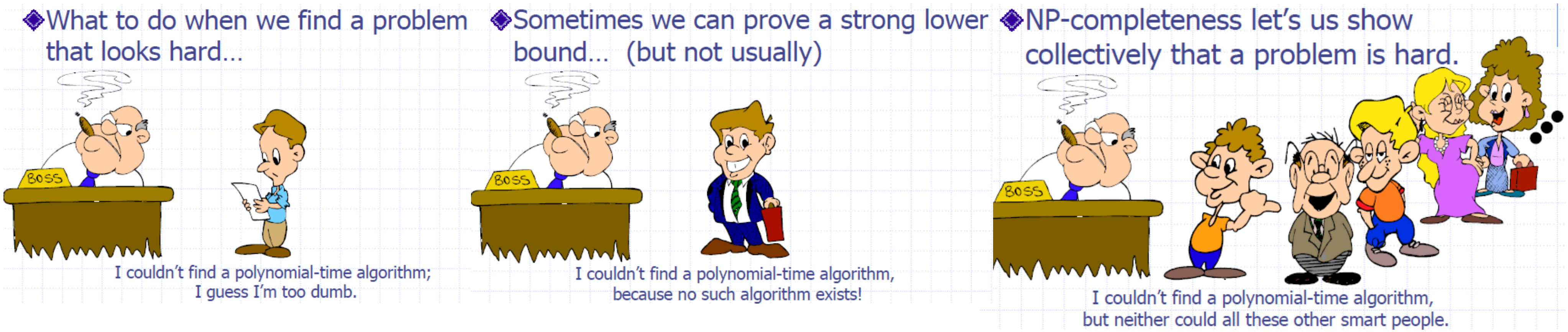
- How hard is it to compute P(X|**E**=**e**)?
- Consider a reduction to 3-SAT with empty evidence E
- Does a satisfying assignment exist?

$$\underbrace{(\bar{X}_1 \vee X_2 \vee X_3)}_{C_1} \wedge \underbrace{(\bar{X}_2 \vee X_3 \vee X_4)}_{C_2} \wedge \underbrace{\ldots}_{C_n}$$


0.5/0.5 prior
X1
X2
X3
X4
Xm
C1
C2
Cn
Y
True with prob 1 iff clause m is satisfied
True with prob 1 iff clause 1 is satisfied

True with prob 1 iff clauses i and i-1 are satisfied

P(Y=t)>0 iff 3-SAT formula is satisfiable



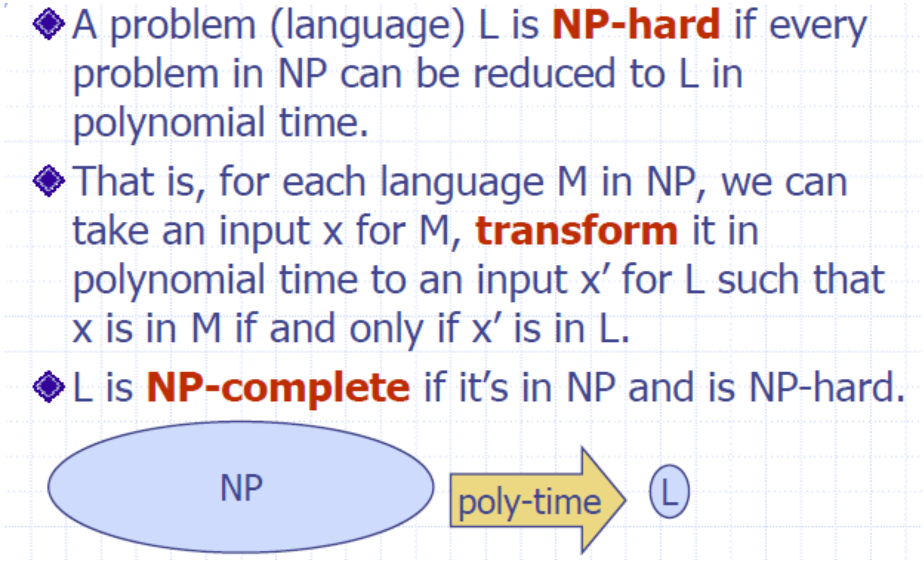
- What to do when we find a problem that looks hard…
- Sometimes we can prove a strong lower bound… (but not usually)
- NP-completeness let's us show collectively that a problem is hard.

I couldn't find a polynomial-time algorithm; I guess I'm too dumb.

I couldn't find a polynomial-time algorithm, because no such algorithm exists!

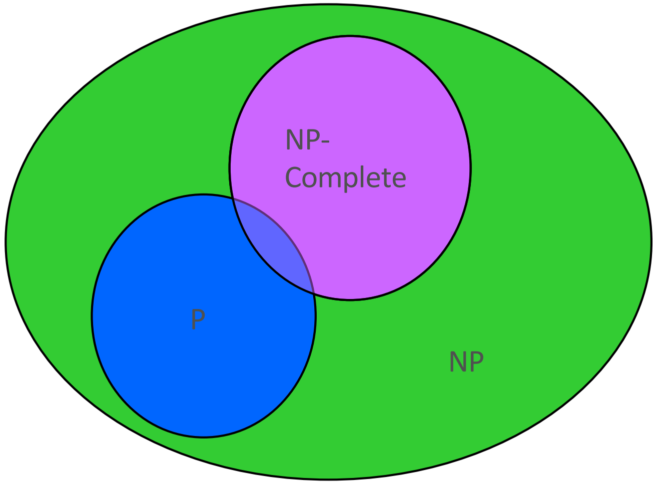
I couldn't find a polynomial-time algorithm, but neither could all these other smart people.

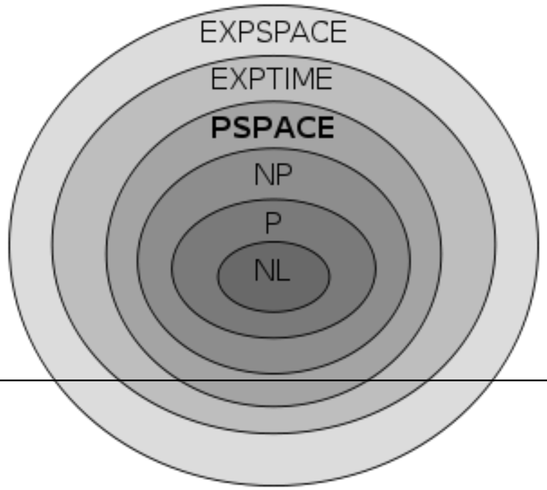
- P = { L | L is accepted by a deterministic Turing Machine in polynomial time }
- NP = { L | L is accepted by a non-deterministic Turing Machine in polynomial time }



- A problem (language) L is **NP-hard** if every problem in NP can be reduced to L in polynomial time.
- That is, for each language M in NP, we can take an input x for M, **transform** it in polynomial time to an input x' for L such that x is in M if and only if x' is in L.
- L is **NP-complete** if it's in NP and is NP-hard.

NP
poly-time
L

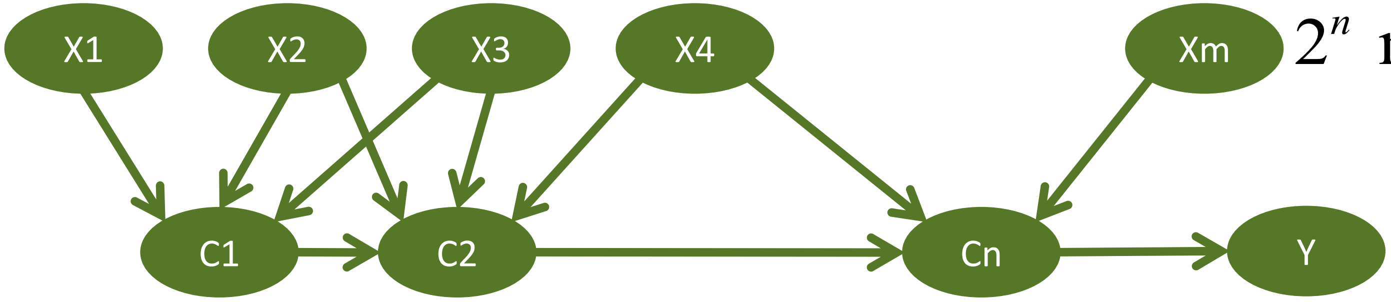




Complexity of conditional probability queries

- How hard is it to compute P(X|**E**=**e**)?
  - At least NP-hard, but even harder!
  - #P problems such as counting the number of satisfiable configurations (model counting)

0.5/0.5 prior



2^n many assignments

$$p(Y = t) = \frac{\#\ \text{sat assignment}}{2^n}$$

Hardness - Notes

- We used deterministic relations in our construction
- The same construction works if we use $(1-\varepsilon, \varepsilon)$ instead of $(1,0)$ in each gate for any $\varepsilon < 0.5$

- **Hardness does not mean we cannot solve inference**
- It implies that we cannot find a general procedure that works efficiently for all networks
- For particular families of networks, we can have provably efficient procedure

What you need to know about inference thus far

- Types of queries
  - probabilistic inference
  - most probable explanation (MPE)
  - maximum a posteriori (MAP)
    - MPE and MAP are truly different (don’t give the same answer)

- Hardness of inference
  - Exact and approximate inference are NP-hard
  - MPE is NP-complete
  - MAP is much harder as we solve the model counting problem

What’s next

- Understanding complexity of variable elimination in more detail
  - Variable elimination as graph transformation
  - Will lead to junction-tree algorithm
  - Will provide some background on MRFs and (loopy) belief propagation

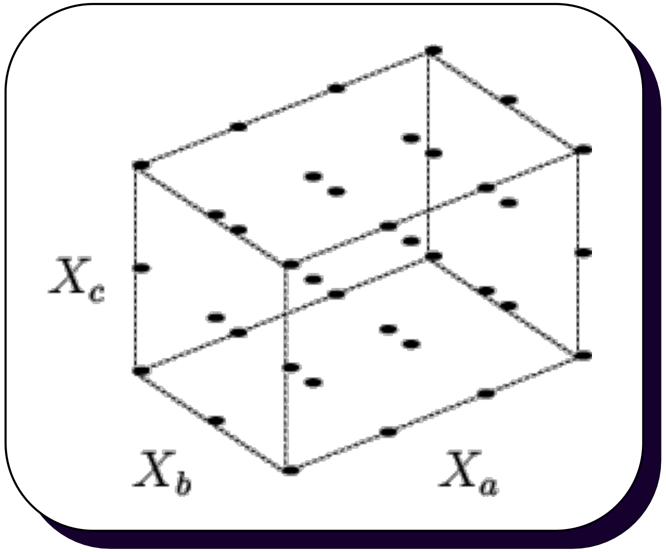
Recap Potentials

A **potential** f_A over a set of variables A is a function that maps each configuration into a **non-negative real number**.

$$\mathrm{dom} f_A = A \quad \text{(domain of } f_A \text{)}$$

Examples: Conditional probability distribution and joint probability distributions are special cases of potentials

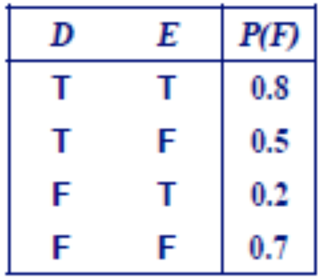
Potentials



Ex: A potential $\phi_{A,B,C}$ over the set of variables {A,B,C}. A has four states, and B and C has three states. $\mathbf{domf}_{A,B,C}$ **={A,B,C}**

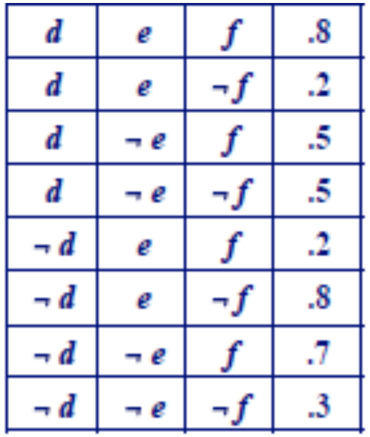
CPTs as Potentials

Potentials: We can represent a CPT in this format…



D	*E*	*P(F)*
T	T	0.8
T	F	0.5
F	T	0.2
F	F	0.7

⇒



d	*e*	*f*	.8
d	*e*	¬ *f*	.2
d	¬ *e*	*f*	.5
d	¬ *e*	¬ *f*	.5
¬ *d*	*e*	*f*	.2
¬ *d*	*e*	¬ *f*	.8
¬ *d*	¬ *e*	*f*	.7
¬ *d*	¬ *e*	¬ *f*	.3

Multiplying Potentials

- Domain of (variables in) result is the union of domains of input potentials
- For each cell in result, multiply all input cells that agree on variable settings

a	b	.1
a	$\neg b$	.2
$\neg a$	b	.5
$\neg a$	$\neg b$	.8

×

b	c	.2
b	$\neg c$	.4
$\neg b$	c	.3
$\neg b$	$\neg c$	.5

=

a	b	c	.02
a	b	$\neg c$	.04
a	$\neg b$	c	.06
a	$\neg b$	$\neg c$	.10
$\neg a$	b	c	.10
$\neg a$	b	$\neg c$	.20
$\neg a$	$\neg b$	c	.24
$\neg a$	$\neg b$	$\neg c$	.40

a	b	.1
a	$\neg b$	.5
$\neg a$	b	.4
$\neg a$	$\neg b$	.1

×

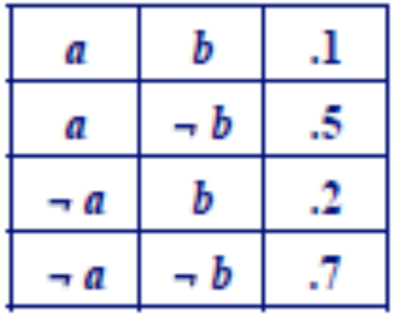
a	b	.8
a	$\neg b$	.7
$\neg a$	b	.9
$\neg a$	$\neg b$	.8

=

a	b	.08
a	$\neg b$	.35
$\neg a$	b	.36
$\neg a$	$\neg b$	.08

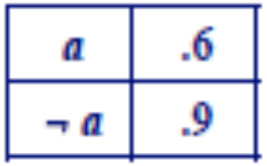
Marginalizing and Normalizing Potentials

- Can also marginalize (sum out a variable) potentials



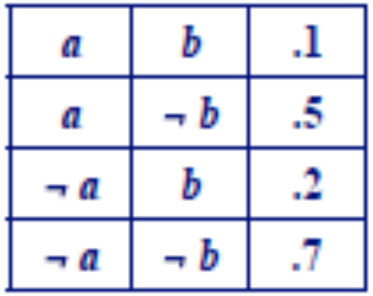
a	b	.1
a	$\neg b$	.5
$\neg a$	b	.2
$\neg a$	$\neg b$	.7

$\Rightarrow$ $\sum_B$



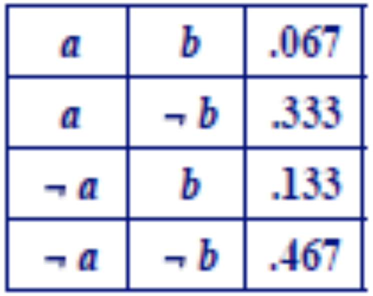
a	.6
$\neg a$	.9

- And normalize them



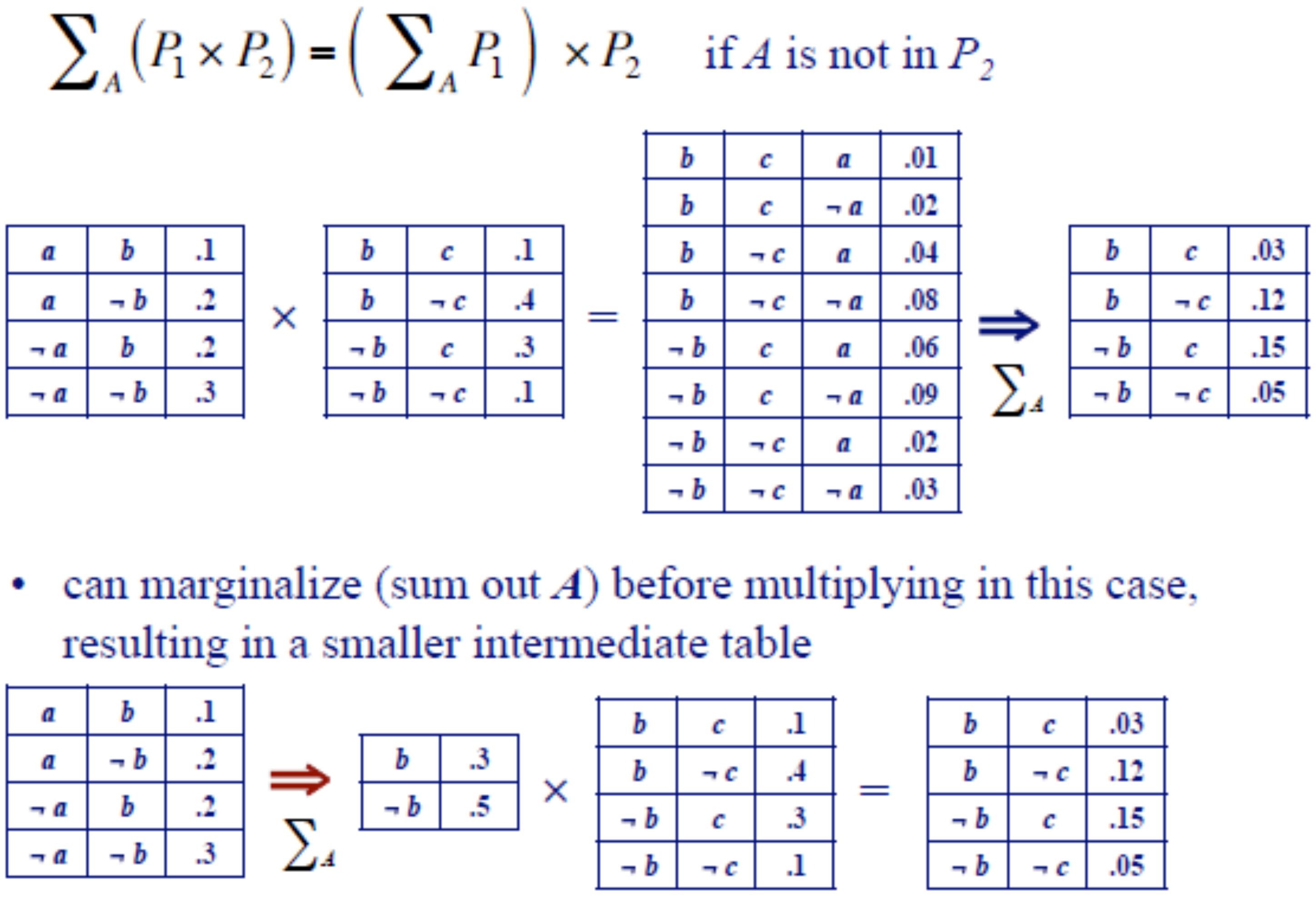
a	b	.1
a	$\neg b$	.5
$\neg a$	b	.2
$\neg a$	$\neg b$	.7

$\Rightarrow$



a	b	.067
a	$\neg b$	.333
$\neg a$	b	.133
$\neg a$	$\neg b$	.467

Key Observation of VE



$$\sum_A (P_1 \times P_2) = \left(\sum_A P_1 \right) \times P_2 \quad \text{if } A \text{ is not in } P_2$$

a	b	.1
a	$\neg b$	.2
$\neg a$	b	.2
$\neg a$	$\neg b$	.3

×

b	c	.1
b	$\neg c$	.4
$\neg b$	c	.3
$\neg b$	$\neg c$	.1

=

b	c	a	.01
b	c	$\neg a$	.02
b	$\neg c$	a	.04
b	$\neg c$	$\neg a$	.08
$\neg b$	c	a	.06
$\neg b$	c	$\neg a$	.09
$\neg b$	$\neg c$	a	.02
$\neg b$	$\neg c$	$\neg a$	.03

$\Rightarrow \sum_A$

b	c	.03
b	$\neg c$	.12
$\neg b$	c	.15
$\neg b$	$\neg c$	.05

- can marginalize (sum out A) before multiplying in this case, resulting in a smaller intermediate table

a	b	.1
a	$\neg b$	.2
$\neg a$	b	.2
$\neg a$	$\neg b$	.3

$\Rightarrow \sum_A$

b	.3
$\neg b$	.5

×

b	c	.1
b	$\neg c$	.4
$\neg b$	c	.3
$\neg b$	$\neg c$	.1

=

b	c	.03
b	$\neg c$	.12
$\neg b$	c	.15
$\neg b$	$\neg c$	.05

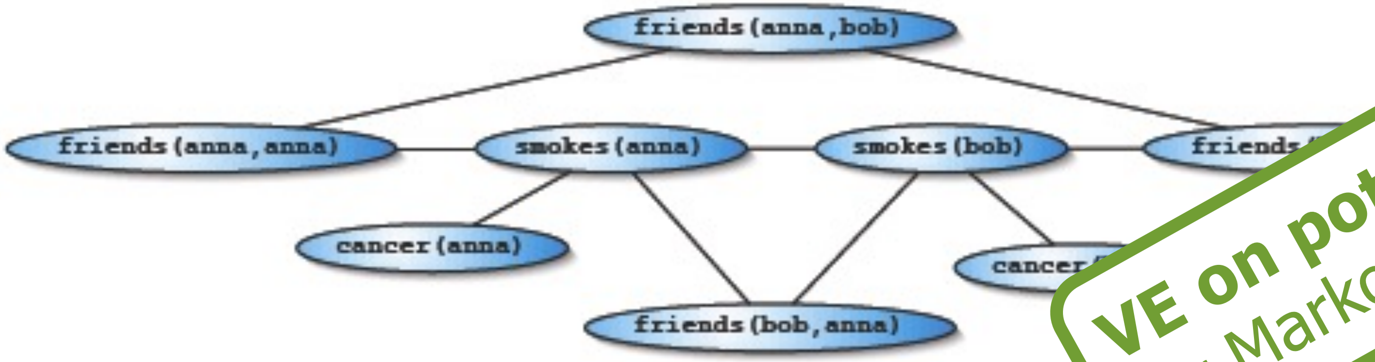
VE using Potentials

Let F be a set of potentials (e.g. CPDs), and let X be a variable. X is eliminated from F:

1. Remove all potentials in F with X in the domain. Let F_X that set.
2. Calculate $\Phi^{-X} = \boxed{\sum_X \prod \Phi_X}$
3. Add Φ^{-X} to F
4. Iterate

Potential where X is not a member of the domain

Recap: Markov Networks / MRFs

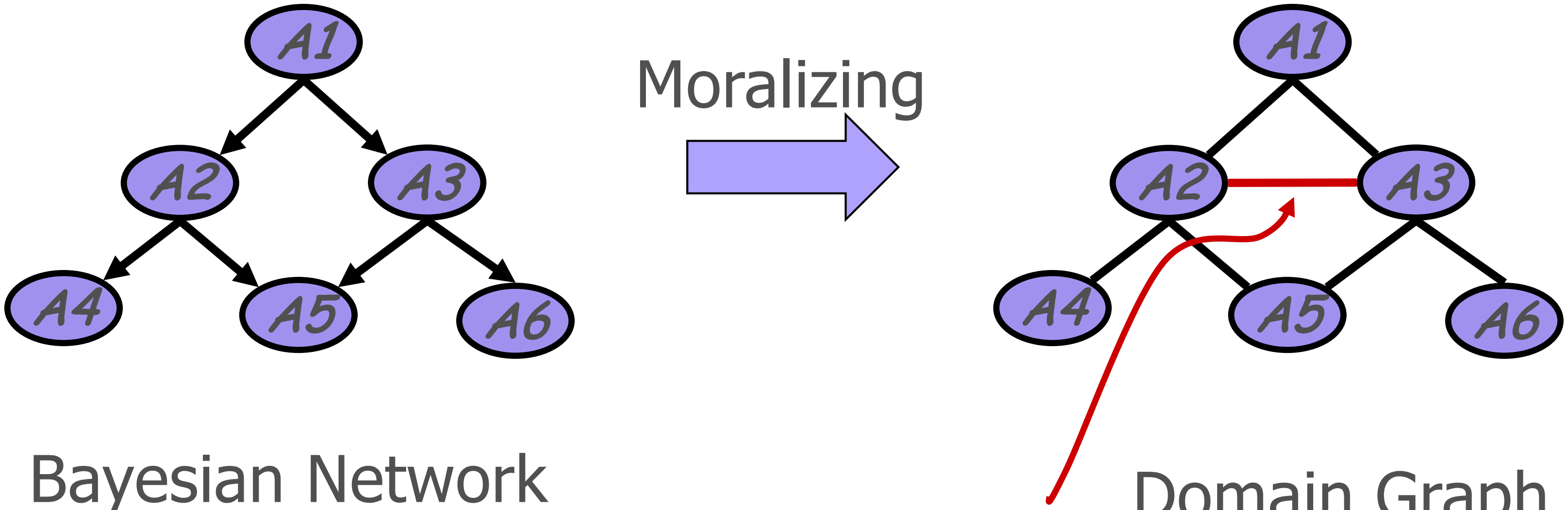


VE on potentials works for Markov networks

- Undirected Graphs
- Nodes = random variables $X_1, \ldots, X_n$
- Cliques = potentials (~ local jpd) ϕ_k

$$P(X = x) = \frac{1}{Z} \prod_k \phi_k(x_{\{k\}})$$

From Directed to Undirected Models: The Domain Graph



Moralizing

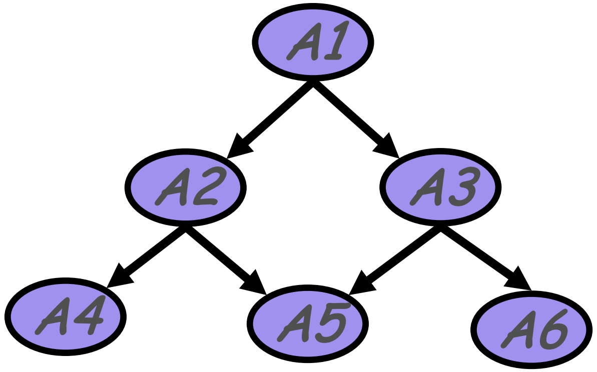
Bayesian Network

moral link

Domain Graph (Moral Graph)

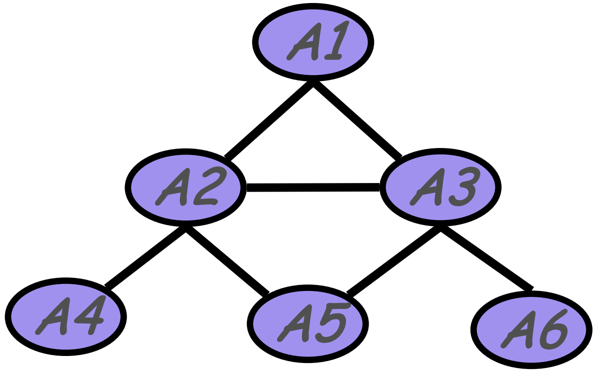
Let $F=\{f_1,...,f_n\}$ be potentials over $U=\{A_1,...,A_m\}$ with $\mathrm{dom} f_i=D_i$. The domain graph for F is the undirected graph with variables of U as nodes and with a link between pairs of variables being members of the same $D_{i.}$

Moralizing



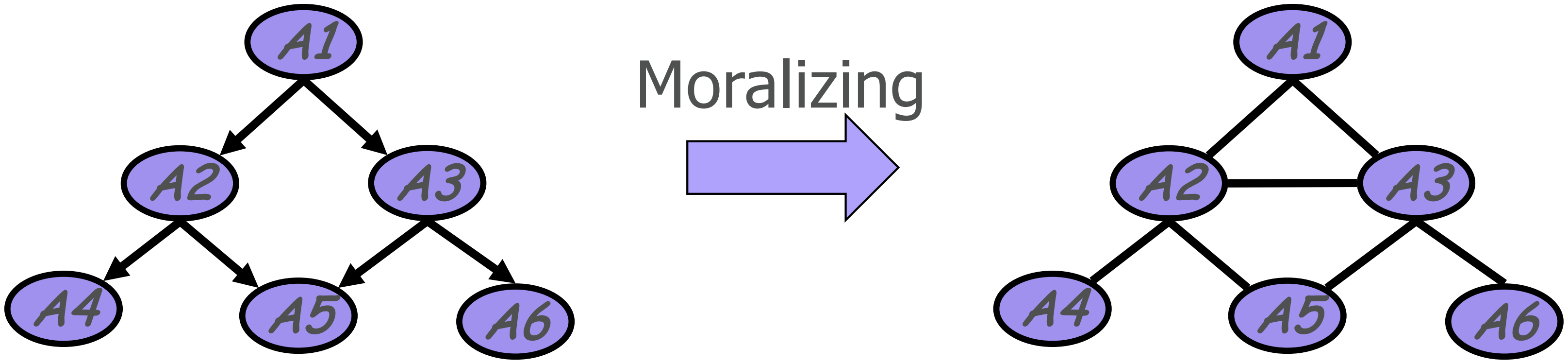
Bayesian Network

Moralizing



Domain Graph
(Moral Graph)

Moralizing



Moralizing

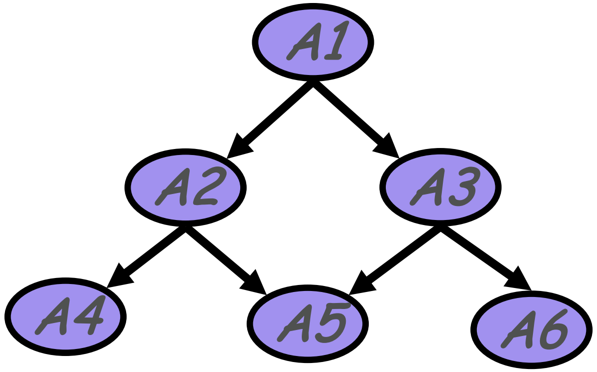
Bayesian Network

Domain Graph
(Moral Graph)

CPDs

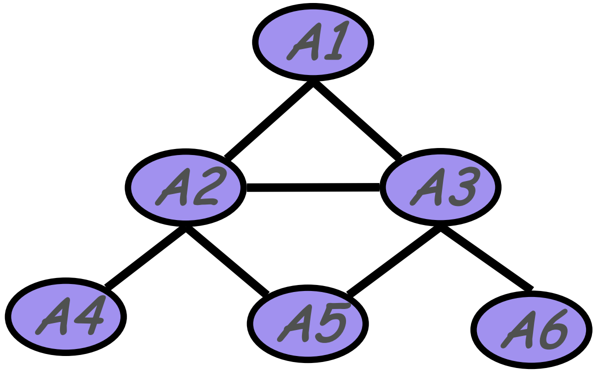
$$P(A_1)$$
$$P(A_2|A_1)$$
$$P(A_3|A_1)$$
$$P(A_4|A_2)$$
$$P(A_5|A_2, A_3)$$
$$P(A_6|A_3)$$

Moralizing



Bayesian Network

Moralizing



Domain Graph
(Moral Graph)

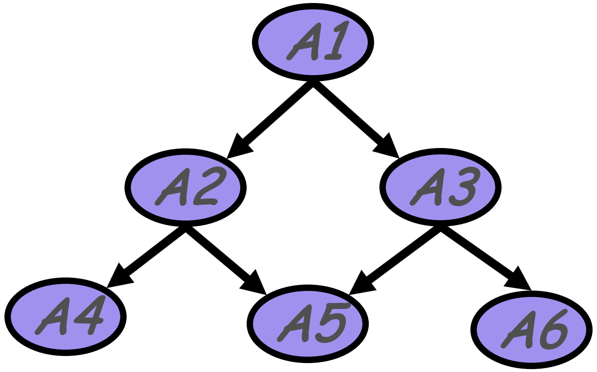
CPDs

$$P(A_1)$$
$$P(A_2|A_1)$$
$$P(A_3|A_1)$$
$$P(A_4|A_2)$$
$$P(A_5|A_2, A_3)$$
$$P(A_6|A_3)$$

CPD
=
potential

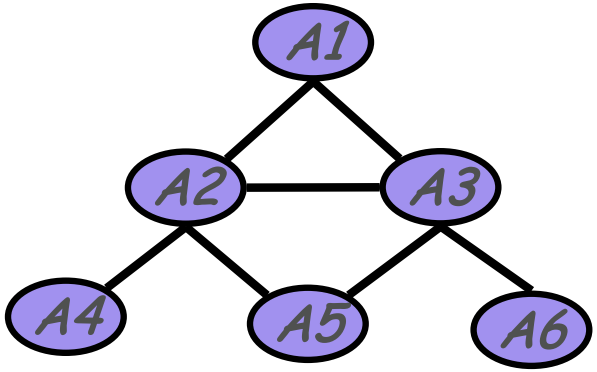
$$dom(\phi_1) = \{A_1\}$$
$$dom(\phi_2) = \{A_2, A_1\}$$
$$dom(\phi_3) = \{A_3, A_1\}$$
$$dom(\phi_4) = \{A_4, A_2\}$$
$$dom(\phi_5) = \{A_5, A_2, A_3\}$$
$$dom(\phi_6) = \{A_6, A_3\}$$

Moralizing



Bayesian Network

Moralizing



Domain Graph
(Moral Graph)

Potentials induce undirected edges

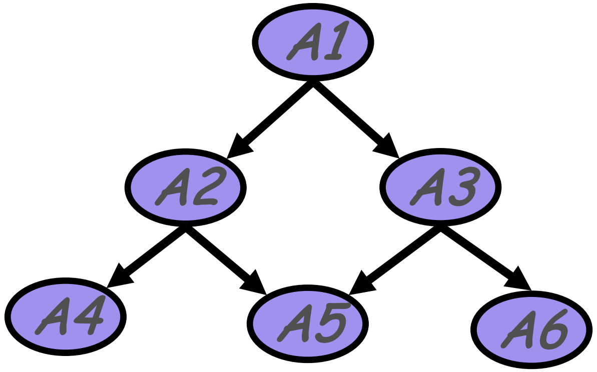
CPDs

$$P(A_1)$$
$$P(A_2|A_1)$$
$$P(A_3|A_1)$$
$$P(A_4|A_2)$$
$$P(A_5|A_2, A_3)$$
$$P(A_6|A_3)$$

CPD
=
potential

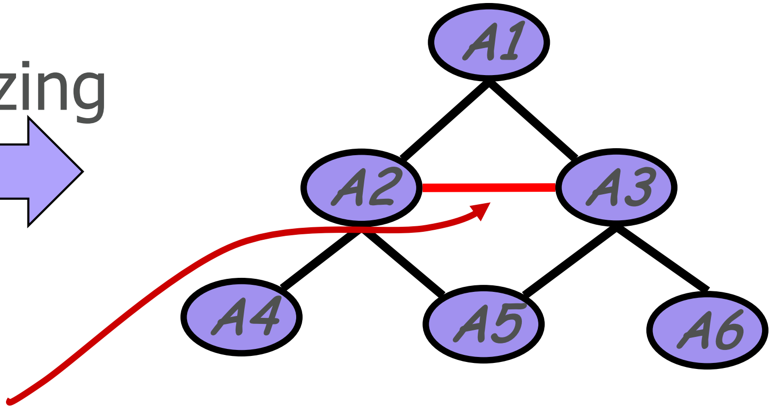
$$dom(\phi_1) = \{A_1\}$$
$$dom(\phi_2) = \{A_2, A_1\}$$
$$dom(\phi_3) = \{A_3, A_1\}$$
$$dom(\phi_4) = \{A_4, A_2\}$$
$$dom(\phi_5) = \{A_5, A_2, A_3\}$$
$$dom(\phi_6) = \{A_6, A_3\}$$

Moralizing



Bayesian Network

Moralizing



moral link

Potentials induce undirected edges

Domain Graph (Moral Graph)

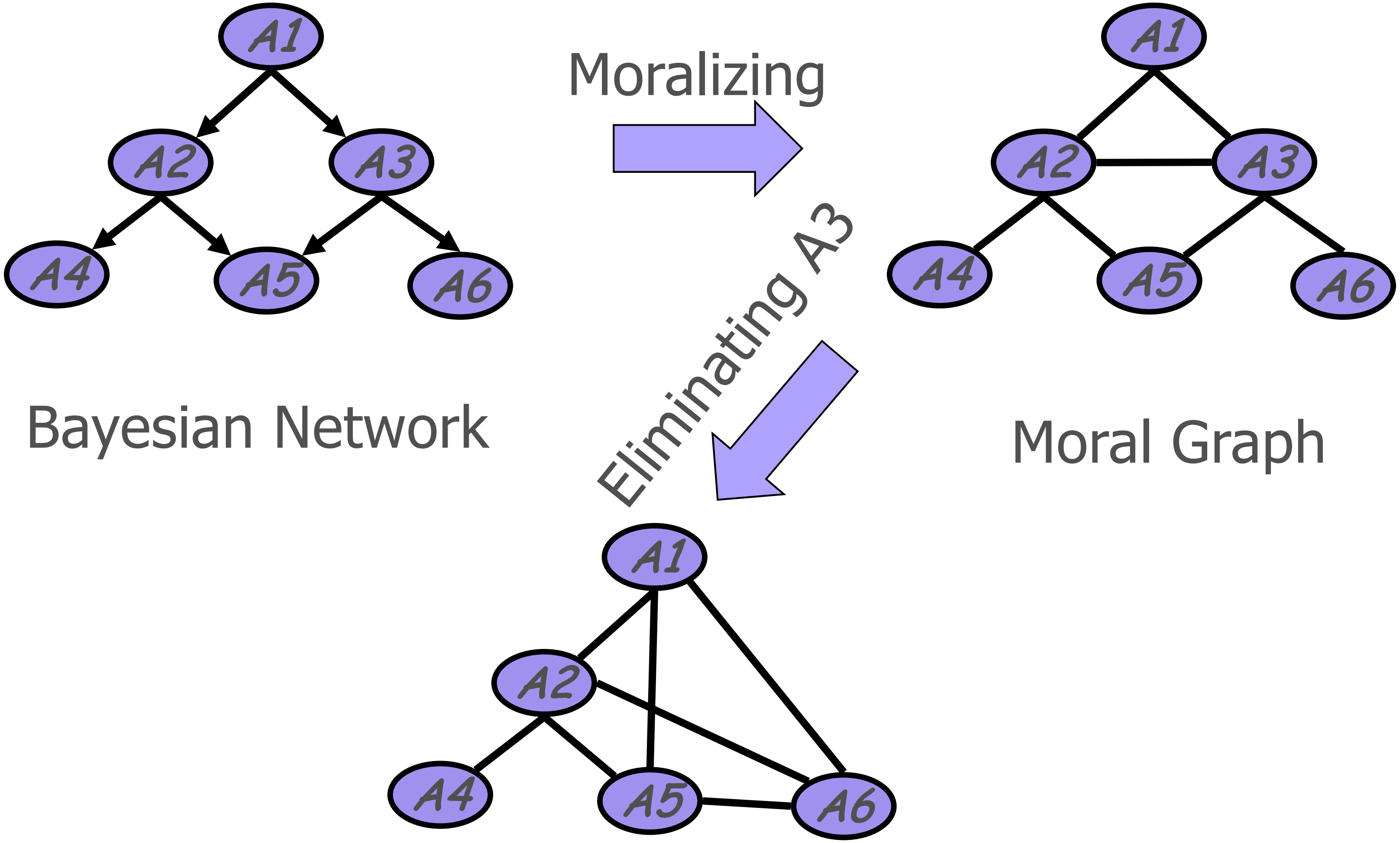
CPDs

$P(A_1)$
$P(A_2|A_1)$
$P(A_3|A_1)$
$P(A_4|A_2)$
$P(A_5|A_2, A_3)$
$P(A_6|A_3)$

CPD = potential

$dom(\phi_1) = \{A_1\}$
$dom(\phi_2) = \{A_2, A_1\}$
$dom(\phi_3) = \{A_3, A_1\}$
$dom(\phi_4) = \{A_4, A_2\}$
$dom(\phi_5) = \{A_5, A_2, A_3\}$
$dom(\phi_6) = \{A_6, A_3\}$

VE on the Moral Graph: Elimination Sequence



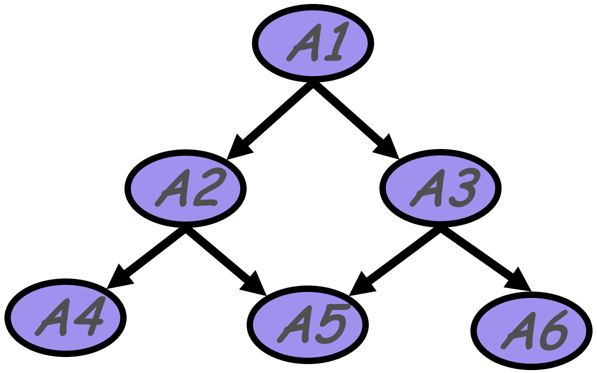
Moralizing

Bayesian Network

Moral Graph

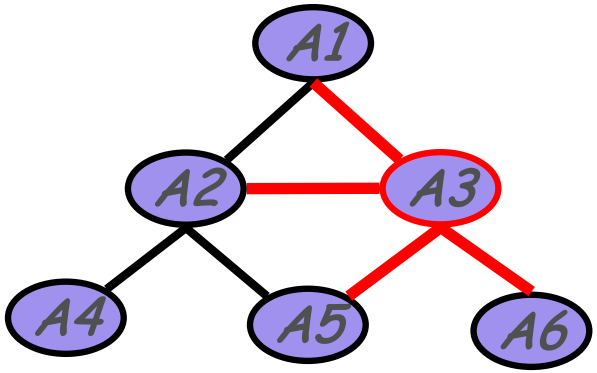
Eliminating A3

Elimination Sequence



Bayesian Network

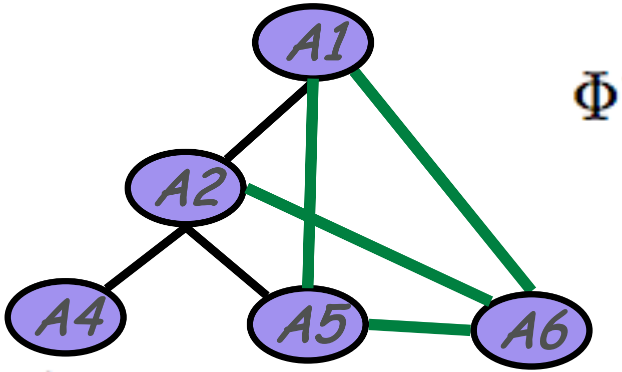
Moralizing



Moral Graph

Eliminating A3

$$\phi_1 = P(A_1)$$
$$\phi_2 = P(A_2|A_1)$$
$$\phi_3 = P(A_3|A_1)$$
$$\phi_4 = P(A_4|A_2)$$
$$\phi_5 = P(A_5|A_2, A_3)$$
$$\phi_6 = P(A_6|A_3)$$

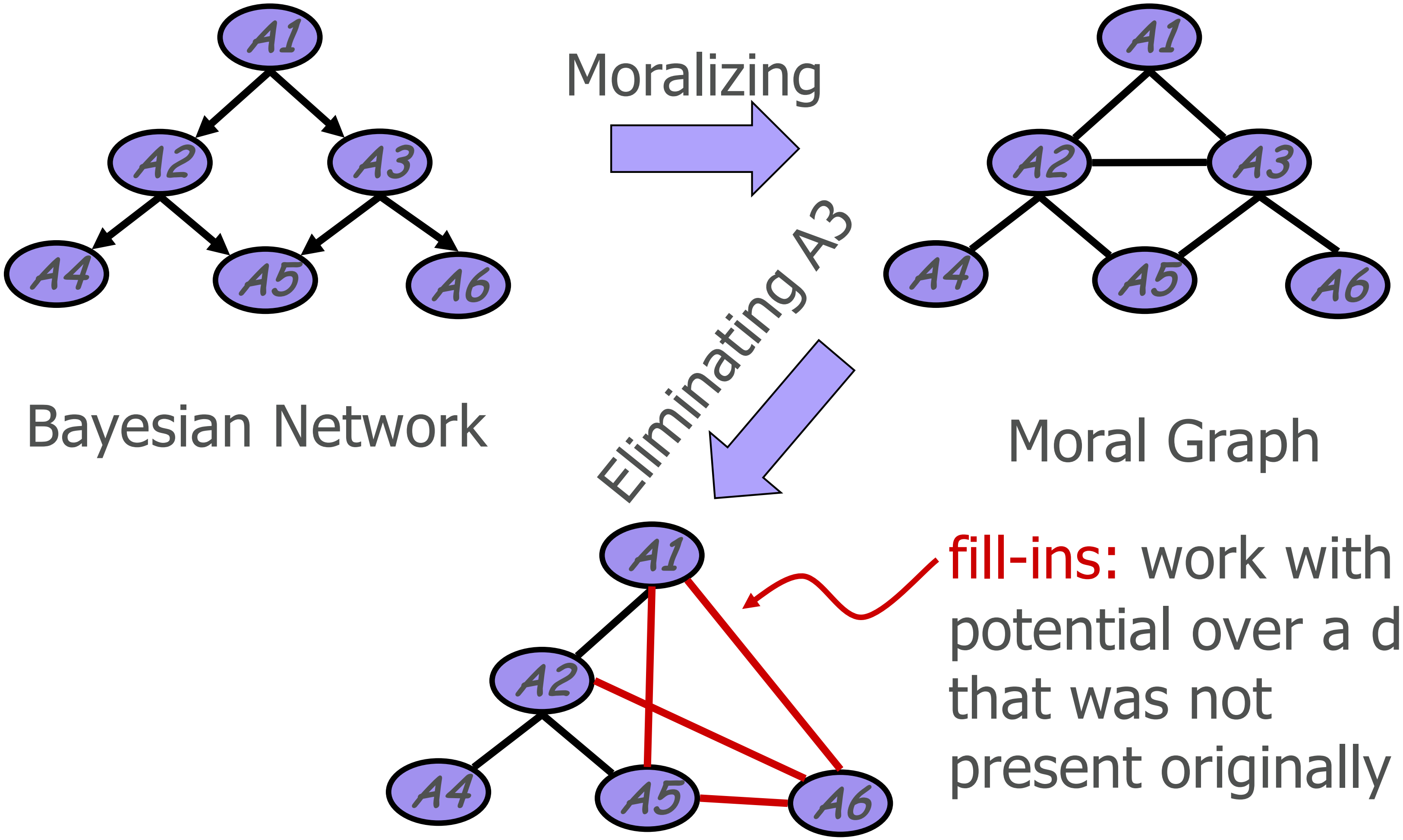


$$\Phi^{-A_3} = \sum\nolimits_{A_3} \Phi_3 \cdot \Phi_5 \cdot \Phi_6$$

Domain: A1,A2,A5,A6

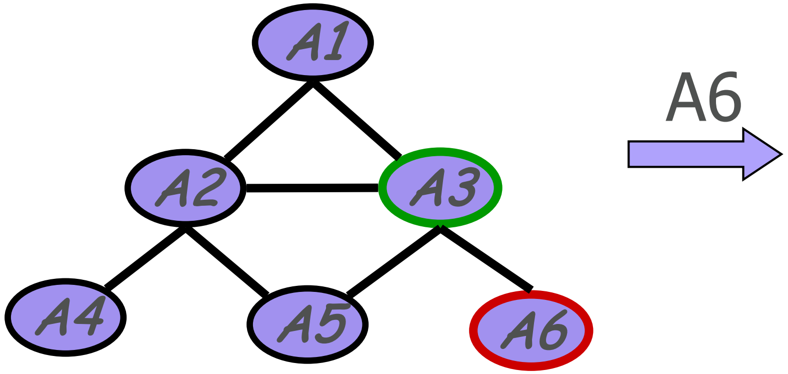
Elimination Sequence

GOAL: Elimination sequence that does not introduce fill-ins

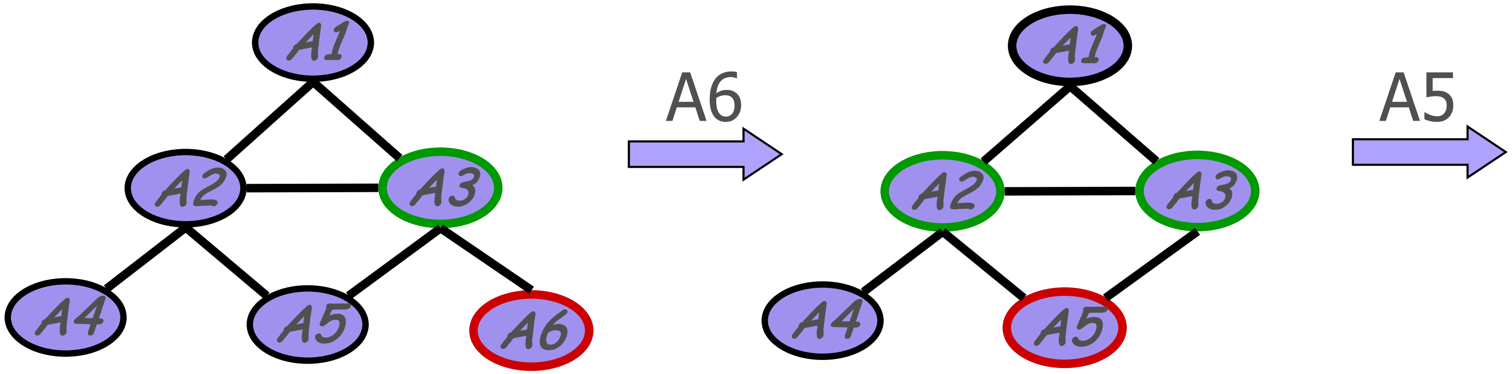


fill-ins: work with a potential over a domain that was not present originally

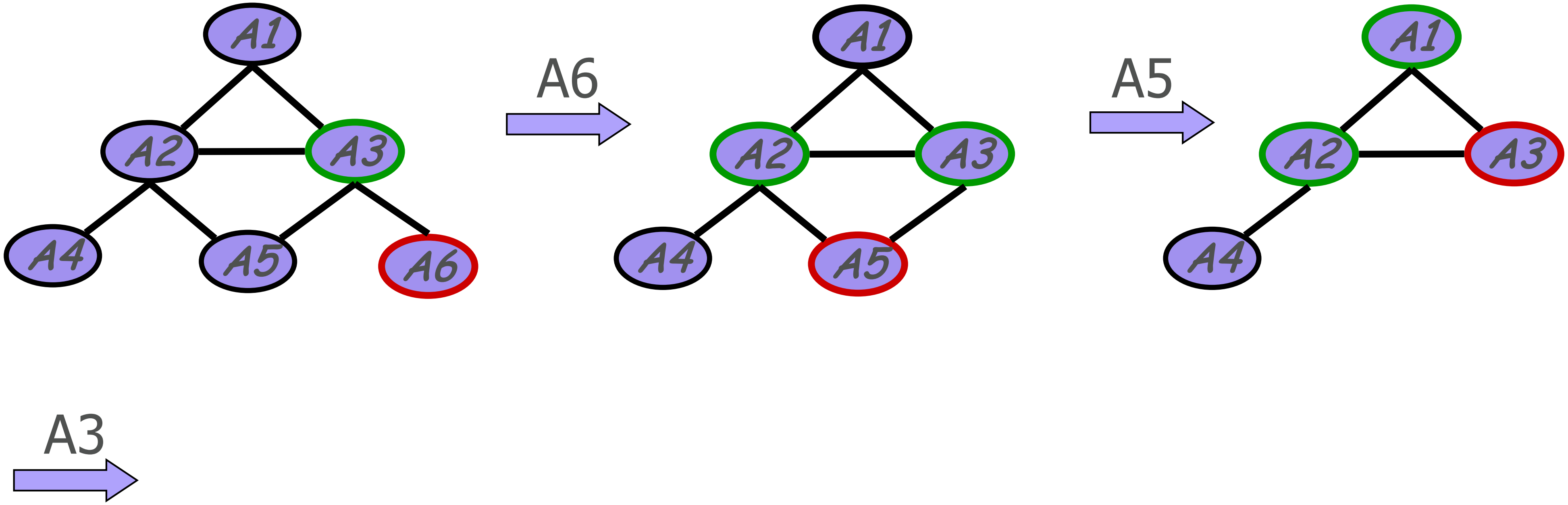
Perfect Elimination Sequence ...



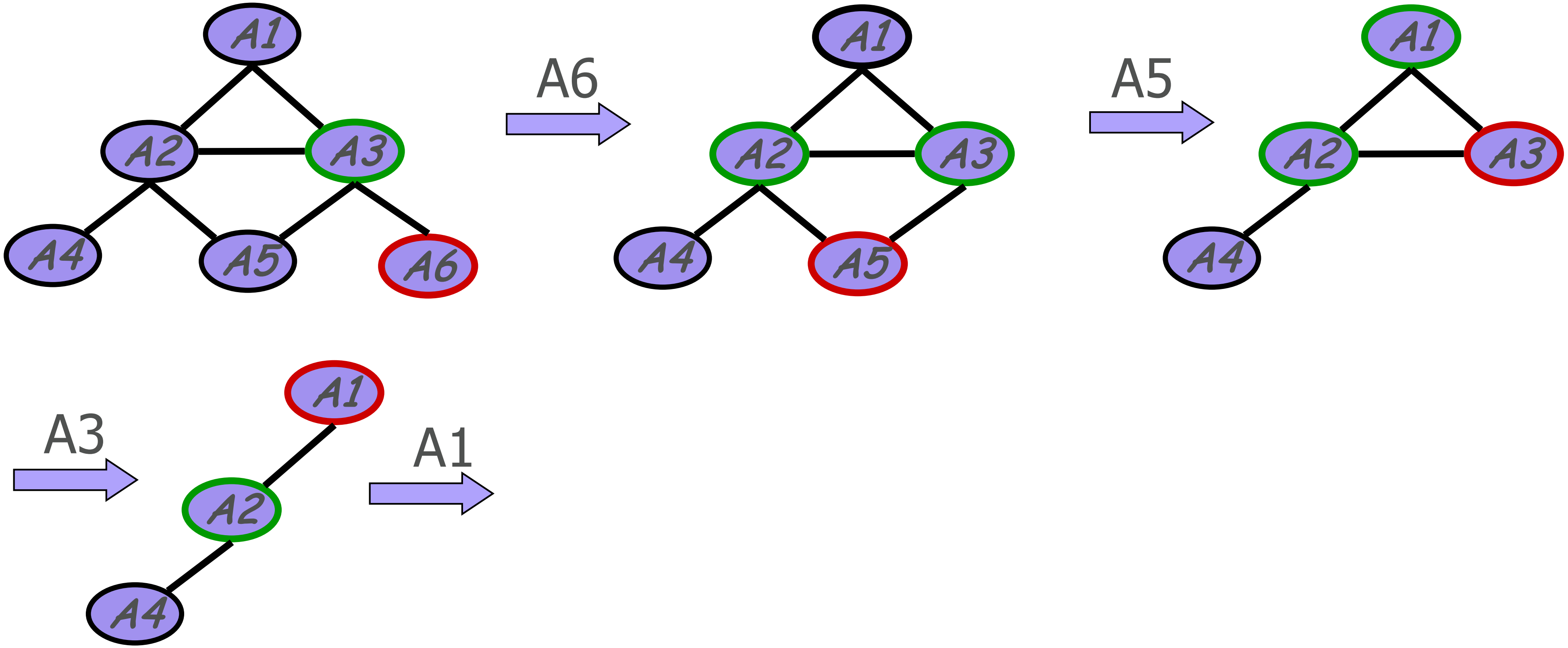
Perfect Elimination Sequence ...



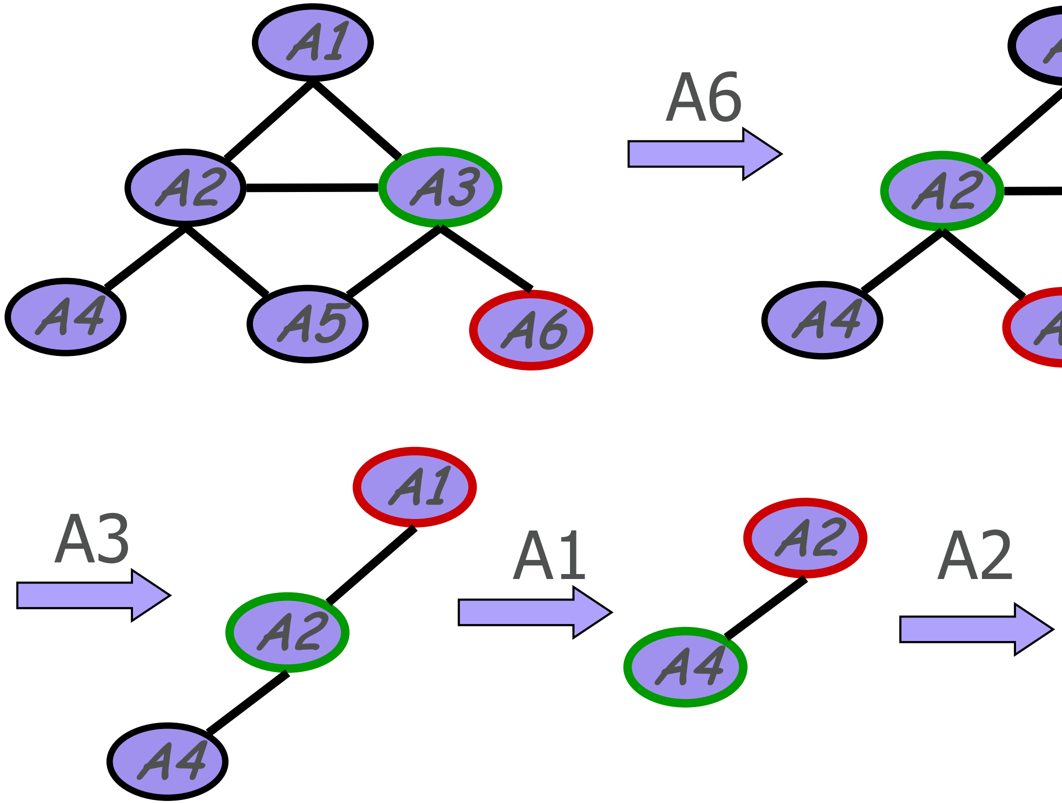
Perfect Elimination Sequence ...



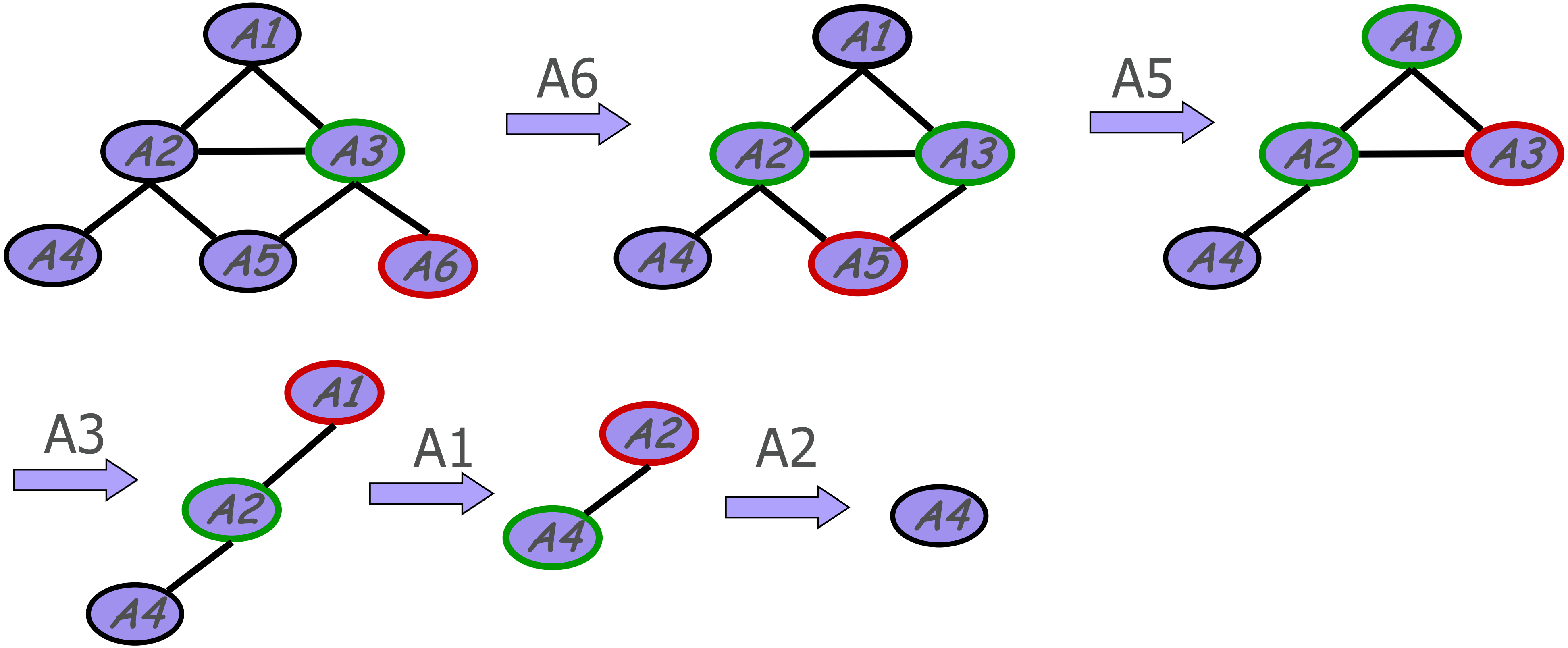
Perfect Elimination Sequence ...



Perfect Elimination Sequence ...

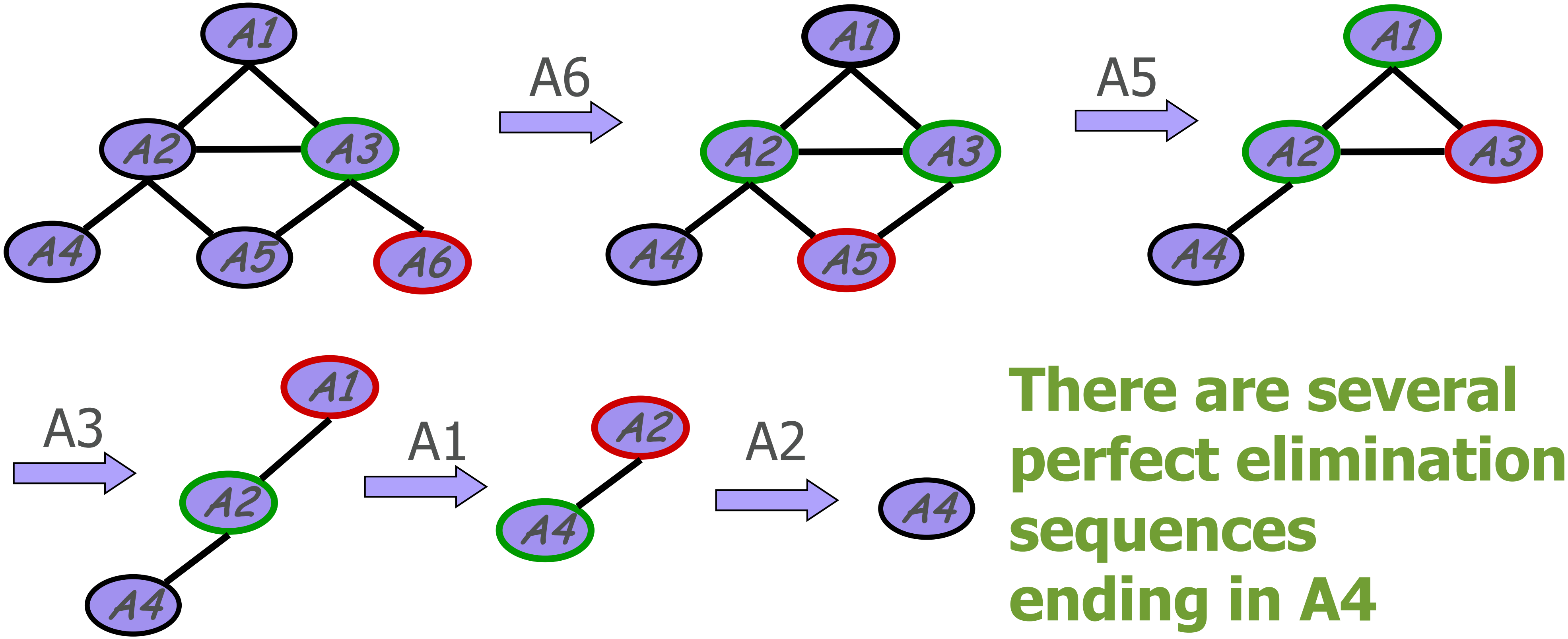


Perfect Elimination Sequence ...



Perfect Elimination Sequence ...

... do not introduce fill-ins

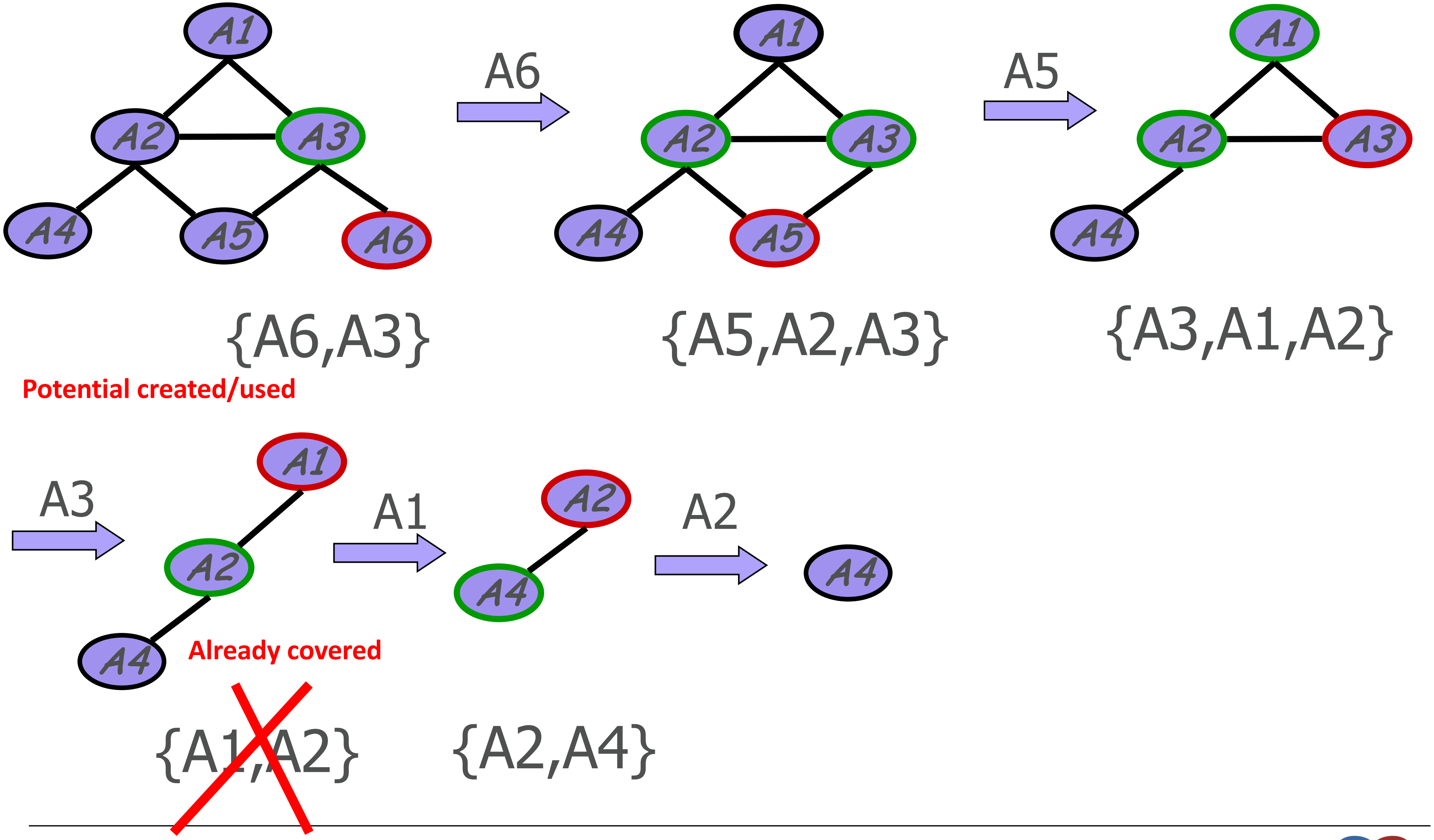


There are several perfect elimination sequences ending in A4

Complexity of VE = Complexity of Elimination Sequence

- Characterized by the set of domains
- Set of domains of potentials produced during the elimination (potentials that are subsets of other potentials are removed).
- A6,A5,A3,A1,A2,A4: {{A6,A3},{A2,A3,A5},{A1,A2,A3},{A2,A4}}

Complexity of Elimination Sequence



A6 → A5 →

{A6,A3}

{A5,A2,A3}

{A3,A1,A2}

Potential created/used

A3 → A1 → A2 →

Already covered

~~{A1,A2}~~

{A2,A4}

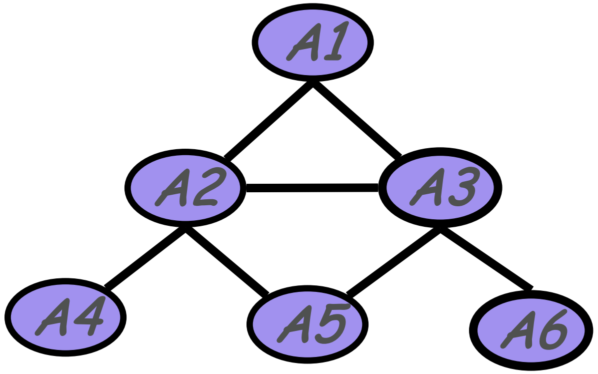
Complexity of Elimination Sequence

- All perfect elimination sequences produce the same domain set, namely the set of cliques of the domain
- Any **perfect elimination sequence** ending with A is **optimal** with respect to **computing P(A)**

Induced Graph

- The induced graph for an elimination order O has an edge $X_i – X_j$ if X_i and X_j appear together in a factor “generated” by VE for elimination order O on factors/potentials F (moral graph is a subgraph)

maximal cliques that cover the induced graph



{A6,A3}

{A5,A2,A3}

{A3,A1,A2}

{A2,A4}

Elimination Order:
A6, A5, A3, A1, A2

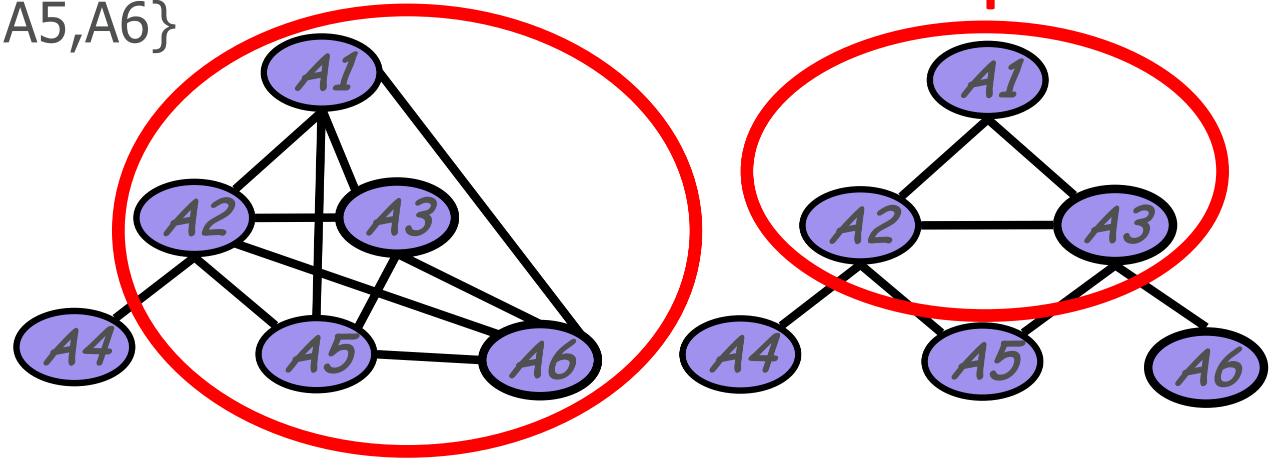
Induced Graph

- The induced graph for an elimination order O has an edge $X_i – X_j$ if X_i and X_j appear together in a factor "generated" by VE for elimination order O on factors/potentials F (moral graph is a subgraph)

Different maximal cliques

{A3,A1,A2,A5,A6}

{A2,A4}



{A6,A3}

{A5,A2,A3}

{A3,A1,A2}

{A2,A4}

A3, A6, A5, A1,A2

A6, A5, A3, A1, A2

Complexity of VE =
Complexity of Elimination Sequence

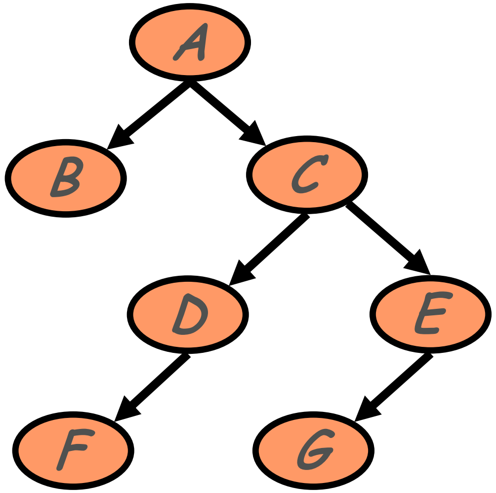
- Main property of induced Graph:
  - Every maximal clique in the induced graph corresponds to an intermediate factor in the VE computations
  - Every factor stored during the VE process is a subset of some maximal clique in the graph
- These facts are true for any variable elimination ordering on any network

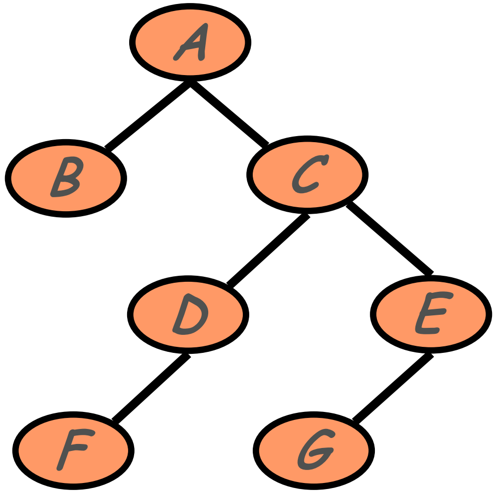
Induced Width (Treewidth)

- **The size of the largest clique in the induced graph is thus an indicator for the complexity of variable elimination**
- This quantity (minus one) is called the **induced width** (or **treewidth**) of a graph according to the specified ordering
- **Finding a good ordering for a graph is equivalent to finding the minimal induced width of the graph**
- **Finding an ordering with minimal induced-width is NP-complete**

Consequence: Elimination on Trees

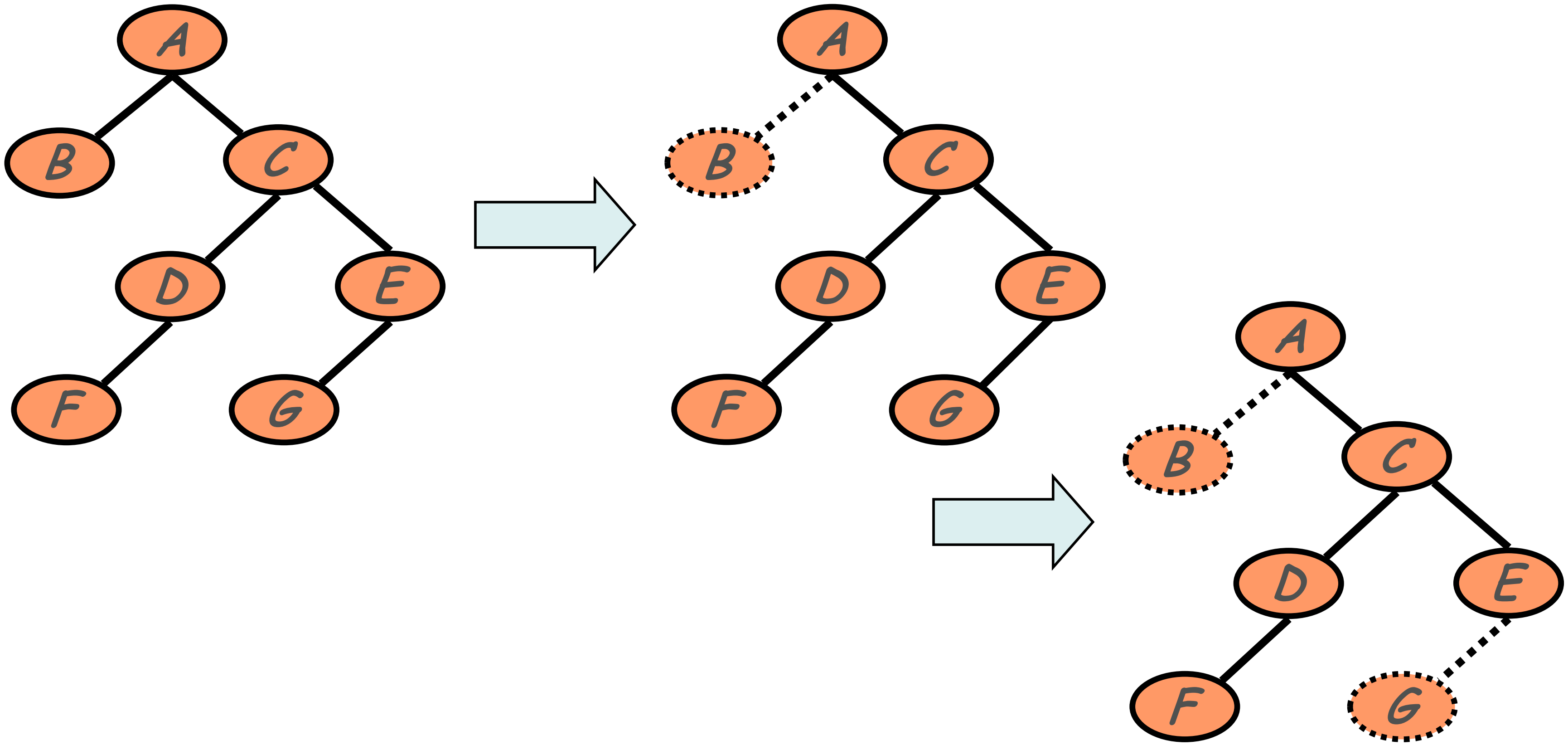
- Suppose we have a **tree**, i.e., a network where each variable has at most one parent. Then:
- All the factors involve at most two variables
- Thus, the moralized graph is also a tree





Elimination on Trees

- We can maintain the tree structure by eliminating extreme variables in the tree



Elimination on Trees

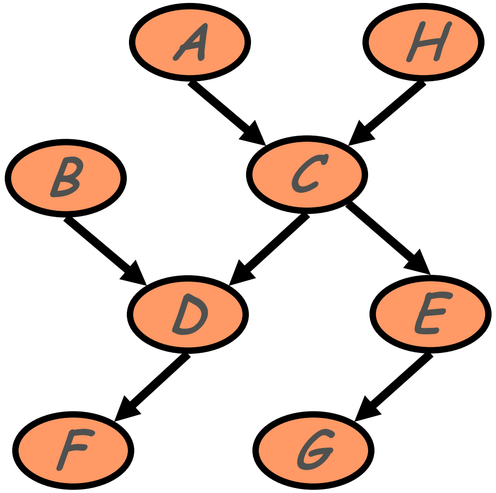
- Formally, for any tree, there is an elimination ordering with **treewidth = 1**

Theorem

- Inference on trees is linear in number of variables

Polytrees

- A polytree is a network where there is at most one path from one variable to another



Theorem:

- Inference in a polytree is linear in the representation size of the network
  - This assumes tabular CPT representation

- Can you see how the argument would work? Maybe this will be a HW

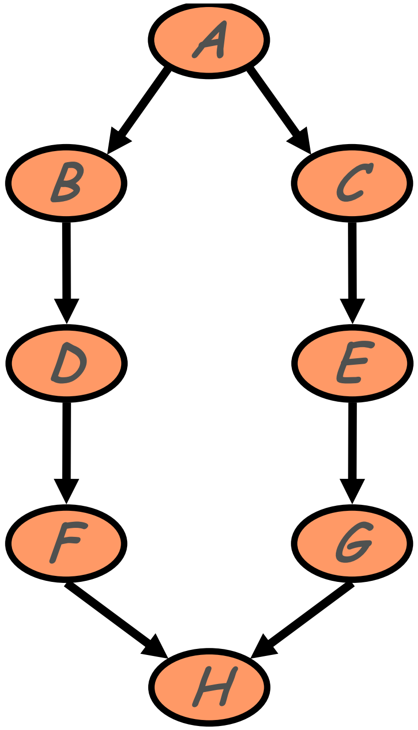
General Networks

What do we do when the network is not a polytree?

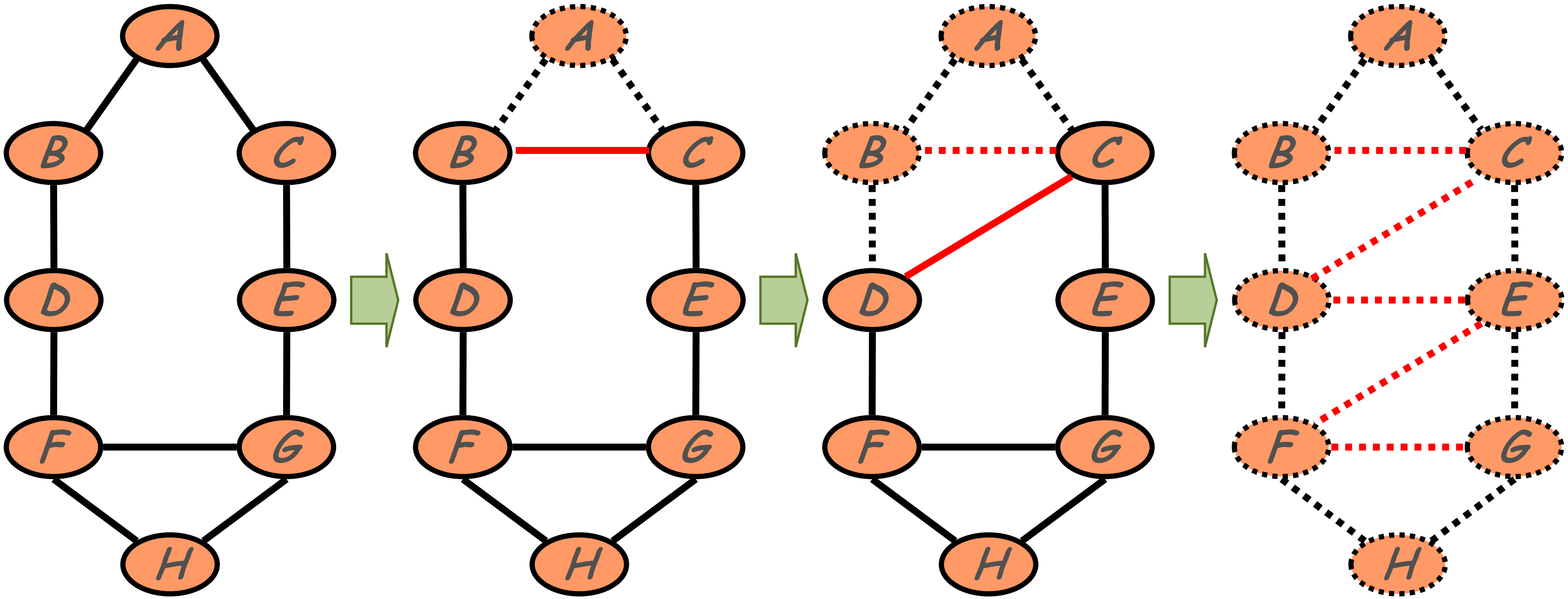
- If network has a cycle, the treewidth for any ordering is greater than 1

Example

- Eliminating A, B, C, D, E,….
- Resulting graph has treewidth 2

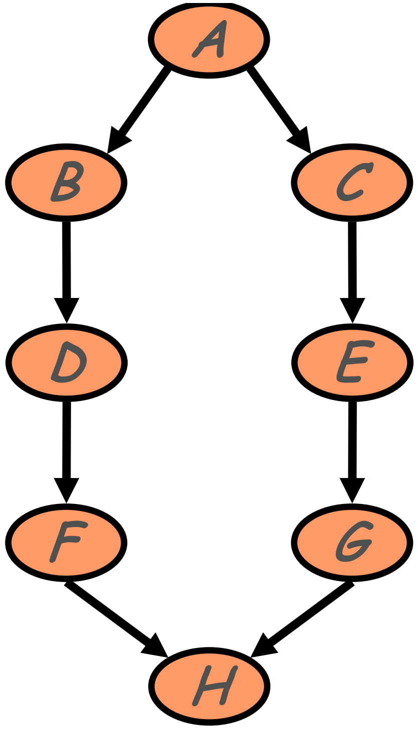


Moral Graph

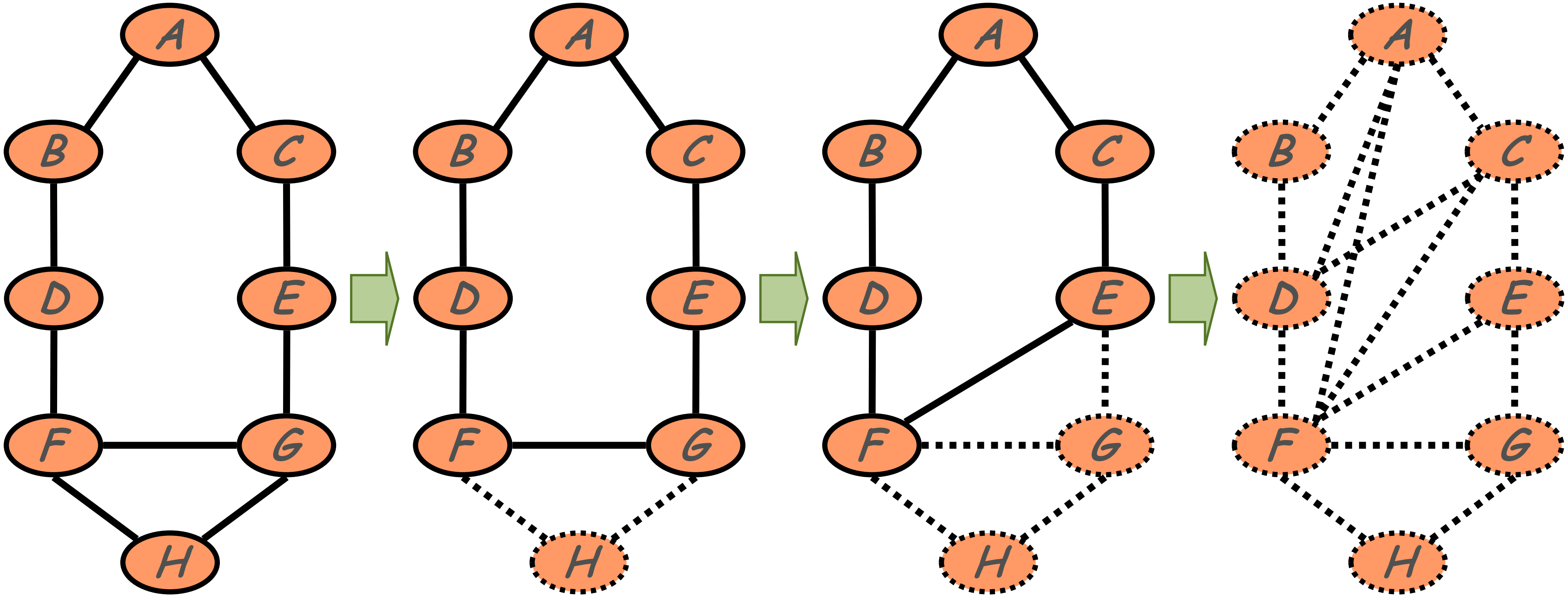


Another Example

- Eliminating H,G, E, C, F, D, B, A



Moral Graph



General Networks

- From graph theory:
  - **Theorem: Finding an ordering that minimizes the treewidth is NP-Hard**

However,

- There are reasonable heuristics for finding “relatively” good ordering
- There are provable approximations to the best treewidth
- If the graph has a small treewidth, there are algorithms that find it in polynomial time

Summary Complexity Results

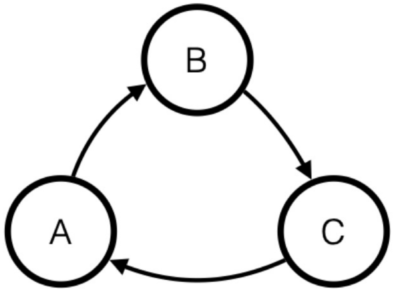
- Probabilistic inference
  - general graphs: #P-complete
  - poly-trees and low tree-width: easy
- Approximate probabilistic inference
  - Absolute error: $|\hat{P} - P| \leq \varepsilon \ldots \quad \mathrm{NP-hard}\ \forall \varepsilon < 0.5$
  - Relative error: $\frac{|\hat{P} - P|}{P} \leq \varepsilon \ldots \quad \mathrm{NP-hard}\ \forall \varepsilon > 0$
- Most probable explanation (MPE)
  - general graphs: NP-complete
  - poly-trees and low tree-width: easy
- Maximum a posteriori (MAP)
  - general graphs: $\mathrm{NP}^{\mathrm{PP}}$-complete
  - poly-trees and low tree-width: NP-hard

What you need to know about inference thus far

- **Variable elimination algorithm**
  - Eliminate a variable:
    - Combine factors that include this var into single factor
    - Marginalize var from new factor
  - **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" (with context-specific independence)
- **Elimination order is important!**
  - **NP-complete problem**
  - Many good heuristics

Acyclicity of Bayes Nets

invalid Bayes net

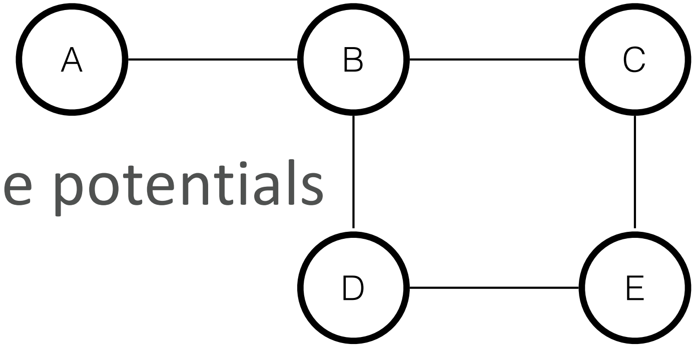


Only “makes sense” if P(A) = P(B) = P(C) = 1

All meaningful Bayes nets are directed, acyclic graphs (DAGs)

We need a different form

Undirected Graphical Models



Intuition: edges encode potentials

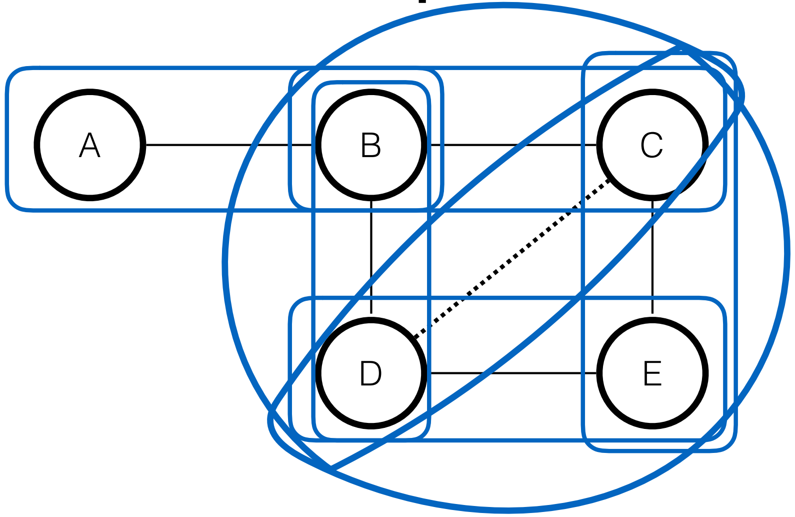
$$P(A,B,C,D,E) \propto \phi(A,B)\phi(B,C)\phi(B,D)\phi(C,E)\phi(D,E)$$

$$P(X) = \frac{1}{Z} \prod_{c \in \text{cliques}(G)} \phi_C(x_c)$$

potential functions

maximal cliques

Undirected Graphical Models



$$P(A,B,C,D,E) \propto \cancel{\phi(A,B)\phi(B,C)\phi(B,D)\phi(C,E)\phi(D,E)}$$

$$\phi(A,B)\phi(B,C,D)\phi(C,D,E)$$

$$P(X) = \frac{1}{Z} \prod_{c \in \text{cliques}(G)} \phi_C(x_c)$$

potential functions

maximal cliques

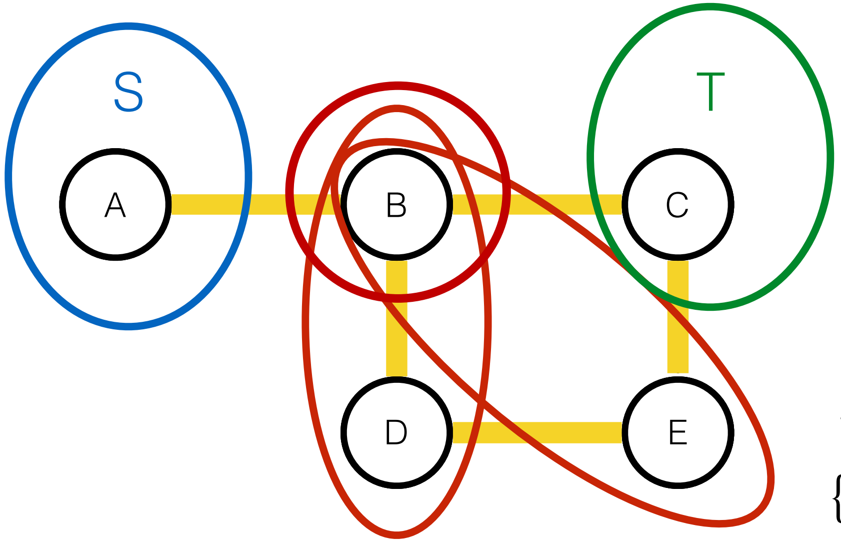
Markov Random Fields

- Any two subsets S and T of variables are conditionally independent given a **separating subset**
  - All paths between S and T must travel through the separating subset

paths:

A-B-C

A-B-D-E-C



separating subsets

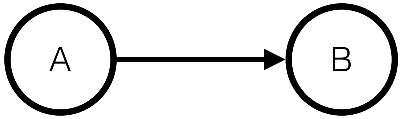
{B,D}, {B,E}, {B,D,E}

Other (implied) independencies

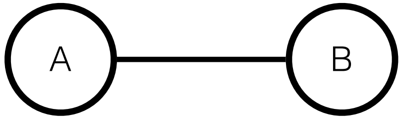
Independence Corollaries

- Any two non-adjacent variables are conditionally independent given all other variables
- Any variable is conditionally independent of the other variables given its neighbors
  - Markov blanket

Bayesian Networks as MRFs



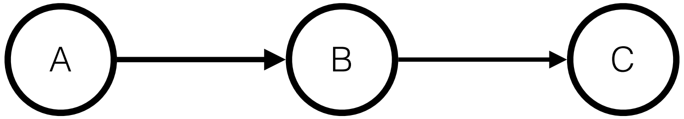
$$p(A, B) = p(A)p(B|A)$$



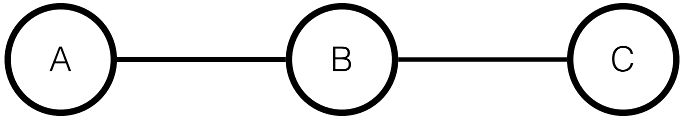
$$p(A, B) \propto \phi(A, B)$$

converting a single edge to a pairwise clique potential is easy

Bayesian Networks as MRFs



$$p(A, B, C) = p(A)p(B|A)P(C|B)$$



$$p(A, B, C) \propto \phi(A, B)\phi(B, C)$$

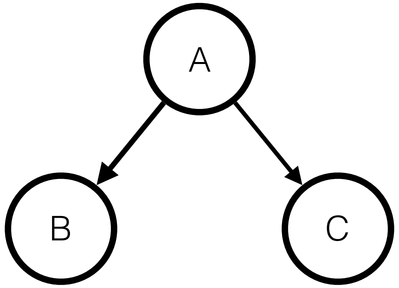
$$\phi(A, B) \leftarrow P(A)P(B|A)$$

$$\phi(B, C) \leftarrow P(C|B)$$

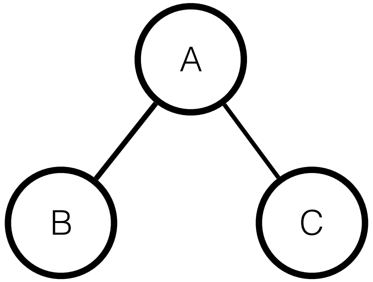
chains are easy too

parameterization is not unique

Bayesian Networks as MRFs



$$p(A, B, C) = p(A)P(B|A)P(C|A)$$



$$p(A, B, C) \propto \phi(A, B), \phi(A, C)$$

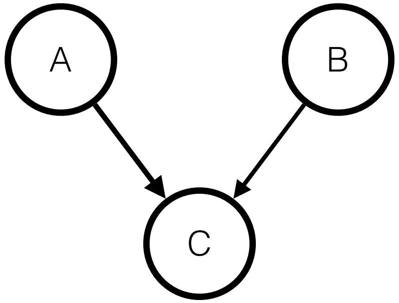
$$\phi(A, B) \leftarrow P(A)P(B|A)$$

$$\phi(A, C) \leftarrow P(C|A)$$

shared parents also easy

Now the v-structure!
Can we also capture this BN in the MRF?

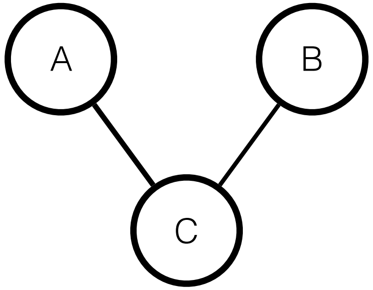
Bayesian Networks as MRFs



$$p(A, B, C) = p(A)p(B)p(C|A, B)$$

A and B are **dependent** given C

What if we observe C?



$$p(A, B, C) \propto \phi(A, C)\phi(B, C)$$

A and B are **independent** given C

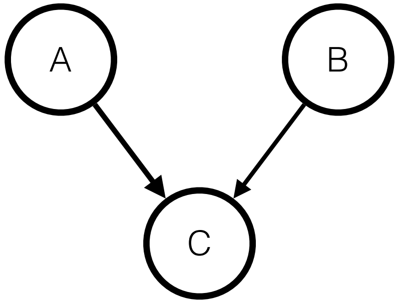
can’t be correct

shared child

We do not have enough information

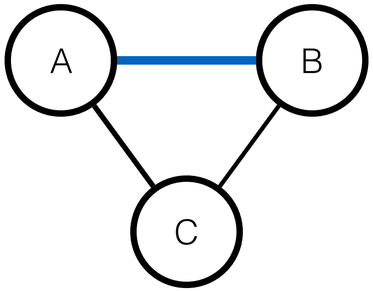
The solution: Moralization!

Moralizing Parents



$$p(A, B, C) = p(A)p(B)p(C|A, B)$$

A and B are **dependent** given C



$$p(A, B, C) \propto \phi(A, C)\phi(B, C)\ \phi(A, B)$$

A and B are **independent** given C

Or we go for the max clique potential,
Where we can code this, too.

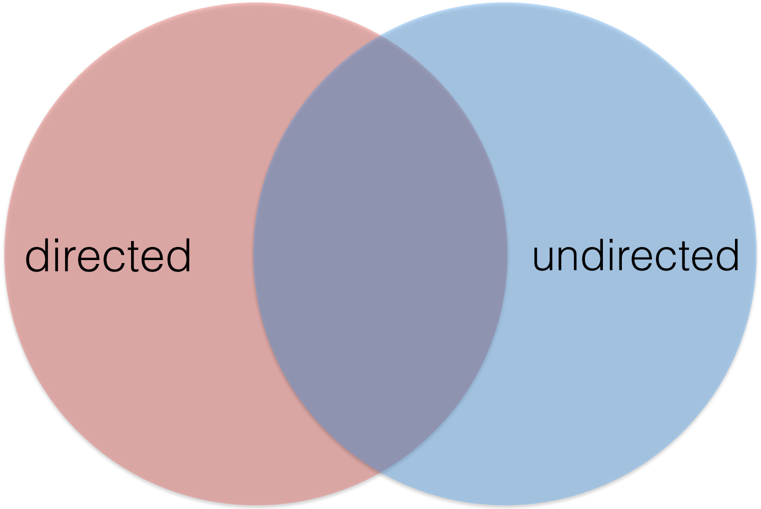
shared child

Explains the moral link we talked about already

Converting Bayes Nets to MRFs

- Moralize all co-parents
- Lose marginal independence of parents

(v-structure: A and B are now almost always dependent when not observing c))



Back to inference
What if we have to run multiple inferences?

- Multiple inference, e.g.,

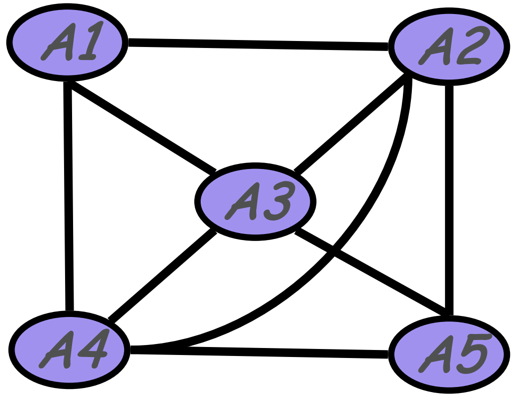
$$P(X_i, e) \qquad\qquad P(X_i|e) = \frac{P(X_i, e)}{P(e)}$$

- For each i do variable elimination?

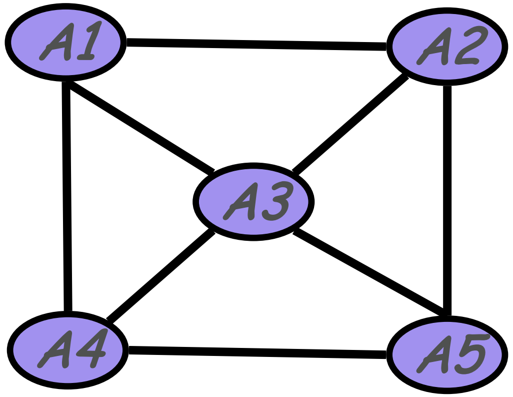
No, instead reuse information resp. computations

Triangulated Graphs and Join Trees

- An undirected graph with **perfect elimination sequence** (no fill-ins) is called a ***triangulated*** graph

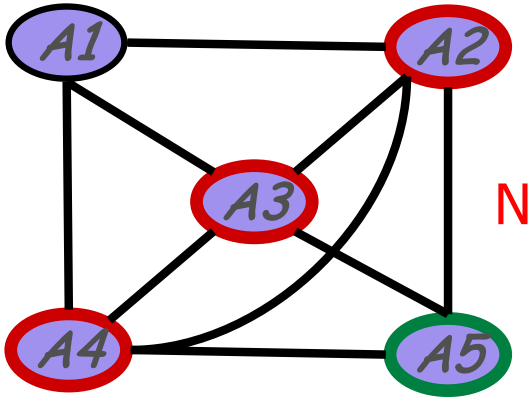


triangulated

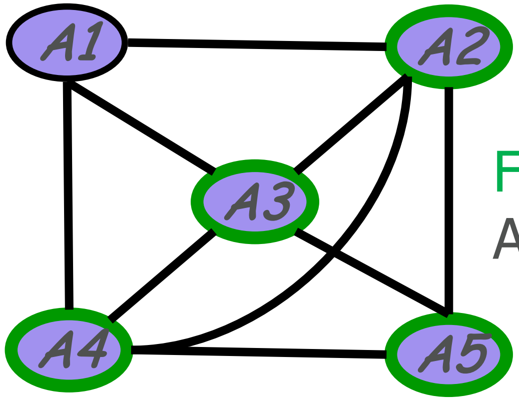


nontriangulated

Triangulated Graphs and Join Trees

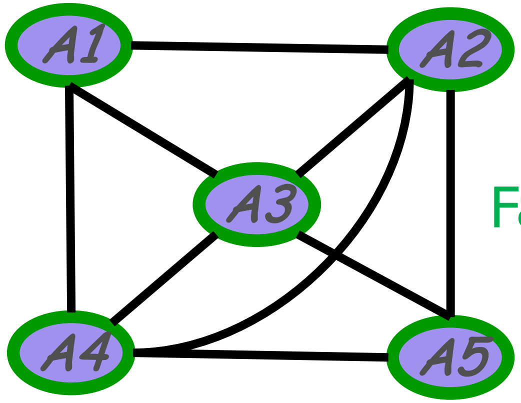


Neighbours of A5



Family of A5, i.e., A5 is simplicial

- Complete neighbour set = all neighbours are pairwise linked = simplicial node
- X is simplicial iff family of X is a clique

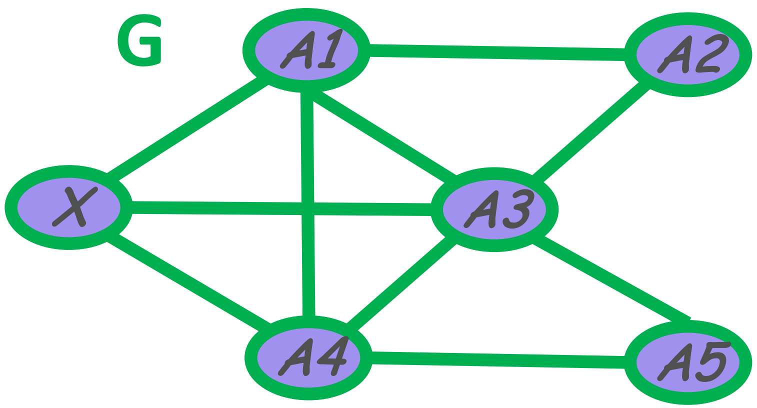


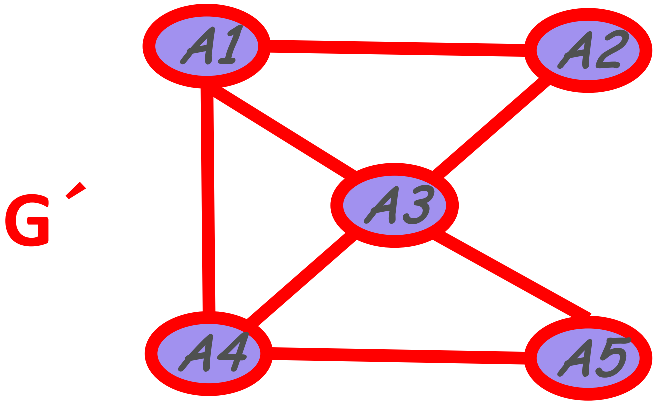
Family of A3, i.e. A3 is **not** simplicial

Triangulated Graphs and Join Trees

Let **G** be a **triangulated** graph, and let **X** be a **simplicial** node. Let G´ be the graph resulting from **eliminating X** (including its edges) from G.

Then G´ is a triangulated graph



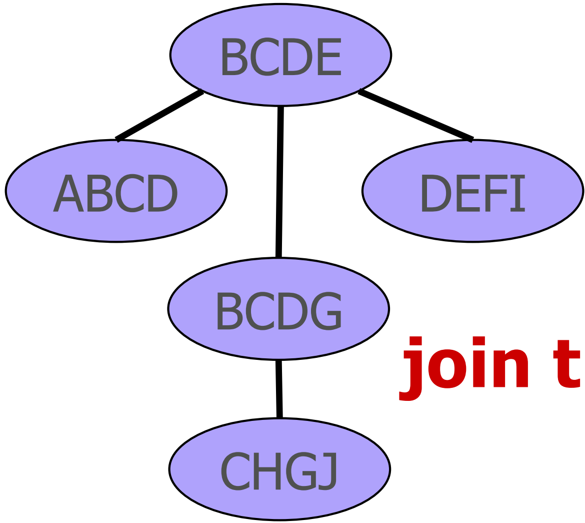


Triangulated Graphs and Join Trees

- **A triangulated graph with at least two nodes has at least two simplicial nodes**
- **In a triangulated graph, each variable A has a perfect elimination sequence ending with A**
- Not all domain graphs are triangulated: An undirected graph is triangulated iff **all nodes can be eliminated by successively eliminating a simplicial node**

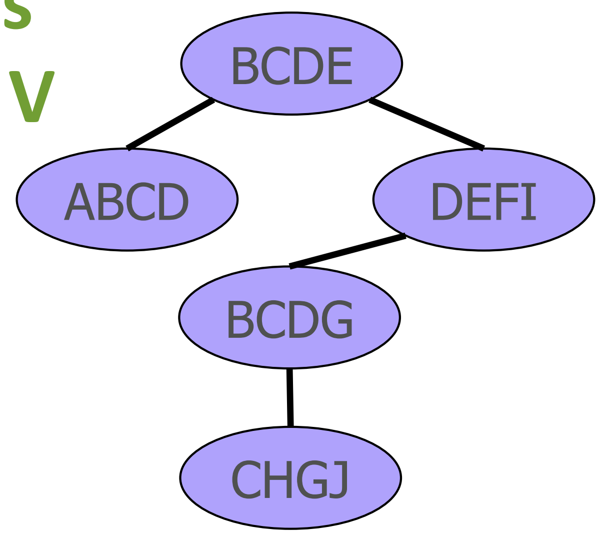
Join Trees

Let G be the set of cliques from an undirected graph, and let the cliques of G be organized in a tree



join tree

- T is a join tree if for any pair of nodes V, W all nodes on the path between V an W contain the intersection V∩W
- This is called „Running Intersection Property“



not a join tree

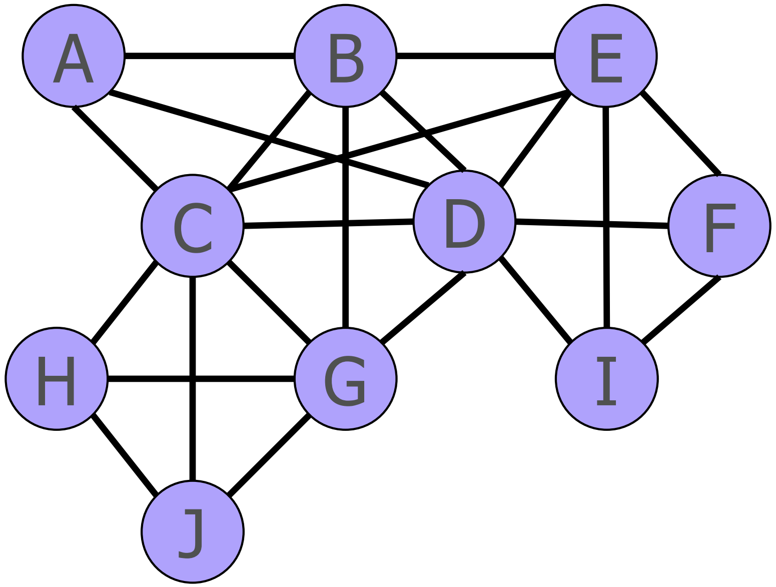
Join Trees ⇔ Triangulated

It can be shown that

- If the cliques of an undirected graph G can be organized into a join tree, then G is triangulated

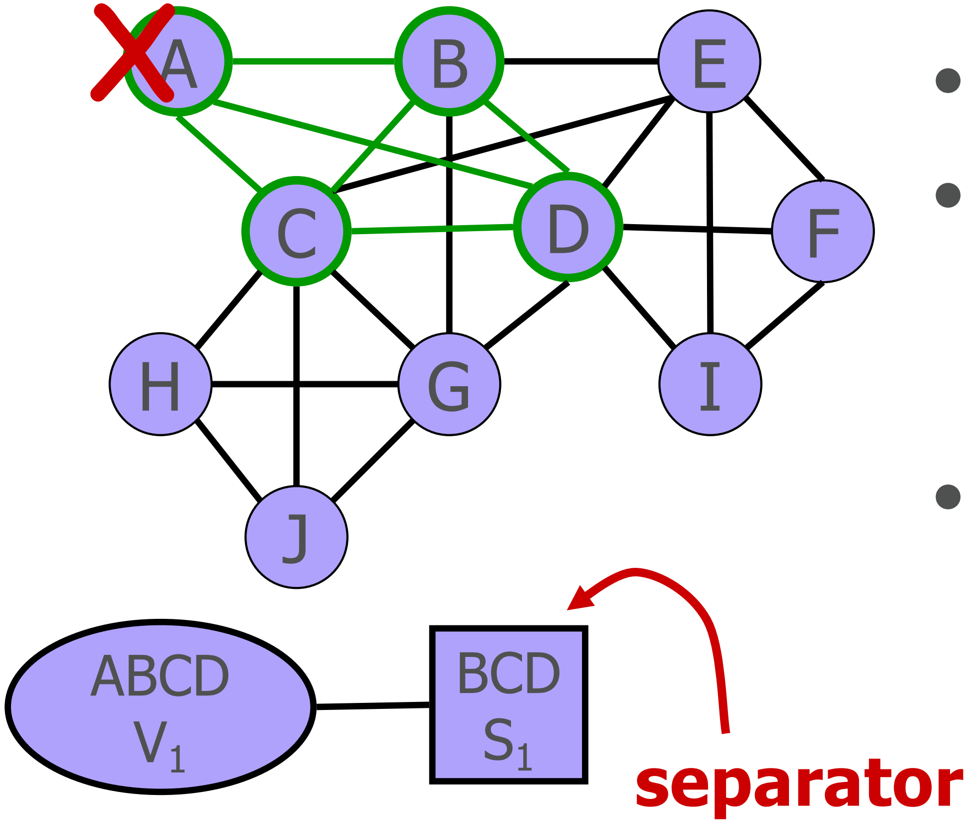
- If the undirected graph is triangulated, then the cliques of G can be organizes into a join tree

Triangulated, undirected Graph -> Join trees



- Simplicial node X
- Family of X is a clique
- Eliminate nodes from family of X which have only neighbours ir the family of X
- Give family of X a number i according to the number of nodes eliminated so far and denote the family by V_i
- Denote the set of remaining nodes S_i

Triangulated, undirected Graph -> Join trees



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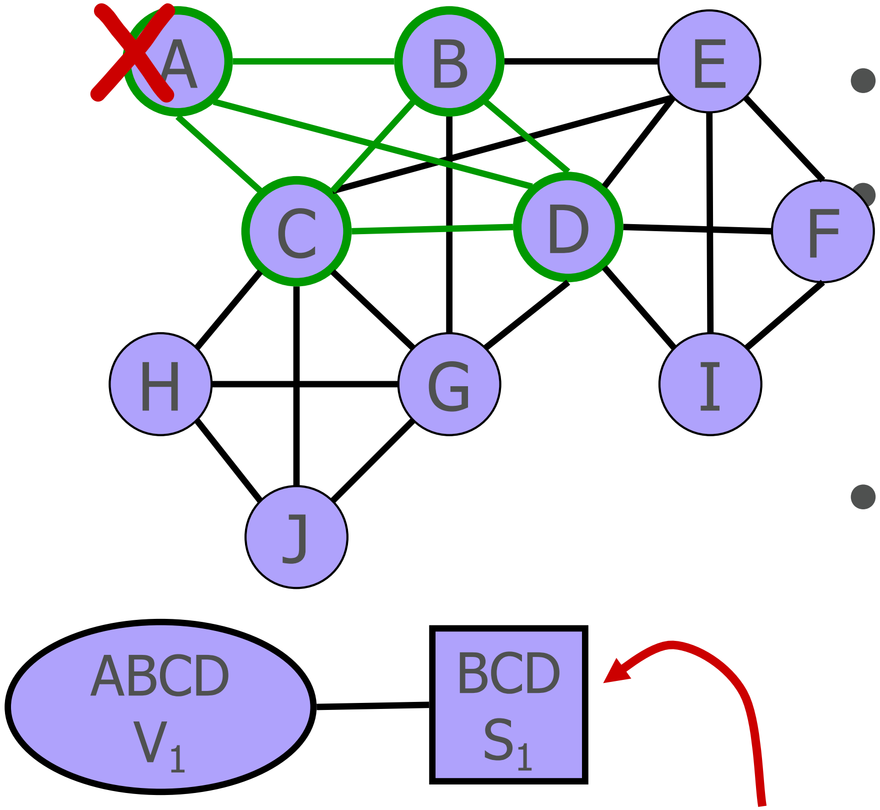
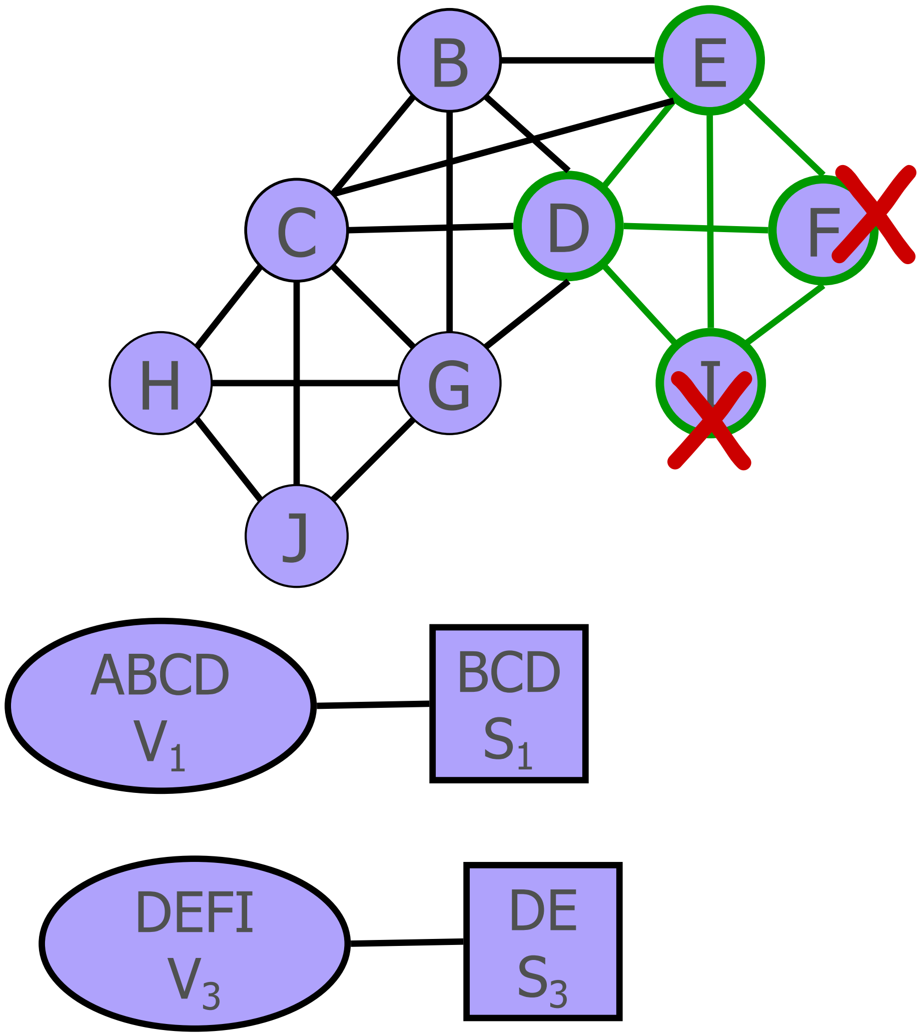
Triangulated, undirected Graph -> Join trees



separator

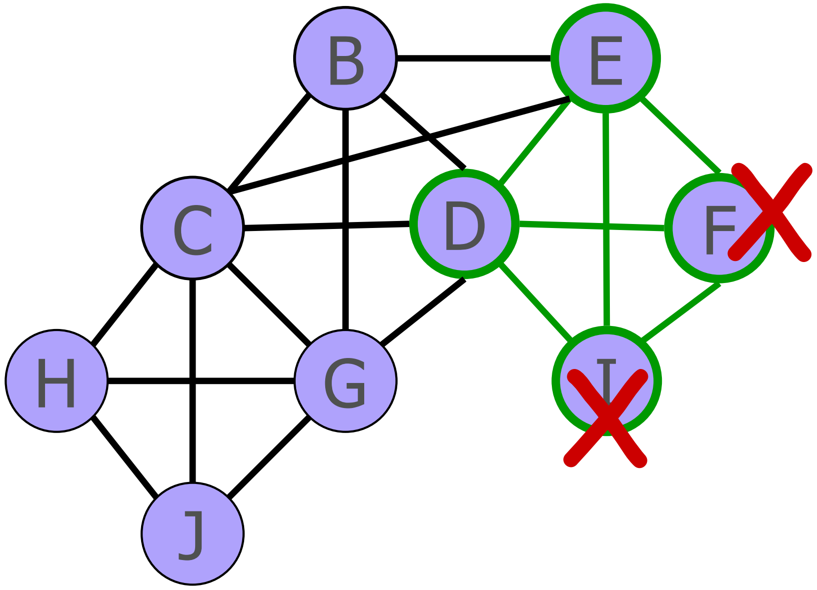
- Simplicial node X **A**
- Family of X is a clique **{A,B,C,D}**
- Eliminate nodes from family of X which have only neighbours in the family of X **{A}{B,C,D}**
- Give family of X a number i according to the number of nodes eliminated so far and denote the family by V_i **V_1**
- Denote the set of remaining nodes S_i **S_1**

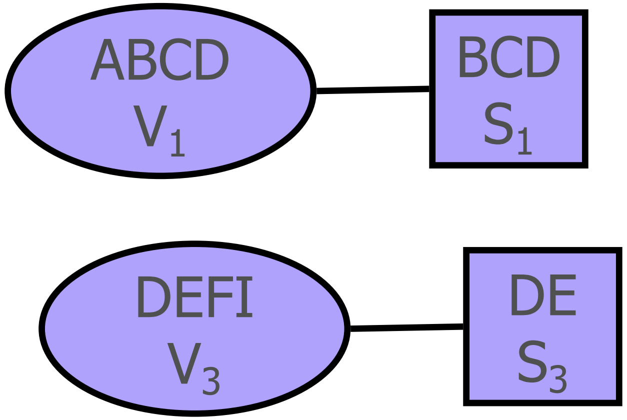
Triangulated, undirected Graph -> Join trees



- Simplicial node X
- Family of X is a clique
- Eliminate nodes from family of X which have only neighbours in the family of X
- Give family of X a number i according to the number of nodes eliminated so far and denote the family by V_i
- Denote the set of remaining nodes S_i

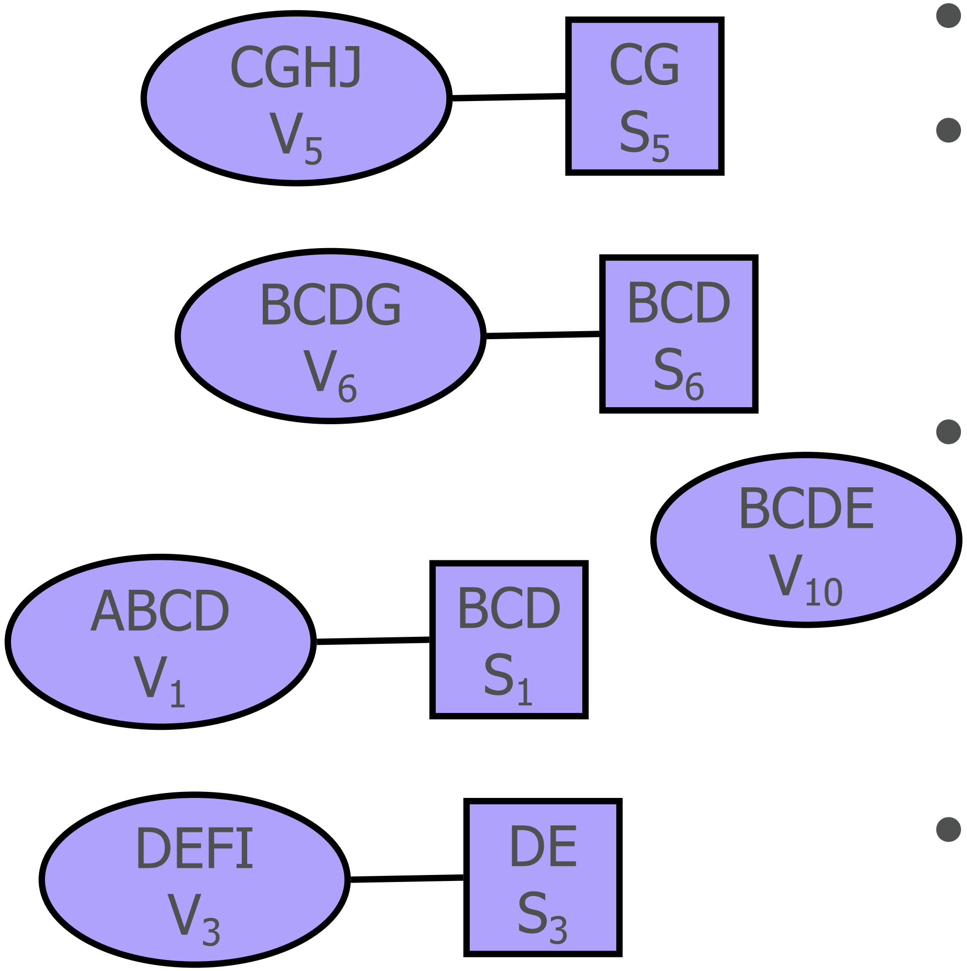
Triangulated, undirected Graph -> Join trees





- Simplicial node X **F**
- Family of X is a clique **{D,E,F,I}**
- Eliminate nodes from family of X which have only neighbours in the family of X **{F,I}{D,E}**
- Give family of X a number i according to the number of nodes eliminated so far and denote the family by V_i $\mathbf{V_3}$
- Denote the set of remaining nodes S_i $\mathbf{S_3}$
- We stopped here

Triangulated, undirected Graph -> Join trees



- Simplicial node X
- Family of X is a clique
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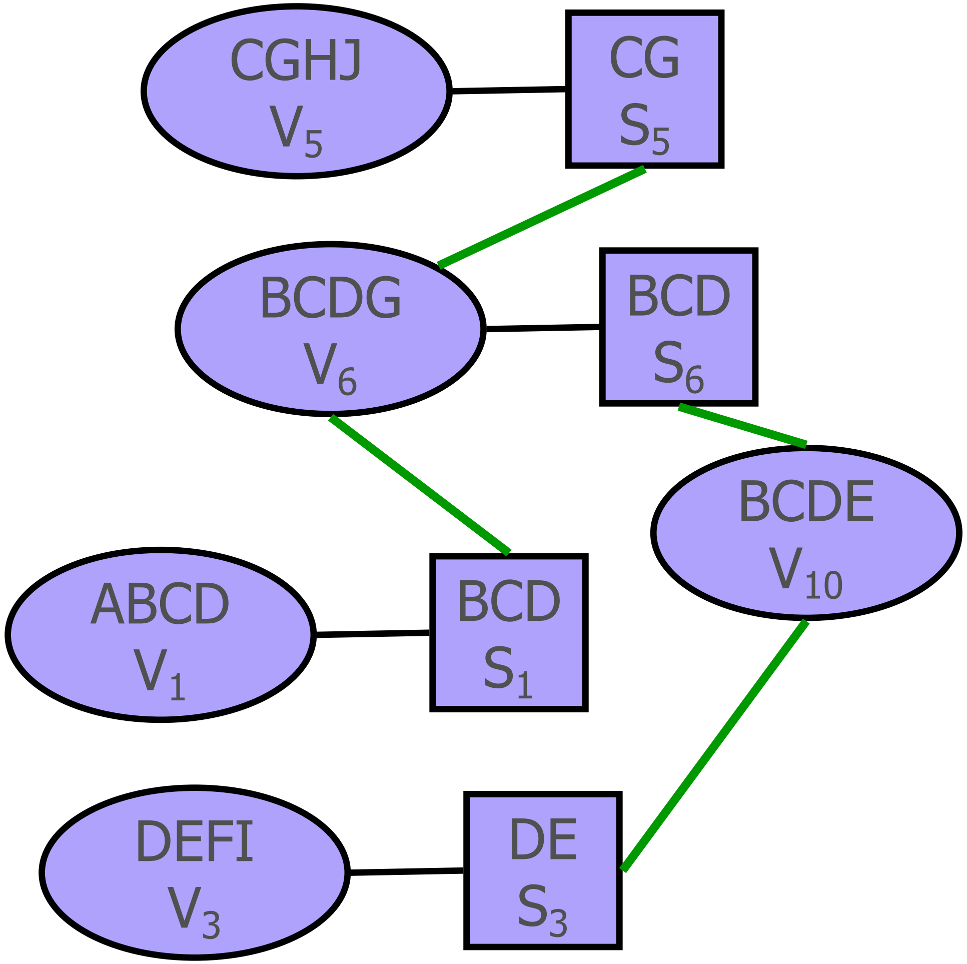
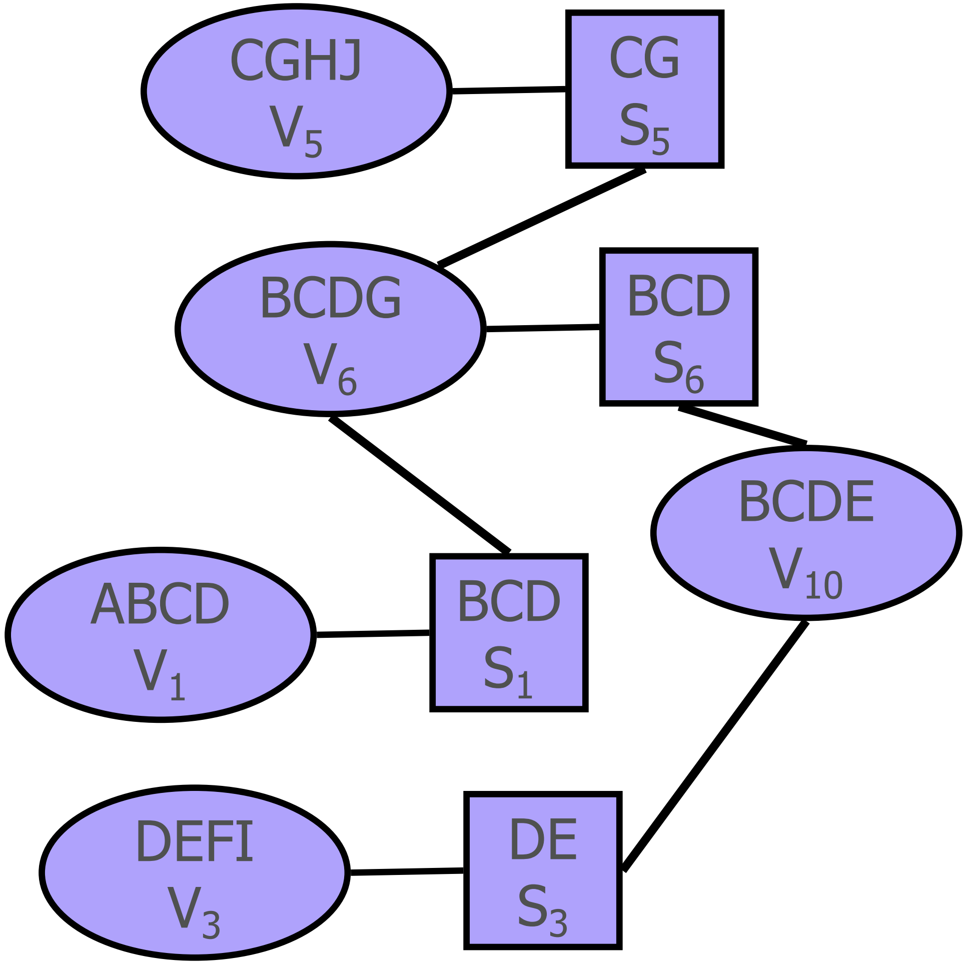
- Denote the set of remaining nodes S_i

Triangulated, undirected Graph -> Join trees



- Connect each separator S_i to a clique V_j, $j>i$, such that S_i is a subset of V_j
- Due to the running intersection property this is always possible

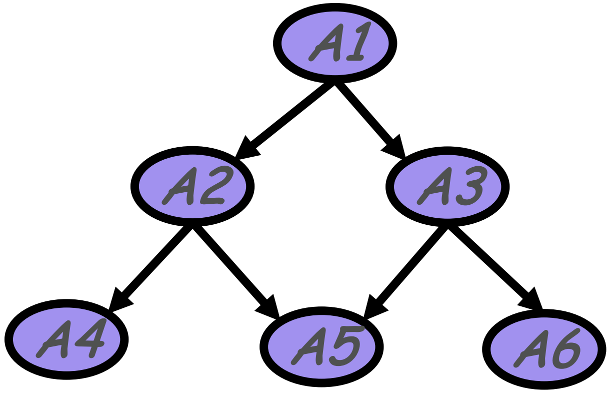
Join Tree

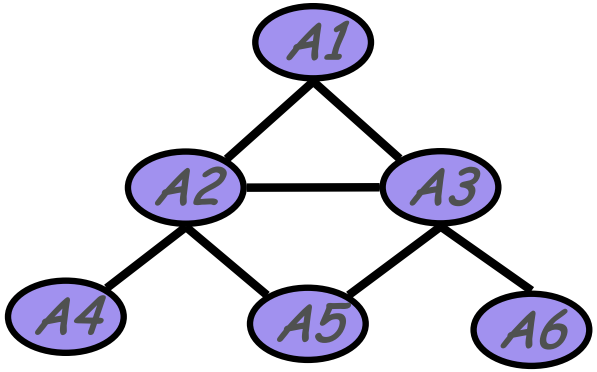


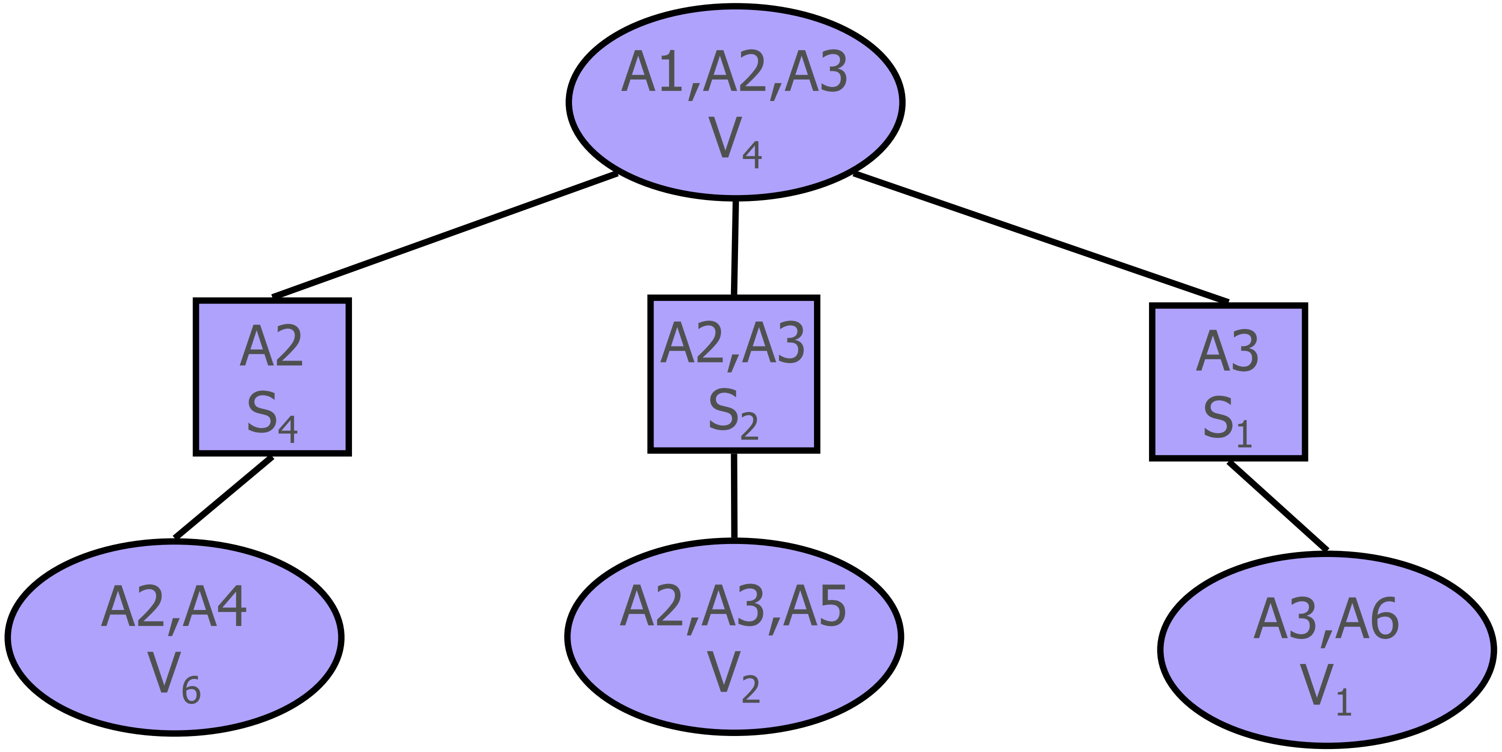
The potential representation of a join tree (aka clique tree) is the product of the clique potentials, dived by the product of the separator potentials.

$$P(\mathbf{X}) = \frac{\prod_c \phi_c(\mathbf{X})}{\prod_s \phi_s(\mathbf{X})}$$

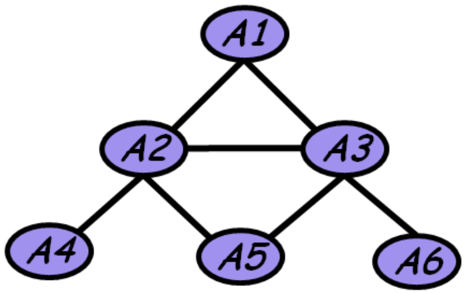
Yet Another Example



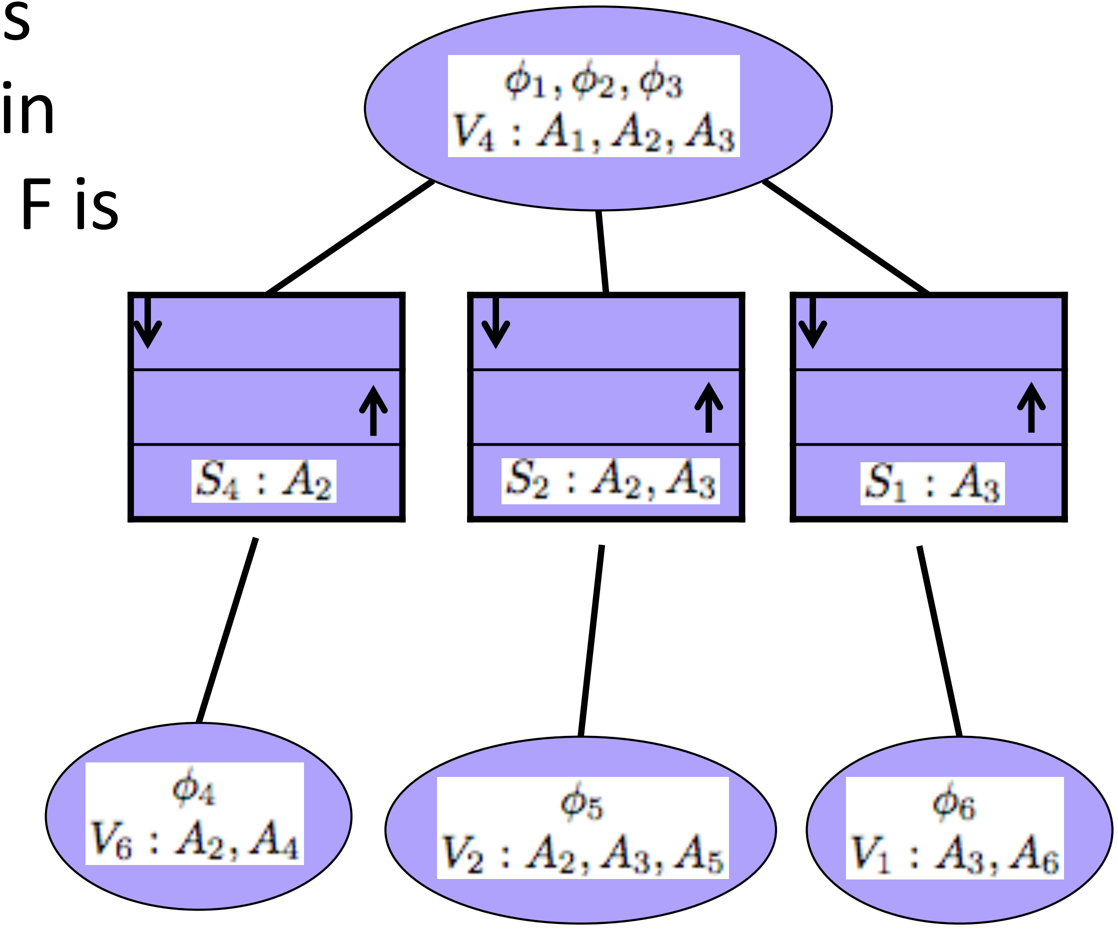




Junction Trees

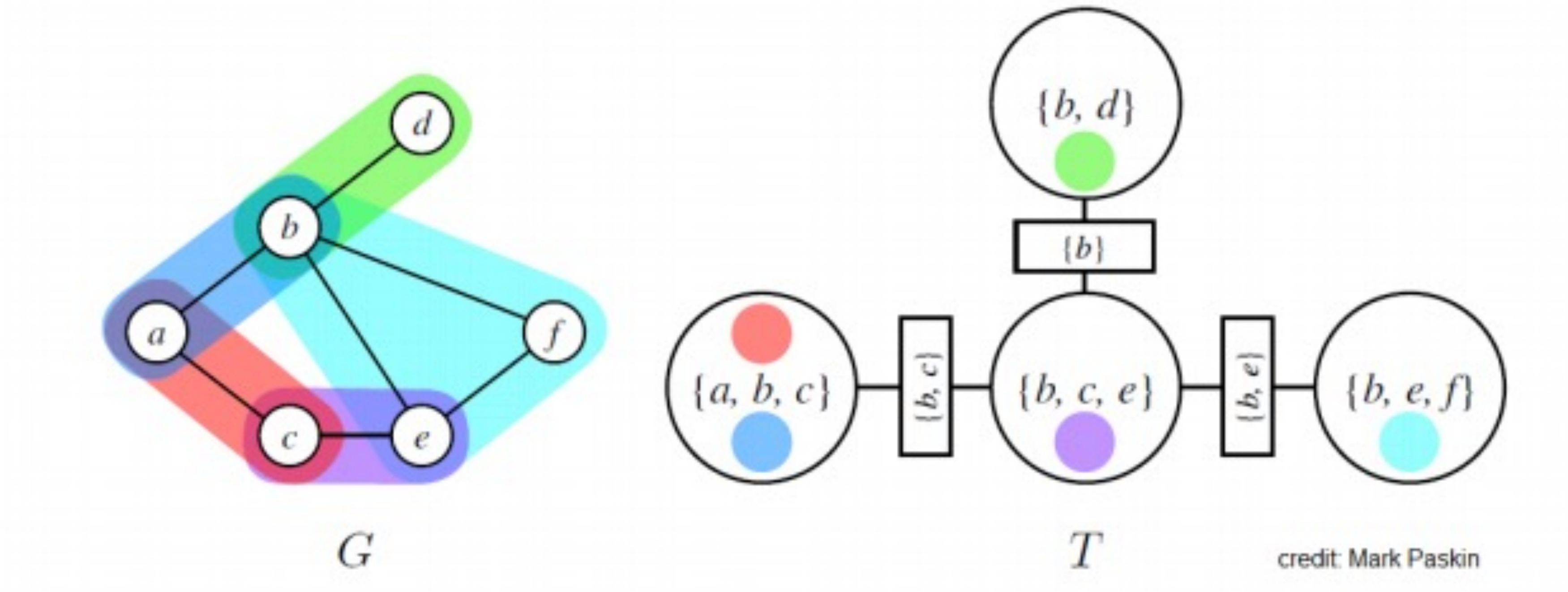


- Let F be a set of potentials with a triangulated domain graph. A junction tree for F is join tree for G with
  - **Each potential f in F is associated to a clique containing dom(f)**
  - Each link has separator attached containing two mailboxes, one for each direction



Works naturally for Markov networks

Family preservation: For each factor f, there is a cluster c such that dom(f)⊆c.



credit: Mark Paskin

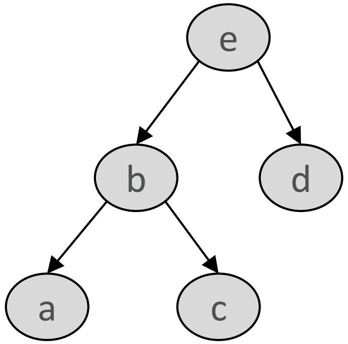
Optimal Junction Trees

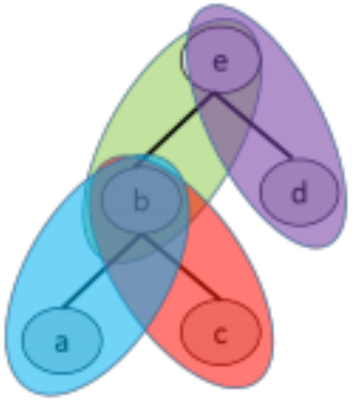
We may always find a **trivial junction tree** with one node containing all the variables in the original graph. However, such trees are useless because they will not result in efficient marginalization algorithms.

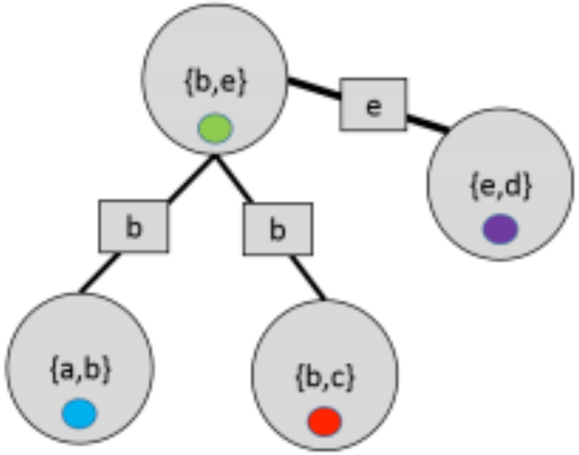
Optimal trees are ones that make the clusters as small and modular as possible; unfortunately, it is again NP-hard to find the optimal tree. We will see below some practical ways in which we can find good junction trees.

Junction tree of tree-structure BN

A special case when we can find the optimal junction tree is when the model itself is a tree. Then, we may define a cluster for each edge in the tree.



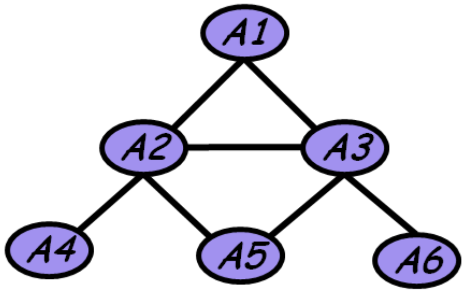




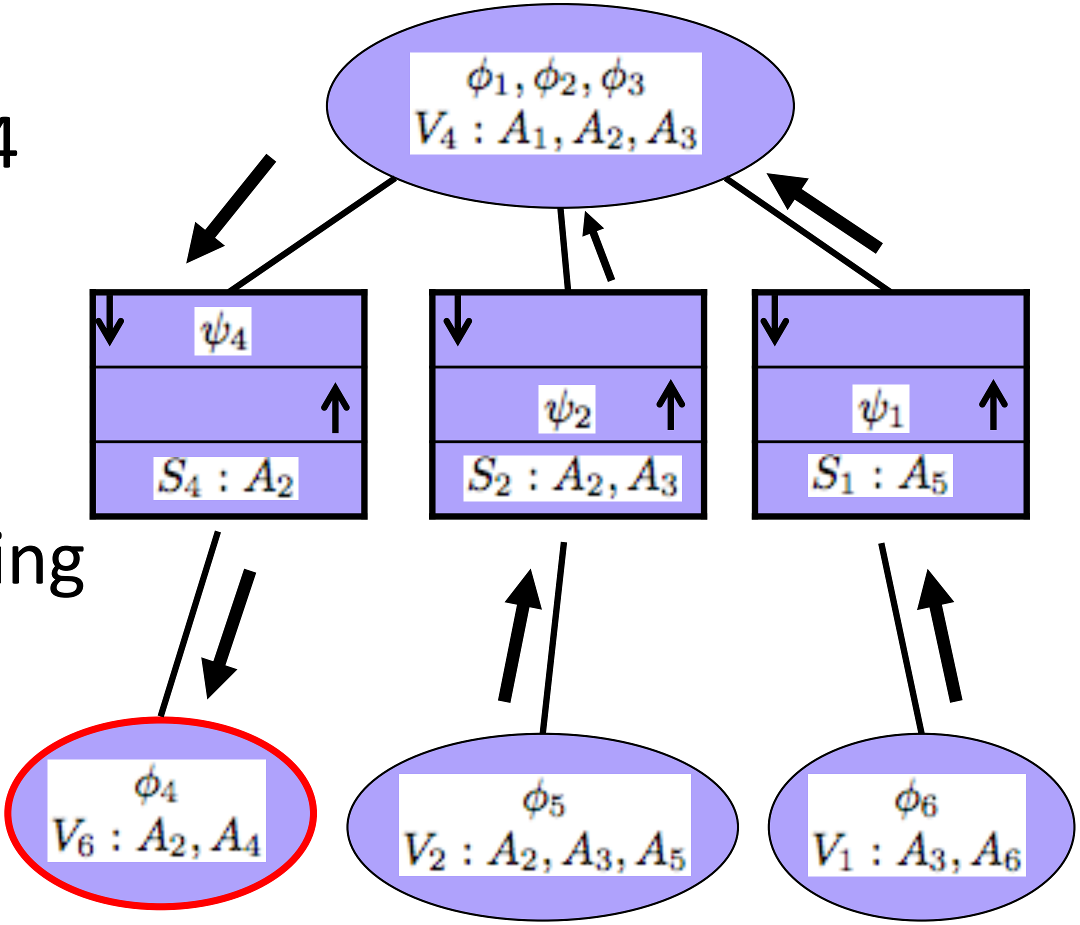
Propagation on a Junction Tree

- Node V can send exactly one message to a neighbour W, and it may only be sent when V has received a message from all of its other neighbours
- Choose one clique (arbitrarily) as a root of the tree; collect message to this node and then distribute messages away from it.
- After collection and distribution phases, we have all we need in each clique to compute potential for variables.

Junction Trees - Collect Evidence



- P(A4) ?
- Find clique containing A4
- V6 temporary root
- Send messages from leaves to root
- V4 assembles the incoming messages, potential



Junction Tree (for Bayesian networks) - Messages

- Propagation/message passing between two adjacent cliques C_1, C_2 (S_0 is their seperator)
  - Marginalize C_1's potential to get new potential for S_0

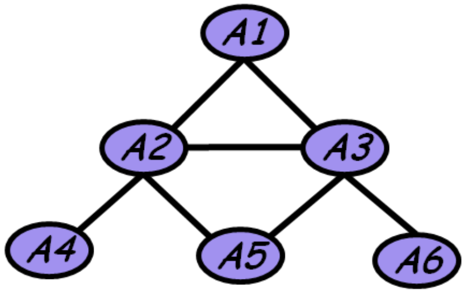
$$\varphi^*_{S_o} = \sum_{C_1 \setminus S_0} \varphi_{C_1}$$

  - Update C_2's potential

$$\varphi^*_{C_2} = \varphi_{C_2} \frac{\varphi^*_{S_0}}{\varphi_{S_0}}$$

  - Update S_0's potential to its new potential. **Initially, its potential is 1**, i.e., $\varphi^*_{C_2} = \varphi_{C_2} \varphi^*_{S_0}$
  - **That is, we sent a message** $\varphi^*_{S_o}$ **from C_1 to C_2**

Junction Trees - Collect Evidence



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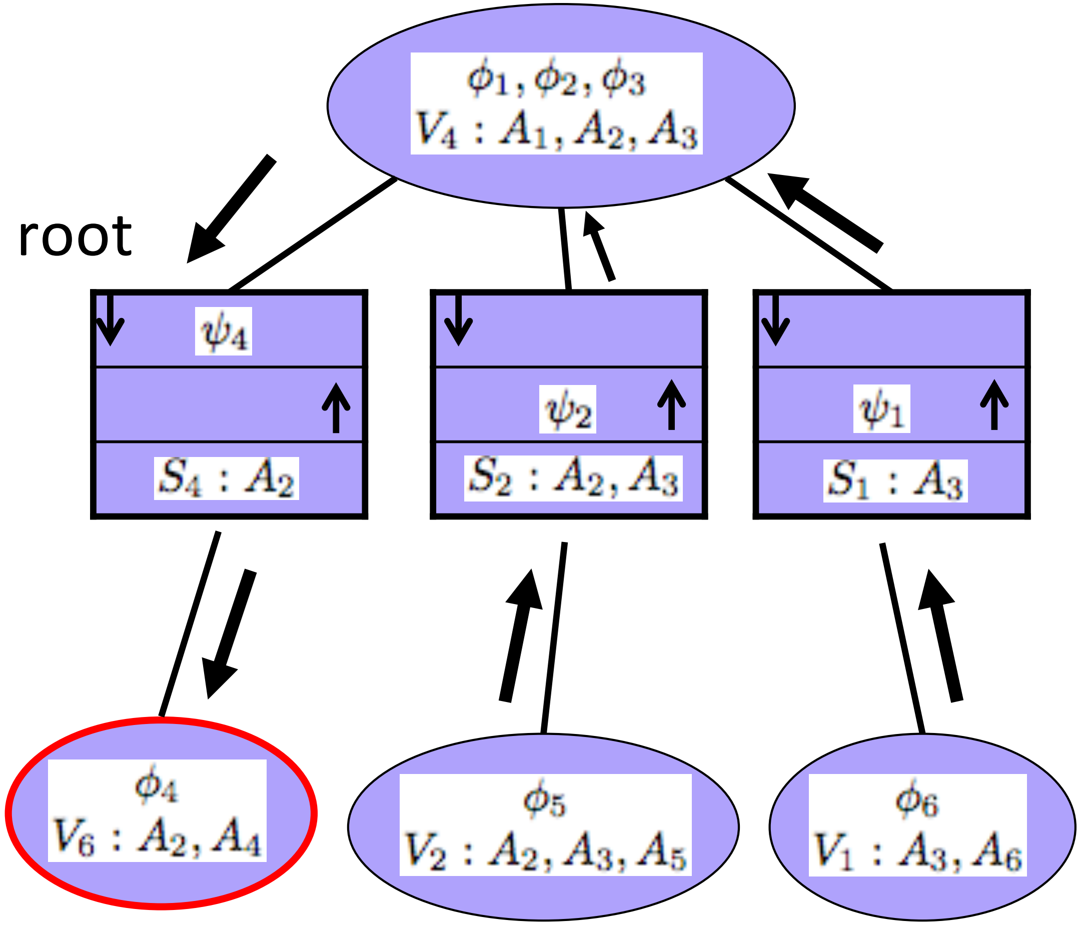
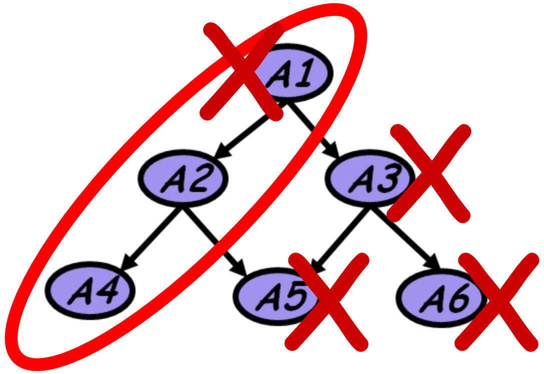


$$\varphi_1 = \sum_{V_1 - \{A_3\}} \phi_6 = \sum_{A_6} \phi_6$$

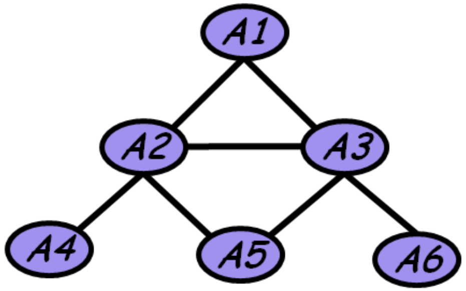
$$\varphi_2 = \sum_{V_2 - \{A_2, A_3\}} \phi_5 = \sum_{A_5} \phi_5$$

$$\psi_4 = \sum\nolimits_{A_1} \phi_1 \cdot \phi_2 \sum\nolimits_{A_3} \phi_3 \cdot \psi_2 \cdot \psi_1$$

(recall, the sperators potential is initialy 1)



This is VE !



First, we have

$$\varphi_1 = \sum_{V_1 - \{A_3\}} \phi_6 = \sum_{A_6} P(A_6 \mid A_3) = 1$$

$$\varphi_2 = \sum_{V_1 - \{A_2, A_3\}} \phi_5 = \sum_{A_5} P(A_5 \mid A_2, A_3) = 1$$

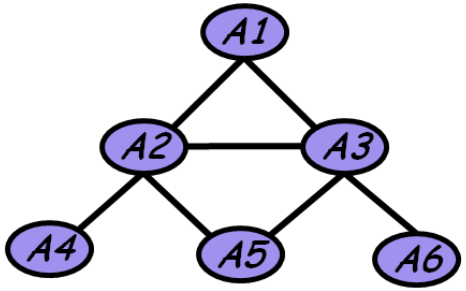
So, we have eliminated A5 and A6

Then

$$\varphi_4 = \sum_{A_1} \phi_1 \cdot \phi_2 \cdot \sum_{A_3} \phi_3 \cdot \varphi_1 \cdot \varphi_2 = \sum_{A_1} \phi_1 \cdot \phi_2 \cdot \sum_{A_3} \phi_3 = \sum_{A_1} \phi_1 \cdot \phi_2 \cdot 1$$

So, we have eliminated A3 and are in the „chain“ situation. First, we eliminate A1 and then …

Junction Trees - Collect Evidence

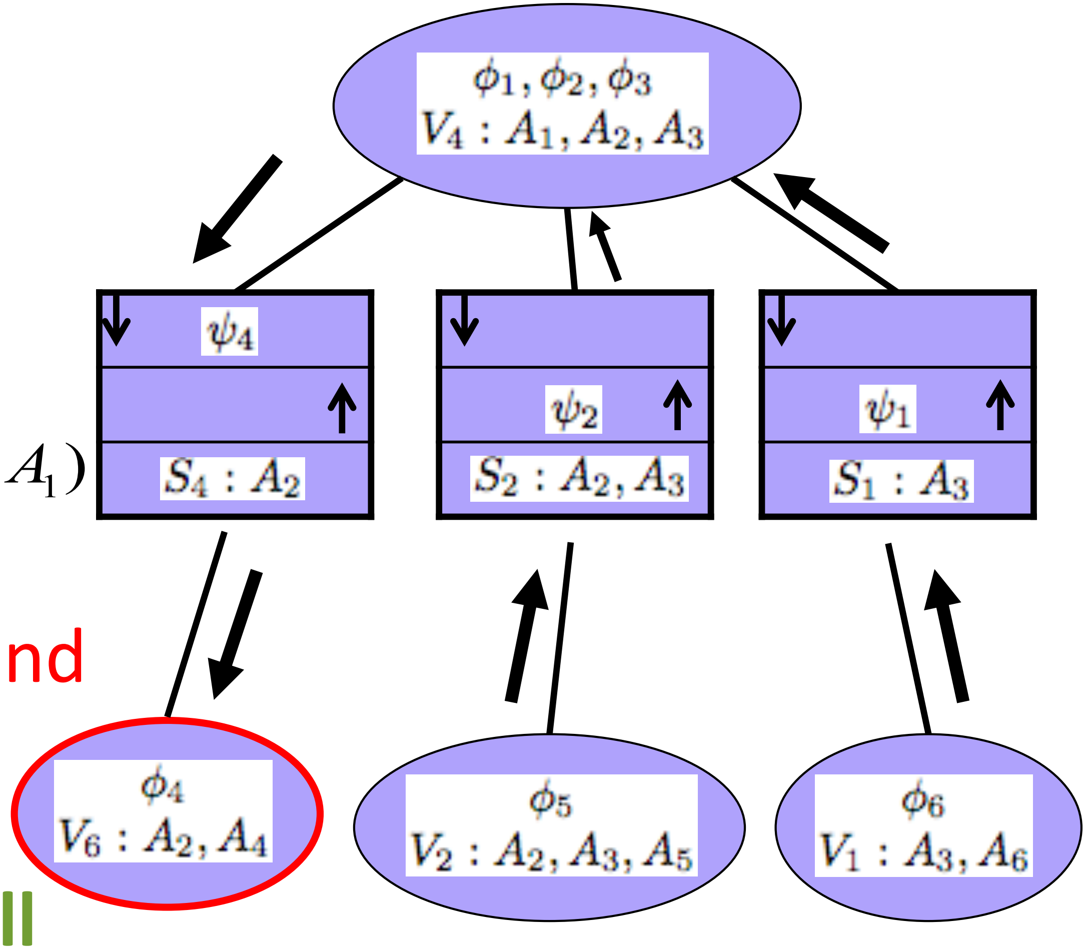


- P(A4) ?

$$P(A_4) = \sum_{A_2} \psi_4 \cdot \phi_4$$

$$P(A_4) = \sum_{A_2} \phi_4 \cdot \sum_{A_1} \phi_1 \cdot \phi_2$$

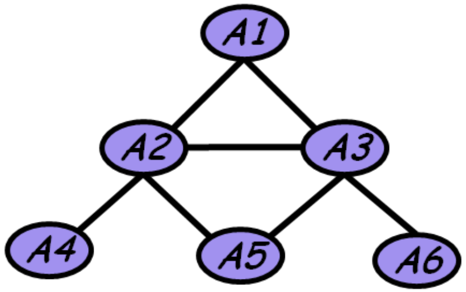
$$= \sum_{A_2} P(A_4 \mid A_2) \cdot \sum_{A_1} P(A_2 \mid A_1) \cdot P(A_1)$$



- That is, we eliminate A2 and get P(A4)

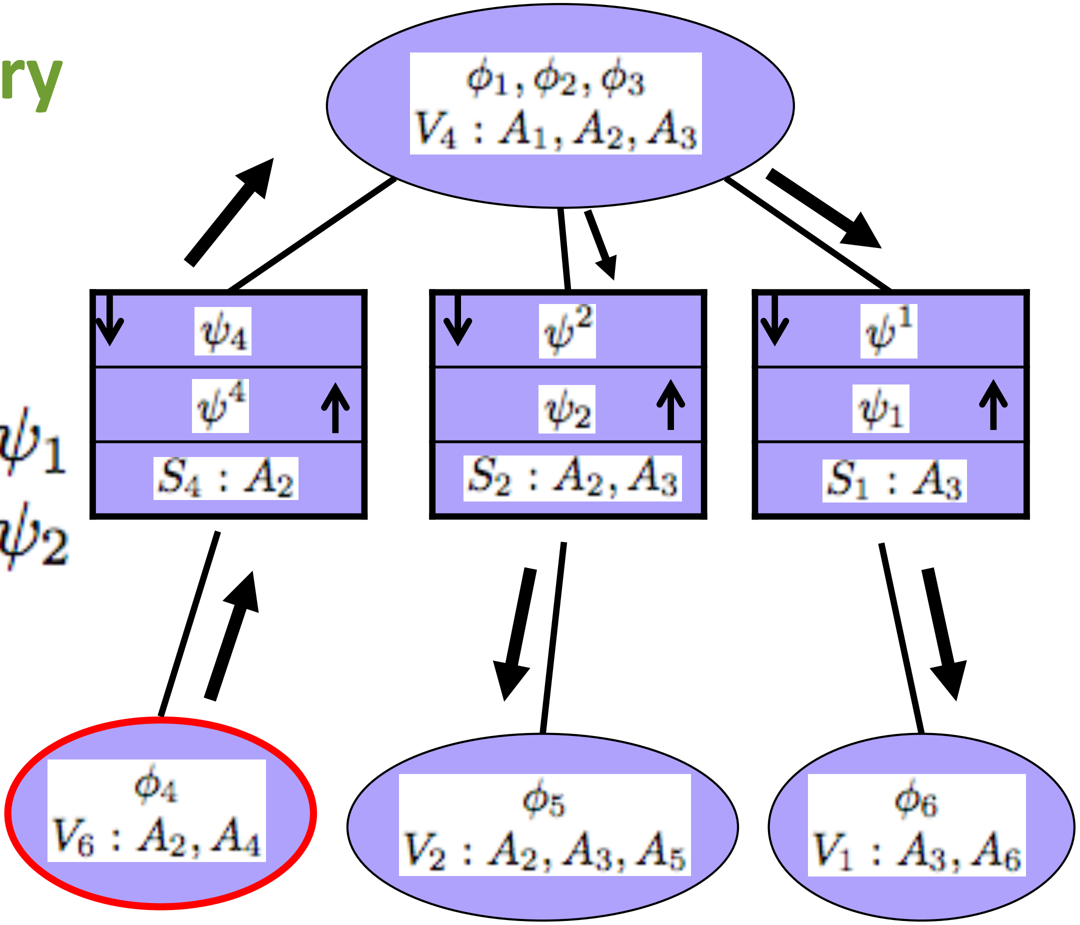
- **What about computing all marginals?**

Junction Trees - Distribute Evidence



- All marginals? **Same story**

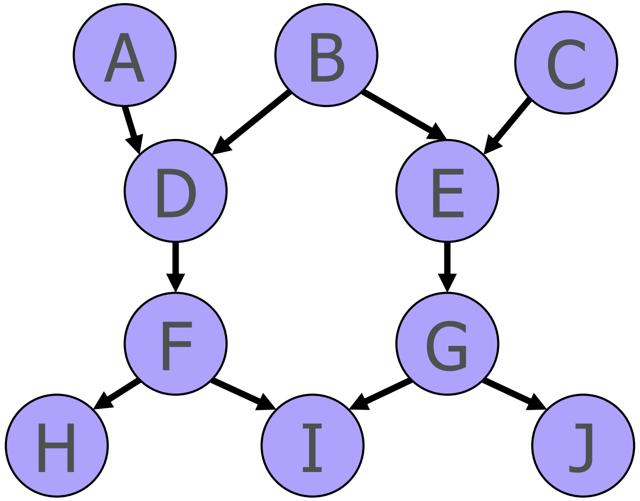
$$
\begin{aligned}
\psi^4 &= \textstyle\sum_{A_2} \phi_4 \\
\psi^2 &= \psi^4 \cdot (\textstyle\sum_{A_1} \phi_1\phi_2\phi_3) \cdot \psi_1 \\
\psi^1 &= \psi^4 \cdot (\textstyle\sum_{A_1} \phi_1\phi_2\phi_3) \cdot \psi_2 \\
P(A_3) &= \textstyle\sum_{A_6} \phi_6 \cdot \psi^1 \\
P(A_6) &= \textstyle\sum_{A_3} \phi_6 \cdot \psi^1 \\
&\ldots
\end{aligned}
$$

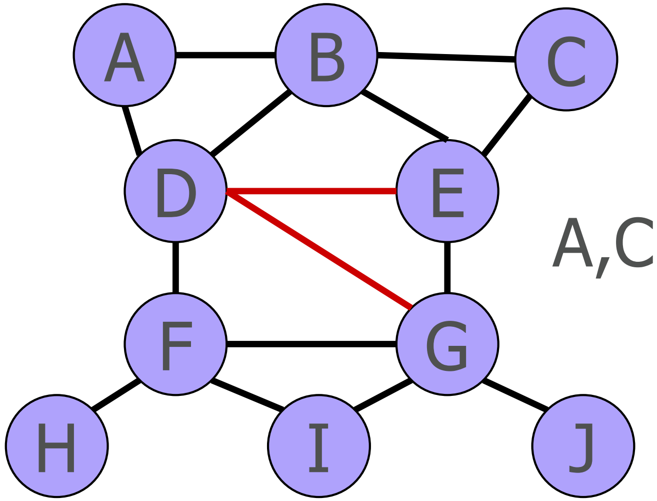


Same can be done for undirected models. Separators also account for their own potentials

Nontriangulated Domain Graphs

- Embed domain graph in a traingulated graph
- Use its junction tree
- Simple idea:
  - Eliminate variables in some order
  - If you wish to eliminate a node with non-complete neighbour set, make it complete by adding fill-ins





A,C,H,I,J,B,G,D,E,F

Summary JTA

- Convert Bayesian network into JT
- Initialize potentials and separators
- Incorporate Evidence (set potentials accordingly)
- Collect and distribute evidence
- Obtain clique marginals by marginalization/normalization

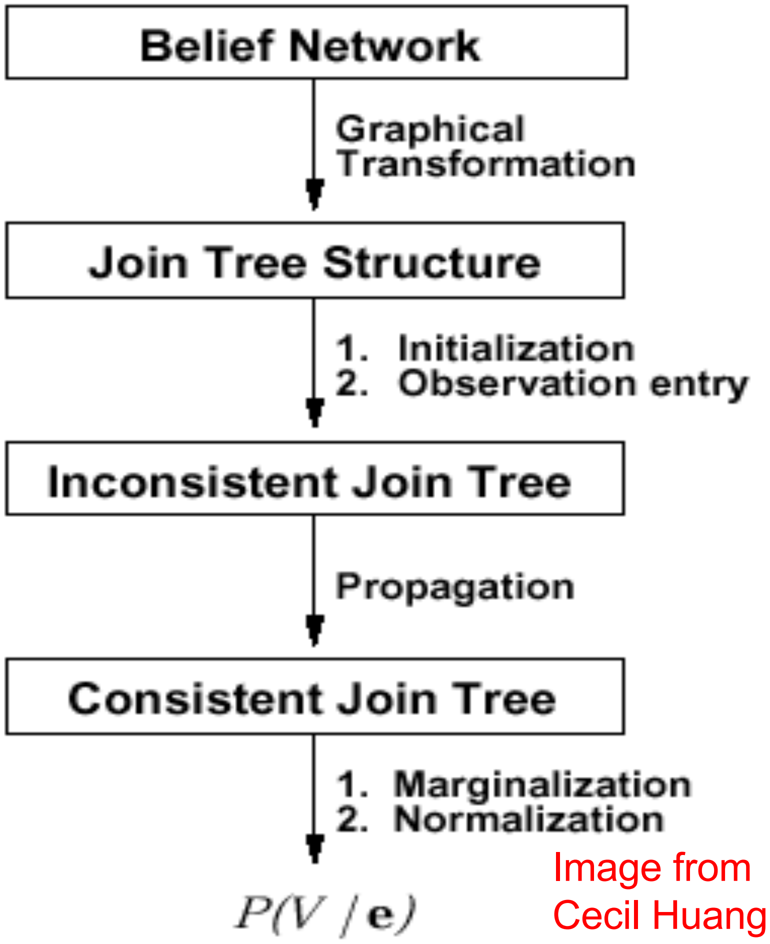


Image from Cecil Huang

Inference Engines

- (Commercial) HUGIN : http://www.hugin.com
- (Commercial) NETICA: http://www.norsys.com
- Bayesian Network Toolbox for Matlab
  www.cs.ubc.ca/~murphyk/Software/BNT/bnt.html
- GENIE/SMILE (JAVA) http://www2.sis.pitt.edu/~genie/
- MSBNx, Microsoft, http://research.microsoft.com/adapt/MSBNx/
- LibDAI http://people.kyb.tuebingen.mpg.de/jorism/libDAI/
- OpenGM2 http://hciweb2.iwr.uni-heidelberg.de/opengm/