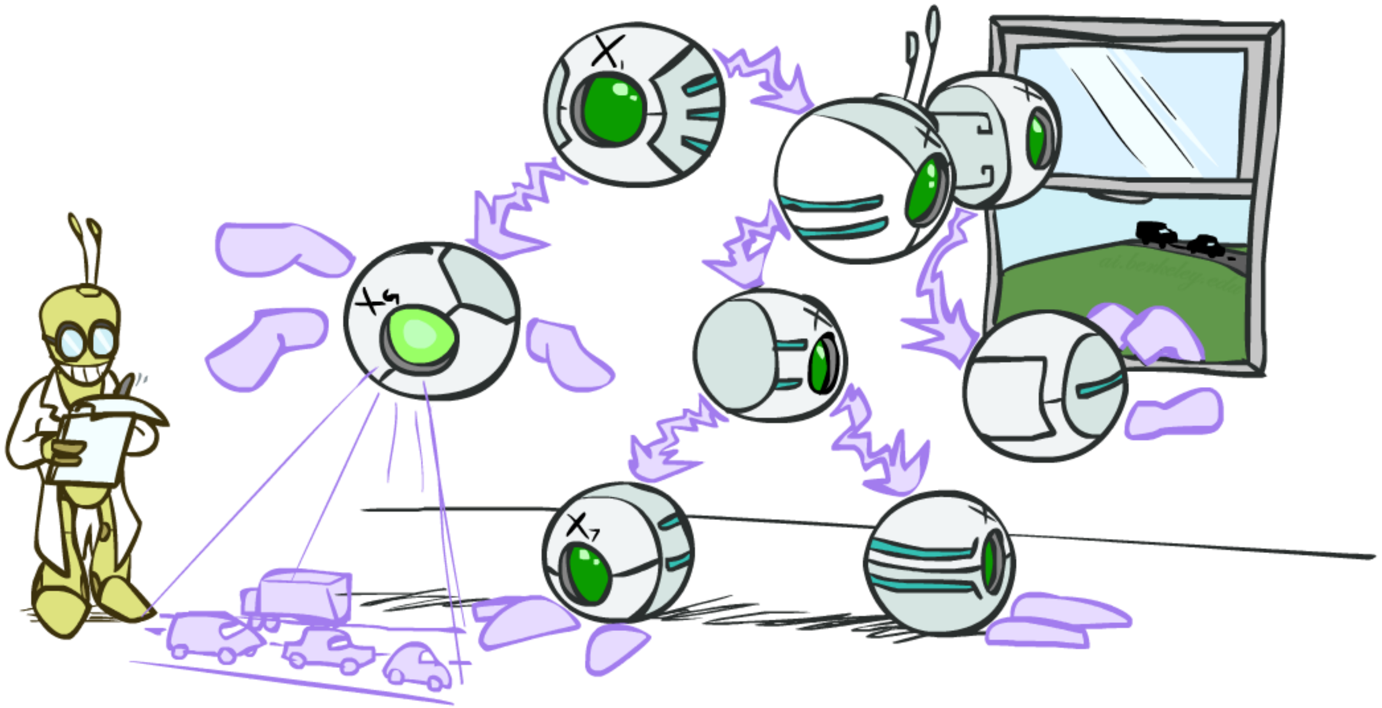
Bayes Nets: Exact Inference



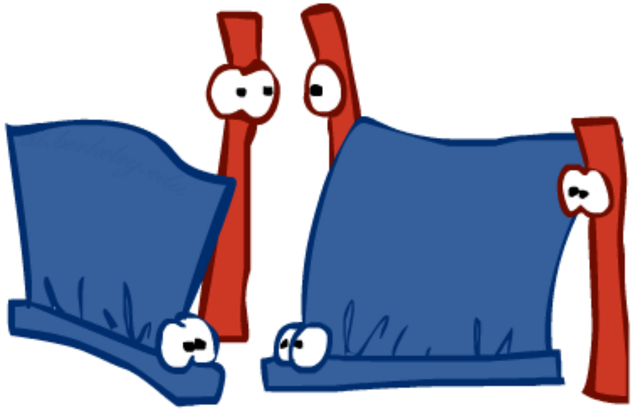
AIMA Chapter 14.4, PRML Chapter 8.4

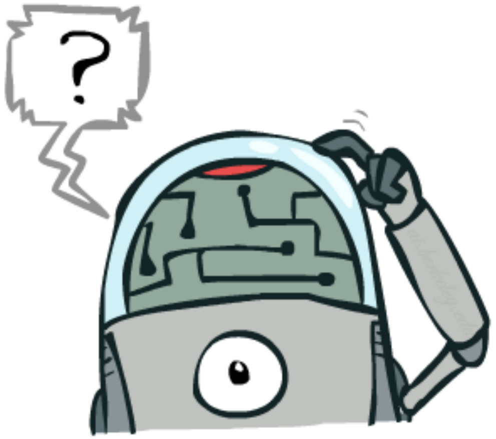
[Adapted from slides by Dan Klein and Pieter Abbeel at UC Berkeley]

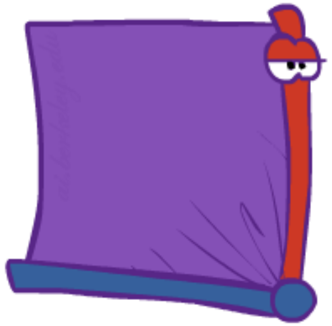
Inference

- Inference: calculating some useful quantity from a probabilistic model (joint probability distribution)

- Examples:
  - Posterior marginal probability
    - $P(Q|e_1,..,e_k)$
    - E.g., what disease might I have?
  - Most likely explanation:
    - $\text{argmax}_q\ P(Q=q|e_1,..,e_k)$
    - E.g., what did he say?







Inference by Enumeration

- General case:
  - Evidence variables: $E_1 \ldots E_k = e_1 \ldots e_k$
  - Query variable: Q
  - Hidden variables: $H_1 \ldots H_r$

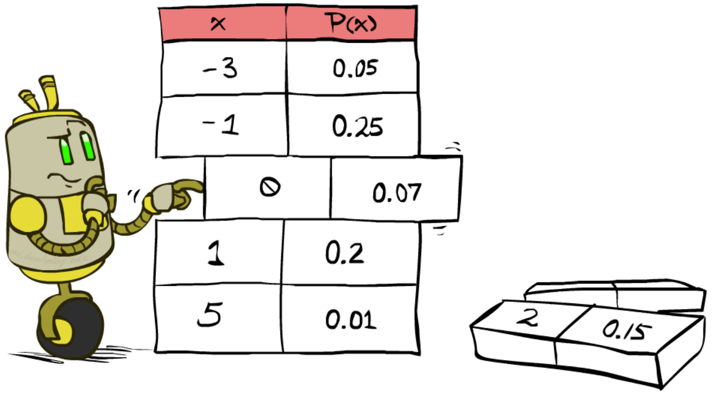
$\left.\begin{matrix} \\ \\ \\ \end{matrix}\right\} \; X_1, X_2, \ldots X_n$

All variables

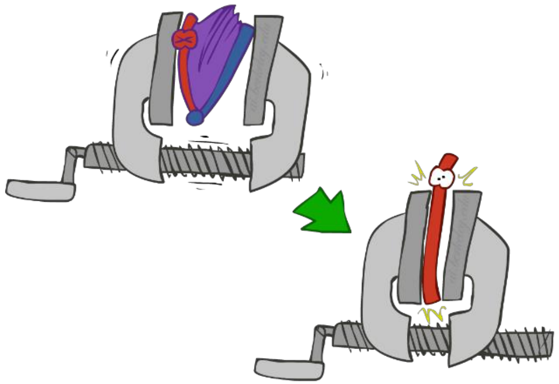
- We want:

$$P(Q|e_1 \ldots e_k)$$

- Step 1: Select the entries consistent with the evidence



- Step 2: Sum out H to get joint of Query and evidence



$$P(Q, e_1 \ldots e_k) = \sum_{h_1 \ldots h_r} \underbrace{P(Q, h_1 \ldots h_r, e_1 \ldots e_k)}_{X_1, X_2, \ldots X_n}$$

- Step 3: Normalize

$$\times \frac{1}{Z}$$

$$Z = \sum_q P(Q, e_1 \cdots e_k)$$

$$P(Q|e_1 \cdots e_k) = \frac{1}{Z} P(Q, e_1 \cdots e_k)$$

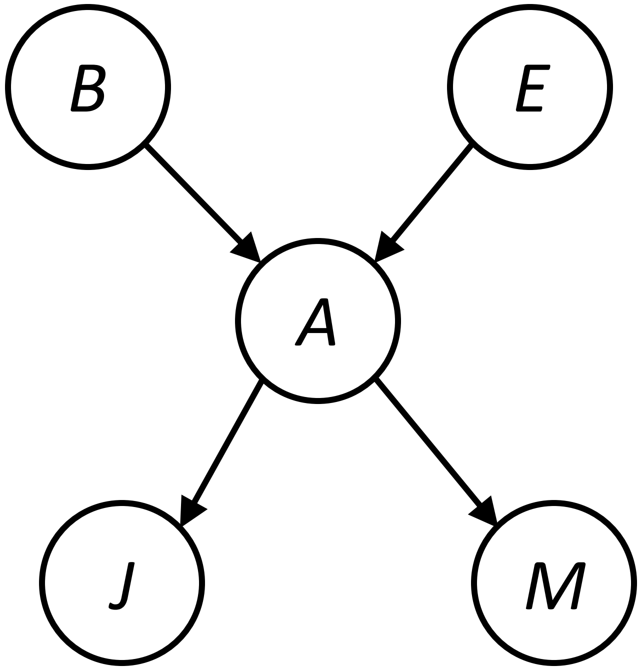
Inference by Enumeration in Bayes Net

- The joint distribution can be computed from a BN by multiplying the conditional distributions
- Then we can do inference by enumeration

$$P(B \mid +j, +m) \ \propto_B P(B, +j, +m)$$

$$= \sum_{e,a} P(B, e, a, +j, +m)$$

$$= \sum_{e,a} P(B)P(e)P(a|B,e)P(+j|a)P(+m|a)$$



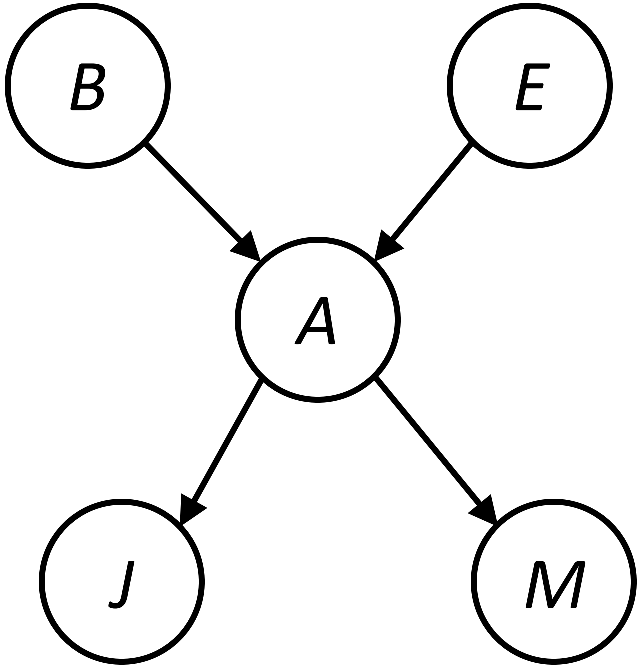
- Problem: sums of ***exponentially many*** products!

Inference by Enumeration in Bayes Net

$$P(B \mid +j, +m) \;\propto_B P(B, +j, +m)$$

$$= \sum_{e,a} P(B, e, a, +j, +m)$$

$$= \sum_{e,a} P(B)P(e)P(a|B,e)P(+j|a)P(+m|a)$$



$$=P(B)P(+e)P(+a|B,+e)P(+j|+a)P(+m|+a) + P(B)P(+e)P(-a|B,+e)P(+j|-a)P(+m|-a)$$
$$+P(B)P(-e)P(+a|B,-e)P(+j|+a)P(+m|+a) + P(B)P(-e)P(-a|B,-e)P(+j|-a)P(+m|-a)$$

Lots of repeated subexpressions!

Can we do better?

- Consider **uwy + uwz + uxy + uxz + vwy + vwz + vxy +vxz**
  - 16 multiplies, 7 adds
  - Lots of repeated subexpressions!
- Rewrite as **(u+v)(w+x)(y+z)**
  - 2 multiplies, 3 adds
- Idea: Move summations inwards as far as possible

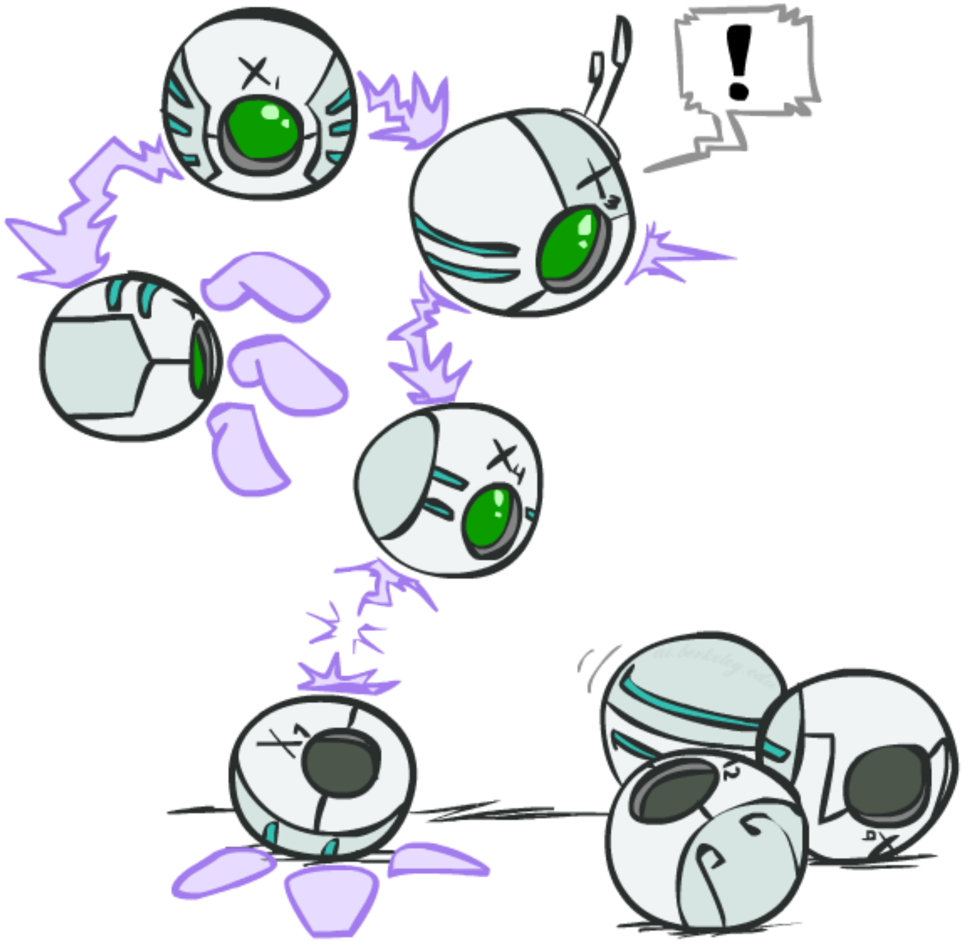
Variable elimination: The basic ideas

- Move summations inwards as far as possible
  - $P(B \mid j, m) = \alpha \sum_{e,a} P(B)\, P(e)\, P(a|B,e)\, P(j|a)\, P(m|a)$

    $= \alpha\, P(B) \sum_{e} P(e) \sum_{a} P(a|B,e)\, P(j|a)\, P(m|a)$

  - Note: $P(a|B,e)$ isn't a single number, it's a bunch of different numbers depending on the values of a, B and e
  - It's clearer to view the computation with operations on ***factors*** (arrays of numbers)

Operations on Factors



Factors

- A factor is a multi-dimensional array to represent $P(Y_1 \dots Y_N \mid X_1 \dots X_M)$
  - If a variable is assigned (represented with lower-case), its dimension is missing from the array

- Joint distribution: P(X,Y)
  - Entries P(x,y) for all x, y
  - Sums to 1

$$P(T,W)$$

T	W	P
hot	sun	0.4
hot	rain	0.1
cold	sun	0.2
cold	rain	0.3

- Selected joint: P(x,Y)
  - A slice of the joint distribution
  - Entries P(x,y) for fixed x, all y
  - Sums to P(x)

$$P(cold,W)$$

T	W	P
cold	sun	0.2
cold	rain	0.3

Factors

- A factor is a multi-dimensional array to represent $P(Y_1 \ldots Y_N \mid X_1 \ldots X_M)$
  - If a variable is assigned (represented with lower-case), its dimension is missing from the array

- Single conditional: P(Y | x)
  - Entries P(y | x) for fixed x, all y
  - Sums to 1

$$P(W|cold)$$

T	W	P
cold	sun	0.4
cold	rain	0.6

- Family of conditionals: P(X |Y)
  - Multiple conditionals
  - Entries P(x | y) for all x, y
  - Sums to |Y|

$$P(W|T)$$

T	W	P
hot	sun	0.8
hot	rain	0.2
cold	sun	0.4
cold	rain	0.6

$P(W|hot)$

$P(W|cold)$

Factors

- A factor is a multi-dimensional array to represent $P(Y_1 \ldots Y_N \mid X_1 \ldots X_M)$
  - If a variable is assigned (represented with lower-case), its dimension is missing from the array
    - Specified family: P(y | X)
      - Entries P(y | x) for fixed y, but for all x
      - Sums to … who knows!

$P(rain|T)$

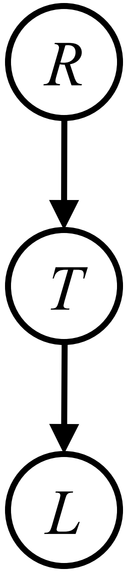
T	W	P
hot	rain	0.2
cold	rain	0.6

$\} P(rain|hot)$

$\} P(rain|cold)$

Running Example: Traffic Domain

- Random Variables
  - R: Raining
  - T: Traffic
  - L: Late



$P(R)$

+r	0.1
-r	0.9

$P(T|R)$

+r	+t	0.8
+r	-t	0.2
-r	+t	0.1
-r	-t	0.9

$P(L|T)$

+t	+l	0.3
+t	-l	0.7
-t	+l	0.1
-t	-l	0.9

Running Example: Traffic Domain

- Initial factors are local CPTs (one per node)

$P(R)$

+r	0.1
-r	0.9

$P(T|R)$

+r	+t	0.8
+r	-t	0.2
-r	+t	0.1
-r	-t	0.9

$P(L|T)$

+t	+l	0.3
+t	-l	0.7
-t	+l	0.1
-t	-l	0.9

- Any known values are selected
  - E.g. if we know $L = +\ell$, the initial factors are

$P(R)$

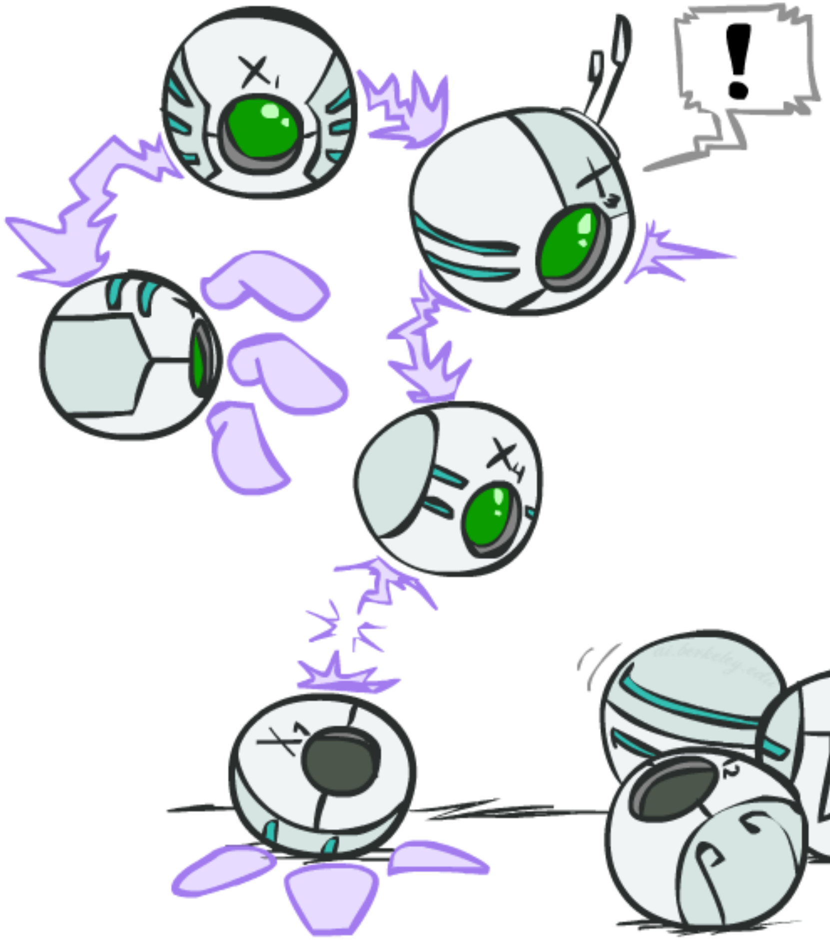
+r	0.1
-r	0.9

$P(T|R)$

+r	+t	0.8
+r	-t	0.2
-r	+t	0.1
-r	-t	0.9

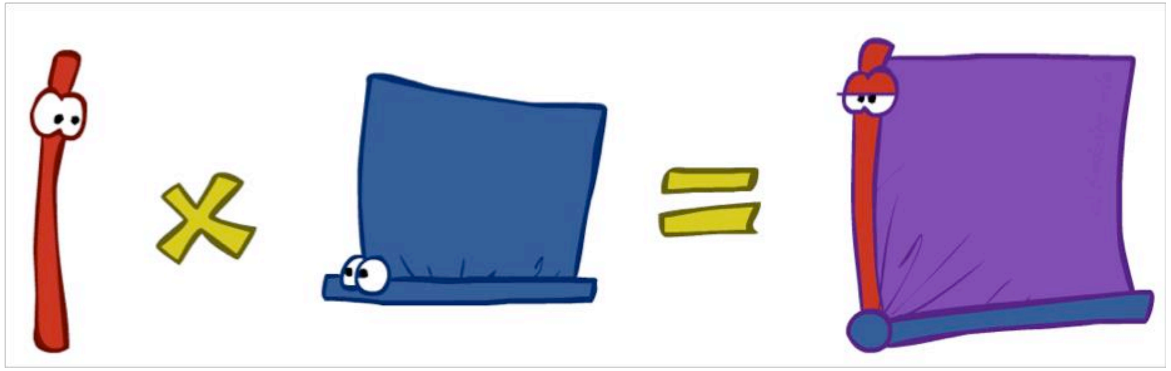
$P(+\ell|T)$

+t	+l	0.3
-t	+l	0.1

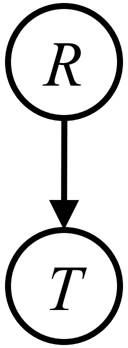


Operation 1: Join Factors

- First basic operation: joining factors
  - Just like a database join
  - Given multiple factors, build a new factor over the union of the variables involved
  - Each entry is computed by pointwise products



- Example:

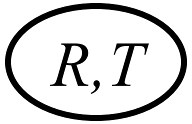


$$P(R) \times P(T|R) \quad \Rightarrow \quad P(R,T)$$

+r	0.1
-r	0.9

+r	+t	0.8
+r	-t	0.2
-r	+t	0.1
-r	-t	0.9

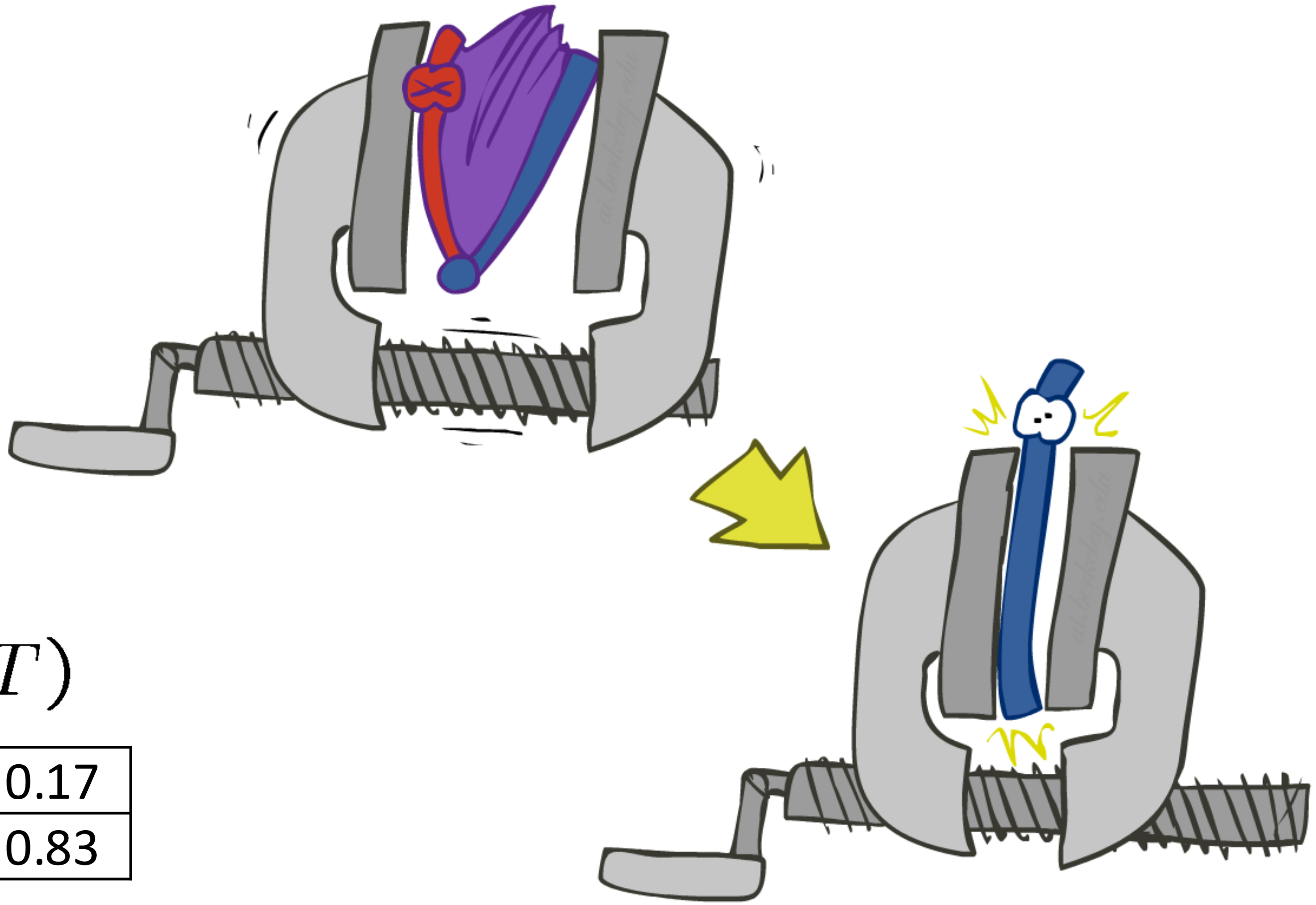
+r	+t	0.08
+r	-t	0.02
-r	+t	0.09
-r	-t	0.81



$$\forall r, t : \quad P(r,t) = P(r) \cdot P(t|r)$$

Operation 2: Eliminate

- Second basic operation: eliminating a variable
  - Take a factor and sum out (marginalize) a variable
- Example:



$P(R,T)$

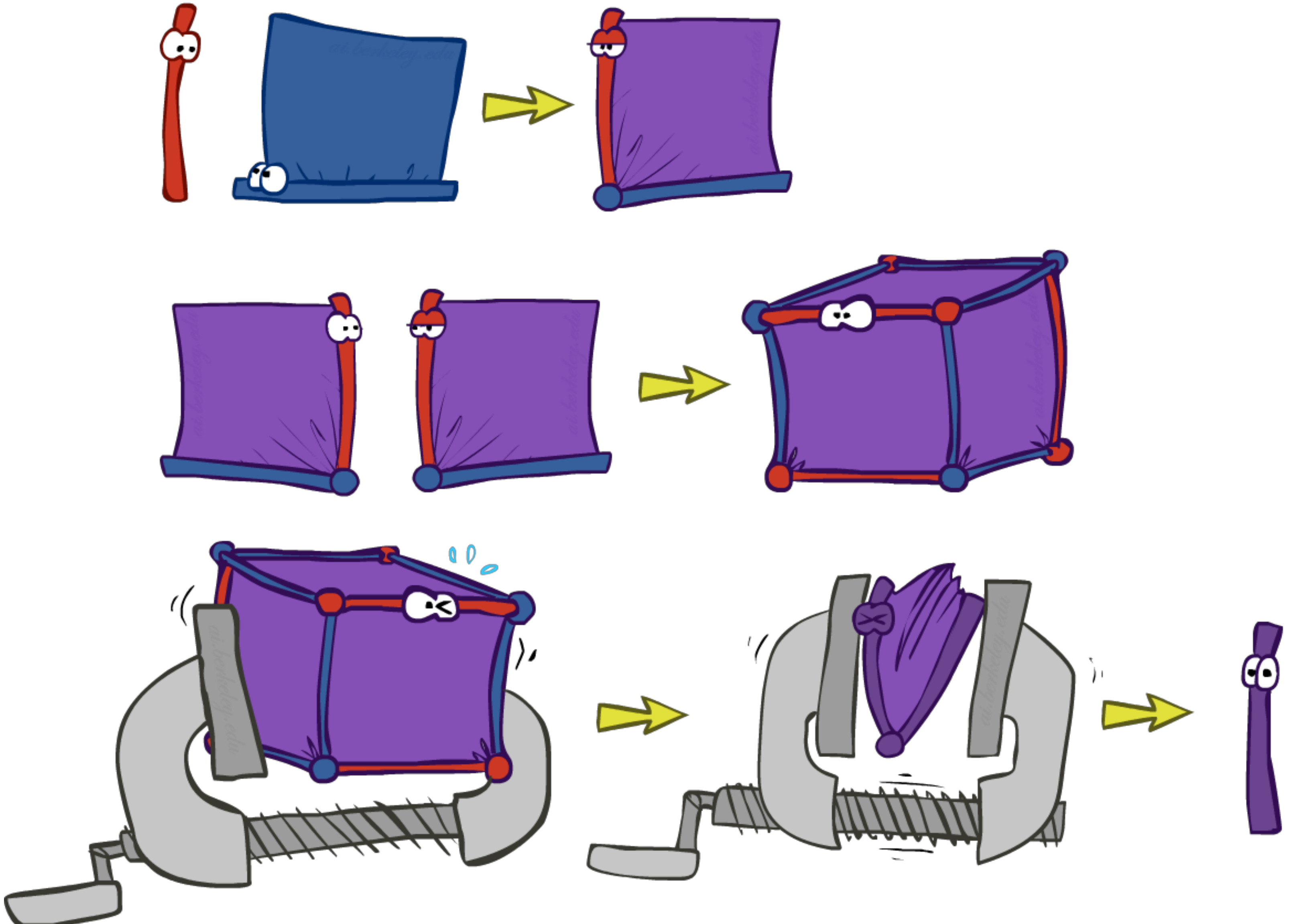
+r	+t	0.08
+r	-t	0.02
-r	+t	0.09
-r	-t	0.81

sum R →

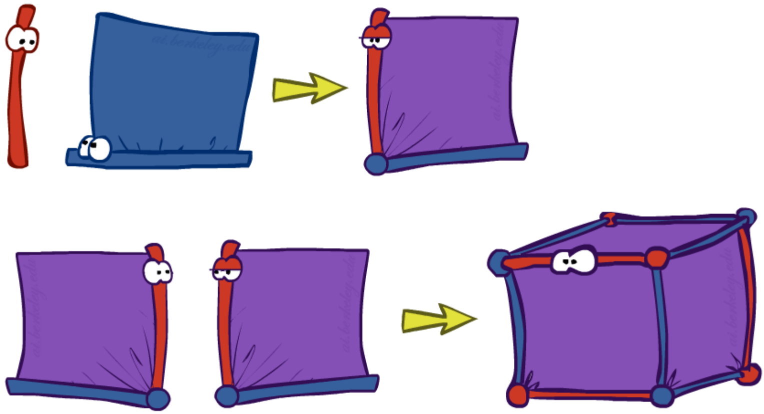
$P(T)$

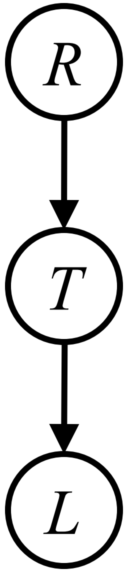
+t	0.17
-t	0.83

Inference by Enumeration in BN = Multiple Join + Multiple Eliminate



Computing $P(L)$: Multiple Joins





$P(R)$

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$P(T|R)$

+r	+t	0.8
+r	-t	0.2
-r	+t	0.1
-r	-t	0.9

$P(L|T)$

+t	+l	0.3
+t	-l	0.7
-t	+l	0.1
-t	-l	0.9

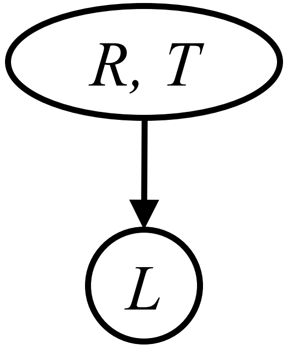
Join

$P(R,T)$

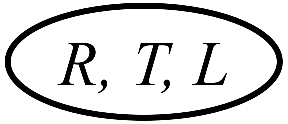
+r	+t	0.08
+r	-t	0.02
-r	+t	0.09
-r	-t	0.81

$P(L|T)$

+t	+l	0.3
+t	-l	0.7
-t	+l	0.1
-t	-l	0.9



Join



$P(R,T,L)$

+r	+t	+l	0.024
+r	+t	-l	0.056
+r	-t	+l	0.002
+r	-t	-l	0.018
-r	+t	+l	0.027
-r	+t	-l	0.063
-r	-t	+l	0.081
-r	-t	-l	0.729

Computing $P(L)$: Multiple Elimination

R, T, L → T, L → L

$P(R,T,L)$

+r	+t	+l	0.024
+r	+t	-l	0.056
+r	-t	+l	0.002
+r	-t	-l	0.018
-r	+t	+l	0.027
-r	+t	-l	0.063
-r	-t	+l	0.081
-r	-t	-l	0.729

A factor of exponential size!

Sum out R

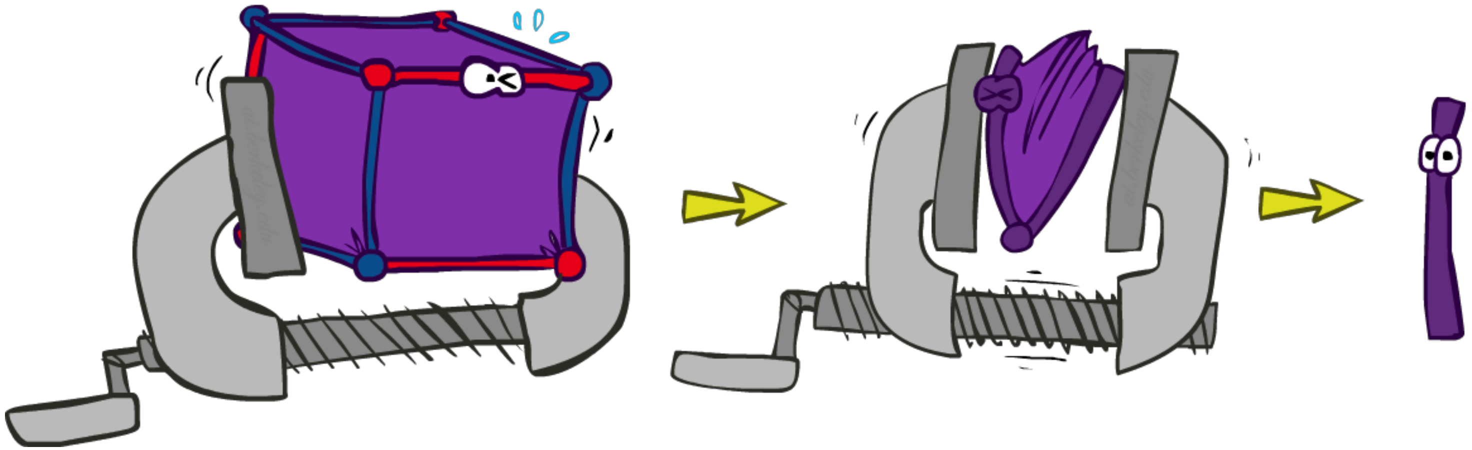
$P(T,L)$

+t	+l	0.051
+t	-l	0.119
-t	+l	0.083
-t	-l	0.747

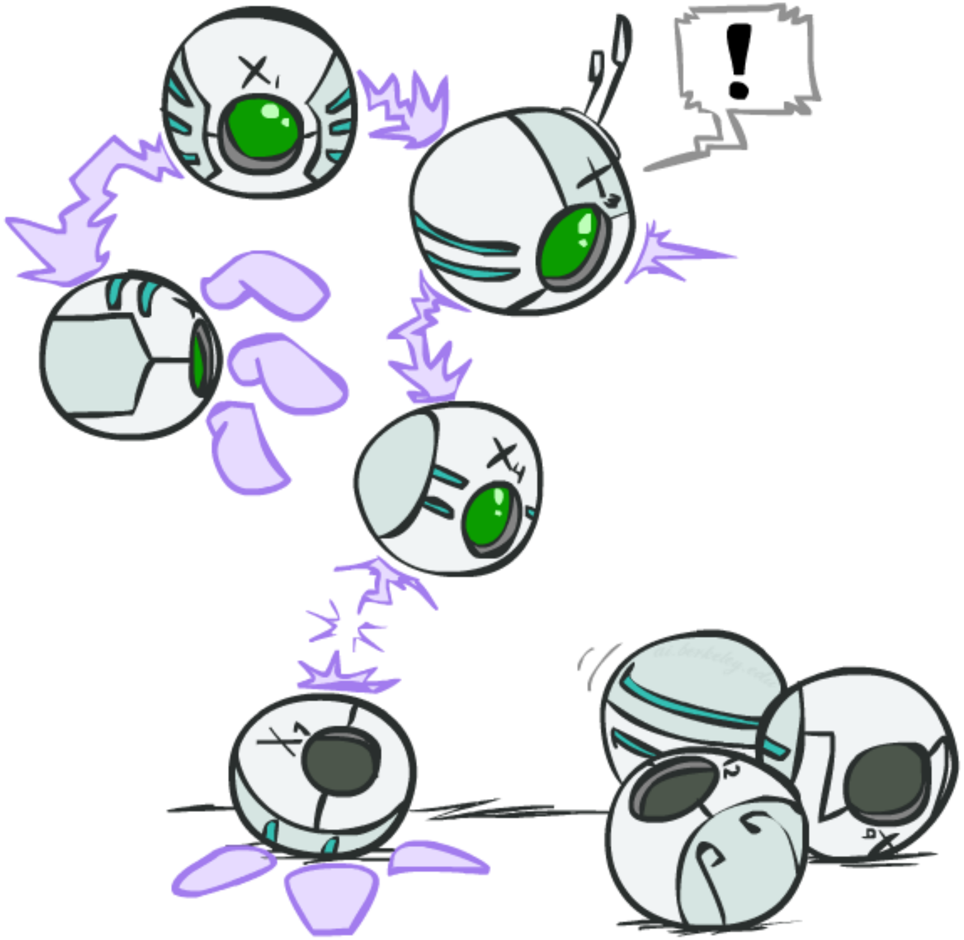
Sum out T

$P(L)$

+l	0.134
-l	0.866

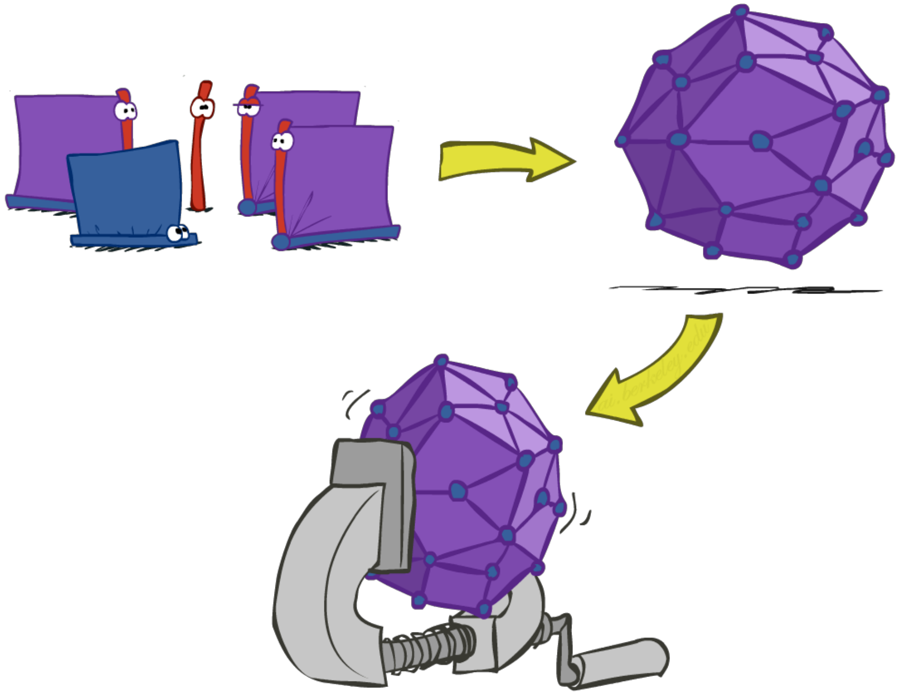


Variable Elimination

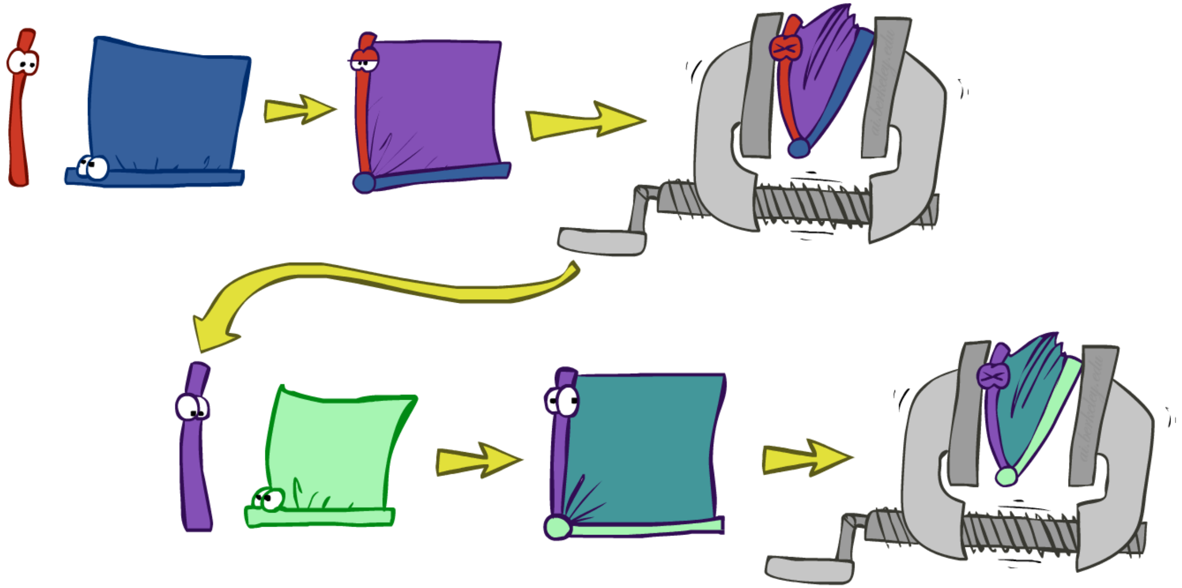


Inference by Enumeration vs. Variable Elimination

- Why is inference by enumeration so slow?
  - You join up the whole joint distribution before you sum out the hidden variables



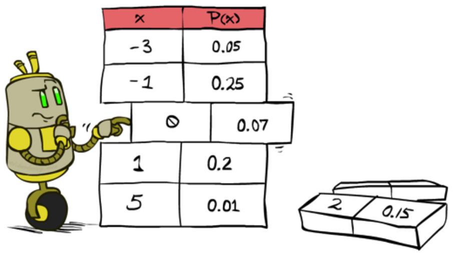
- Idea: interleave joining and elimination!
  - Called "Variable Elimination"
  - Still NP-hard, but usually much faster than inference by enumeration



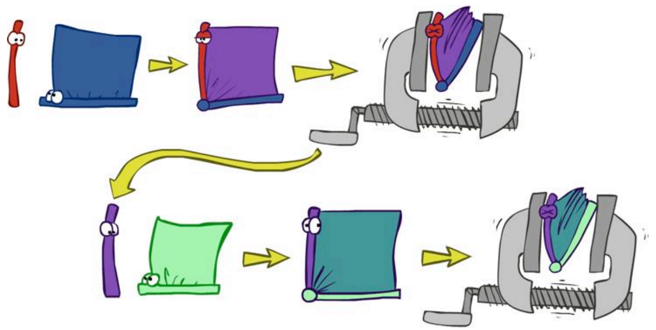
Variable Elimination

- Query: $P(Q|E_1 = e_1, \dots E_k = e_k)$

- Start with initial factors:
  - Local CPTs (but instantiated by evidence)



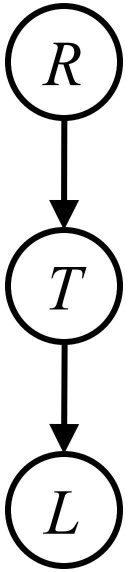
- While there are still hidden variables (not Q or evidence):
  - Pick a hidden variable H
  - Join all factors mentioning H
  - Eliminate (sum out) H



- Join all remaining factors and normalize

$\times \frac{1}{Z}$

Traffic Domain



$$P(L) = ?$$

- Inference by Enumeration

$$= \underbrace{\sum_t \underbrace{\sum_r \underbrace{P(L|t)\underbrace{P(r)P(t|r)}_{\text{Join on r}}}_{\text{Join on t}}}_{\text{Eliminate r}}}_{\text{Eliminate t}}$$

- Variable Elimination

$$= \underbrace{\sum_t \underbrace{P(L|t) \underbrace{\sum_r \underbrace{P(r)P(t|r)}_{\text{Join on r}}}_{\text{Eliminate r}}}_{\text{Join on t}}}_{\text{Eliminate t}}$$

Variable Elimination

$P(R)$

+r	0.1
-r	0.9

$P(T|R)$

+r	+t	0.8
+r	-t	0.2
-r	+t	0.1
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$P(L|T)$

+t	+l	0.3
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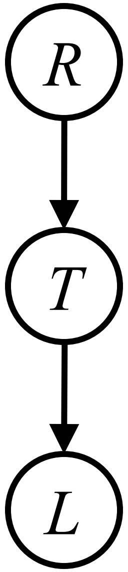

Join R

$P(R,T)$

+r	+t	0.08
+r	-t	0.02
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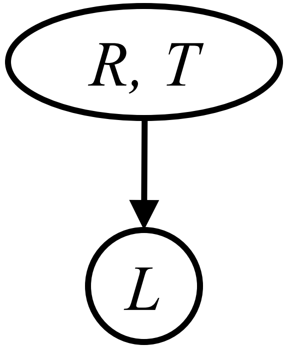


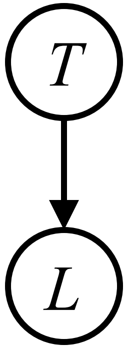
$P(L|T)$

+t	+l	0.3
+t	-l	0.7
-t	+l	0.1
-t	-l	0.9

Sum out R

$P(T)$

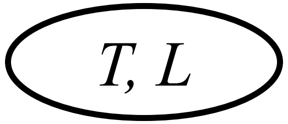
+t	0.17
-t	0.83



$P(L|T)$

+t	+l	0.3
+t	-l	0.7
-t	+l	0.1
-t	-l	0.9

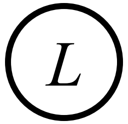
Join T



$P(T,L)$

+t	+l	0.051
+t	-l	0.119
-t	+l	0.083
-t	-l	0.747

Sum out T

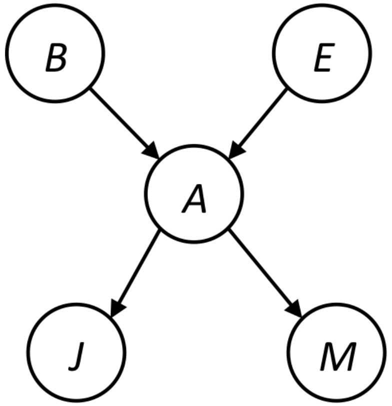


$P(L)$

+l	0.134
-l	0.866

Example

$$P(B|j,m) \propto P(B,j,m)$$



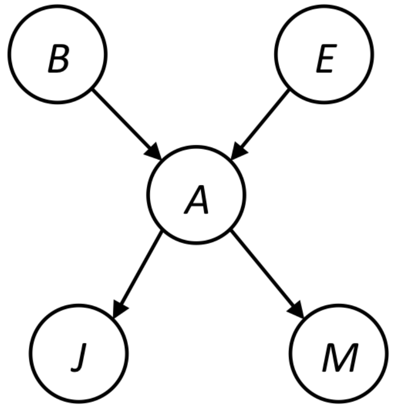
$$\boxed{P(B) \qquad P(E) \qquad P(A|B,E) \qquad P(j|A) \qquad P(m|A)}$$

Choose A

$$\begin{array}{l} P(A|B,E) \\ P(j|A) \\ P(m|A) \end{array} \xrightarrow{\times} \xrightarrow{\Sigma} P(j,m|B,E)$$

$$\boxed{P(B) \qquad P(E) \qquad P(j,m|B,E)}$$

Example



$$P(B) \qquad P(E) \qquad P(j,m|B,E)$$

Choose E

$$\left.\begin{matrix} P(E) \\ P(j,m|B,E) \end{matrix}\right. \xrightarrow{\times} \xrightarrow{\Sigma} P(j,m|B)$$

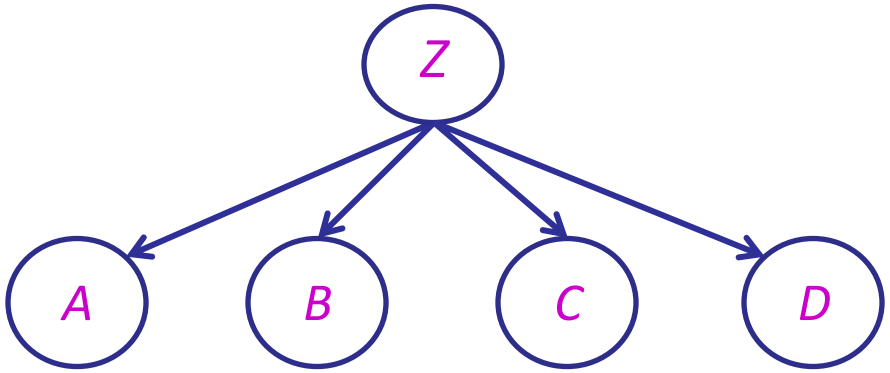
$$P(B) \qquad P(j,m|B)$$

Finish with B

$$\left.\begin{matrix} P(B) \\ P(j,m|B) \end{matrix}\right. \xrightarrow{\times} P(j,m,B) \xrightarrow{\text{Normalize}} P(B|j,m)$$

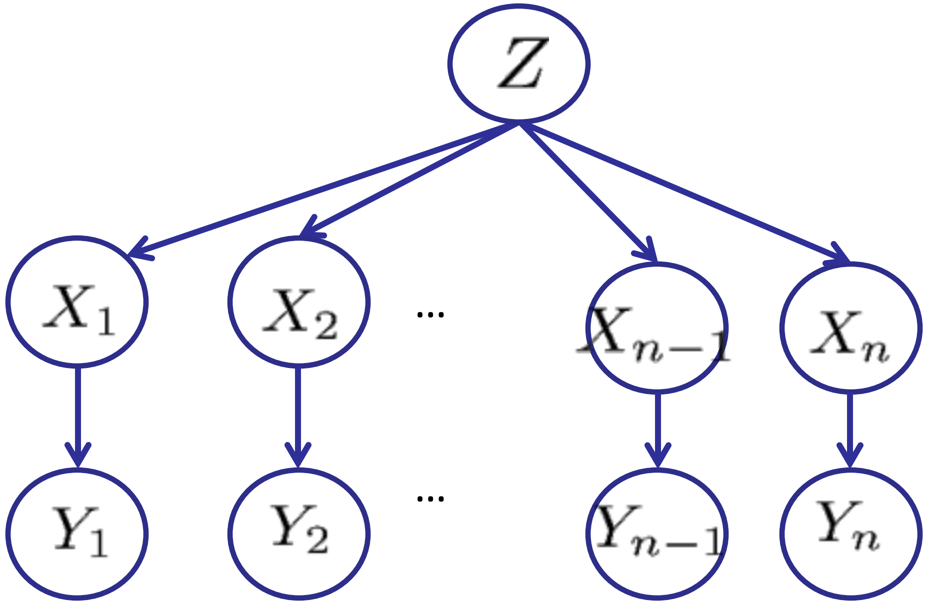
Order matters

- We care about P(D)
- What is the size of the largest factor during VE?
  - Eliminating C, B, A, Z
    - $P(D) = \alpha \sum_{z,a,b,c} P(z)\, P(a|z)\, P(b|z)\, P(c|z)\, P(D|z)$
    - $\quad = \alpha \sum_z P(z)\, P(D|z) \sum_a P(a|z) \sum_b P(b|z) \sum_c P(c|z)$
    - Largest factor during computation has 2 variables
  - Eliminating Z, C, B, A
    - $P(D) = \alpha \sum_{a,b,c,z} P(a|z)\, P(b|z)\, P(c|z)\, P(D|z)\, P(z)$
    - $\quad = \alpha \sum_a \sum_b \sum_c \sum_z P(a|z)\, P(b|z)\, P(c|z)\, P(D|z)\, P(z)$
    - Largest factor during computation has 5 variables
- With n leaves, it is 2^2 vs. 2^{n+1}



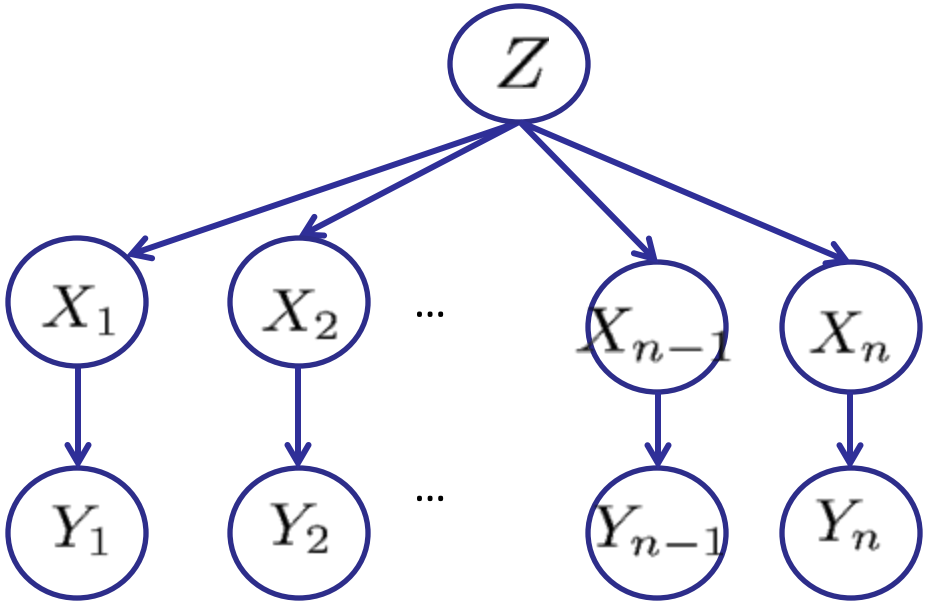
Variable Elimination Ordering

- Query: $P(X_n|y_1,\ldots,y_n)$
- Two different orderings: $Z, X_1, \ldots, X_{n-1}$ and $X_1, \ldots, X_{n-1}, Z$.
- What is the <u>size of the maximum factor</u> generated for each of the orderings?



Variable Elimination Ordering

- Z, X_1, …, X_{n-1}



$$P(Z)P(X_1|Z)P(X_2|Z),\ldots,P(X_n|Z)$$

$$\Downarrow$$

$$f_1(X_1, X_2, \ldots, X_n)$$

$$\Downarrow$$

$$f_2(y_1, X_2, \ldots, X_n)$$

$$\Downarrow$$

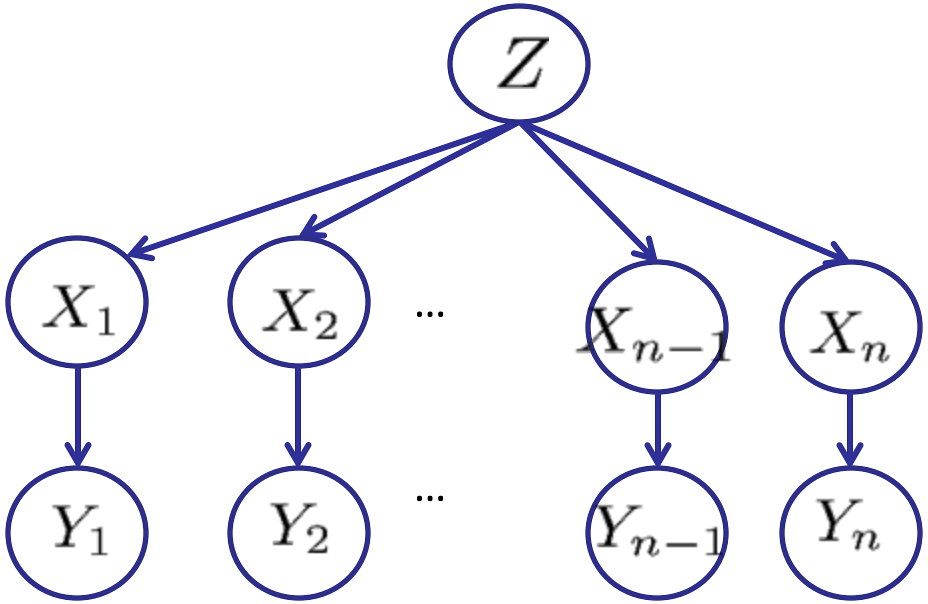
$$f_3(y_1, y_2, \ldots, X_n)$$

$$\vdots$$

$$2^{n+1}$$

Variable Elimination Ordering

- $X_1, \ldots, X_{n-1}, Z$



$$P(X_1|Z)P(y_1|X_1)$$

$$f_1(Z, y_1)$$

$$f_1(Z, y_1), f_2(Z, y_2), \ldots, f_{n-1}(Z, y_{n-1}), P(Z), P(X_n|Z)$$

$$f_n(X_n, y_1, \ldots, y_{n-1})$$

$$2^2$$

VE: Computational Complexity

- The size of the largest factor determines the time and space complexity of VE
- The elimination ordering can greatly affect the size of the largest factor.
  - E.g., previous slide's example 2^{n+1} vs. 2^2

- Does there always exist an ordering that only results in small factors?
  - No!
  - The factor size is influenced by the tree-width of the graph

Reduction from 3SAT

$$(x_1 \vee x_2 \vee \neg x_3) \wedge (\neg x_1 \vee x_3 \vee \neg x_4) \wedge (x_2 \vee \neg x_2 \vee x_4) \wedge (\neg x_3 \vee \neg x_4 \vee \neg x_5) \wedge (x_2 \vee x_5 \vee x_7) \wedge (x_4 \vee x_5 \vee x_6) \wedge (\neg x_5 \vee x_6 \vee \neg x_7) \wedge (\neg x_5 \vee \neg x_6 \vee x_7)$$

$P(X_i = 0) = P(X_i = 1) = 0.5$

$Y_1 = X_1 \vee X_2 \vee \neg X_3$

...

$Y_8 = \neg X_5 \vee X_6 \vee X_7$

$Y_{1,2} = Y_1 \wedge Y_2$

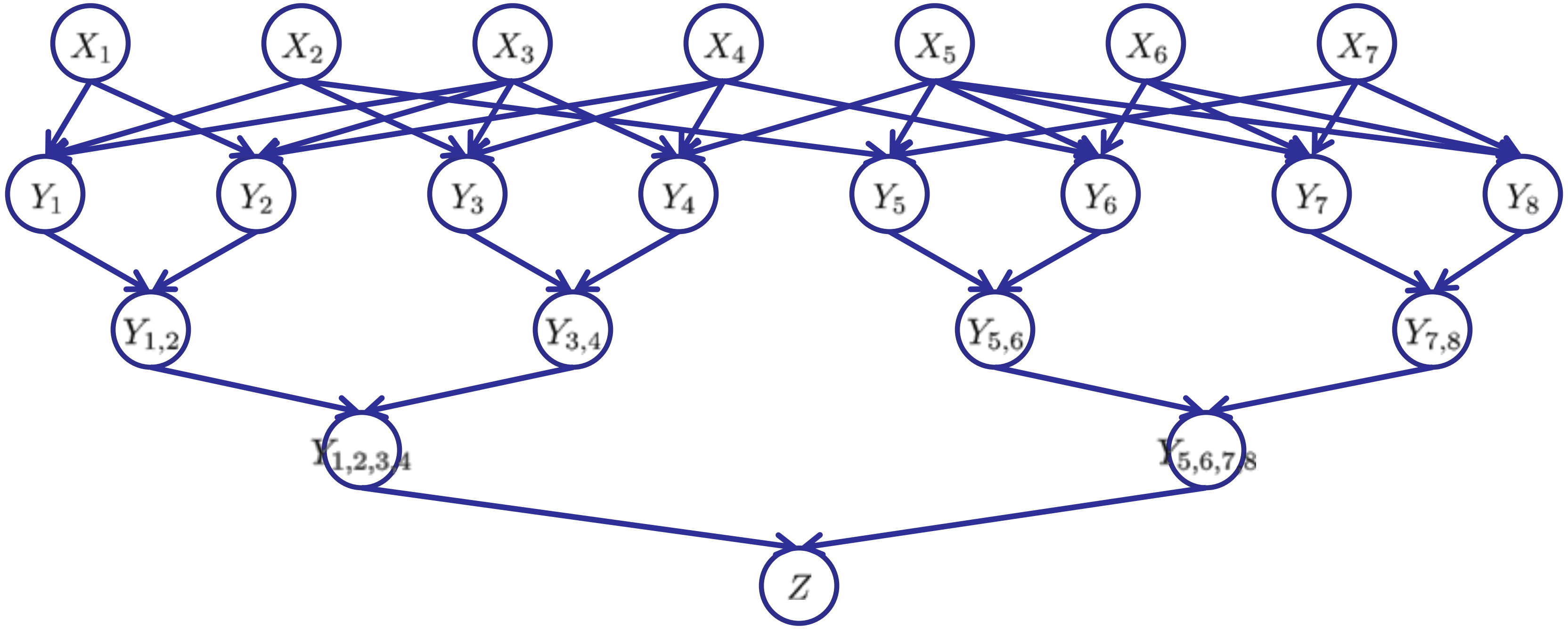
...

$Y_{7,8} = Y_7 \wedge Y_8$

$Y_{1,2,3,4} = Y_{1,2} \wedge Y_{3,4}$

$Y_{5,6,7,8} = Y_{5,6} \wedge Y_{7,8}$

$Z = Y_{1,2,3,4} \wedge Y_{5,6,7,8}$

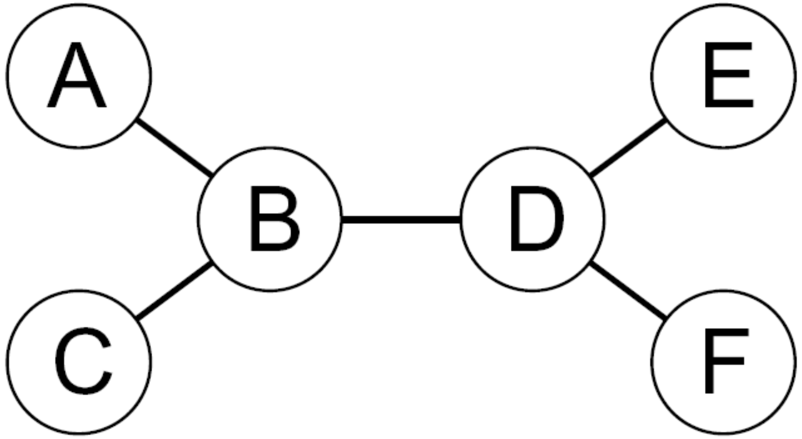


$$P(+z) = \sum_{\mathbf{x},\mathbf{y}} P(\mathbf{x}, \mathbf{y}, +z) = \sum_{\mathbf{x} \text{ s.t. } z=T} P(\mathbf{x})$$

- P(+z) > 0 iff the sentence is satisfiable ➔ NP-hard
- P(+z) = S×0.5^7 where S is the number of satisfying assignments ➔ #P-hard

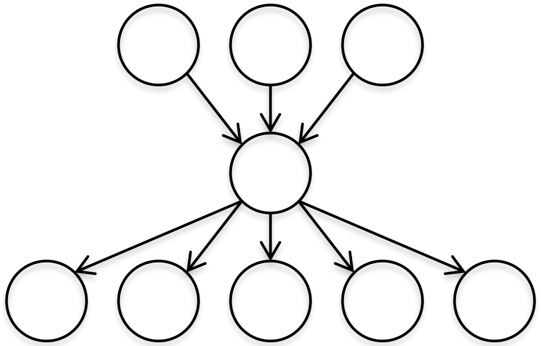
When do we have tractable inference?

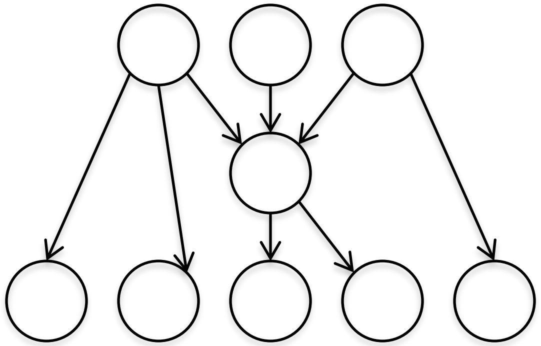
- Recall: Tree-Structured CSPs
  - CSP is NP-hard in general
  - If the constraint graph has no loops (i.e., tree), the CSP can be solved in linear time!

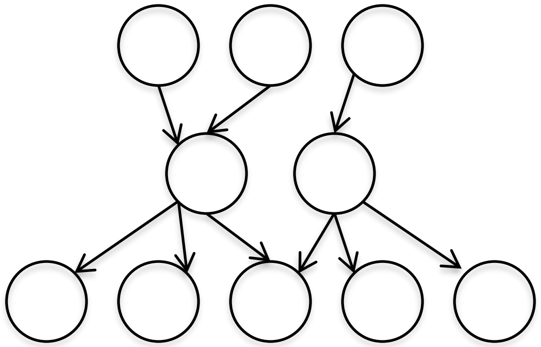


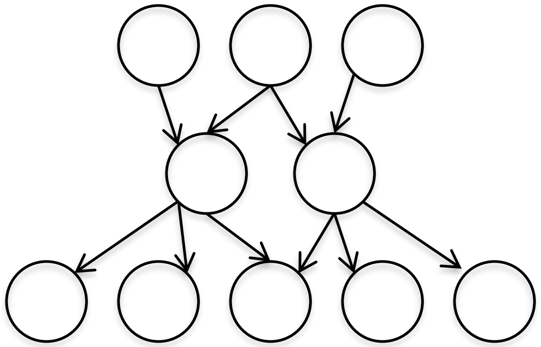
Polytrees

- A polytree is a directed graph with no undirected cycles



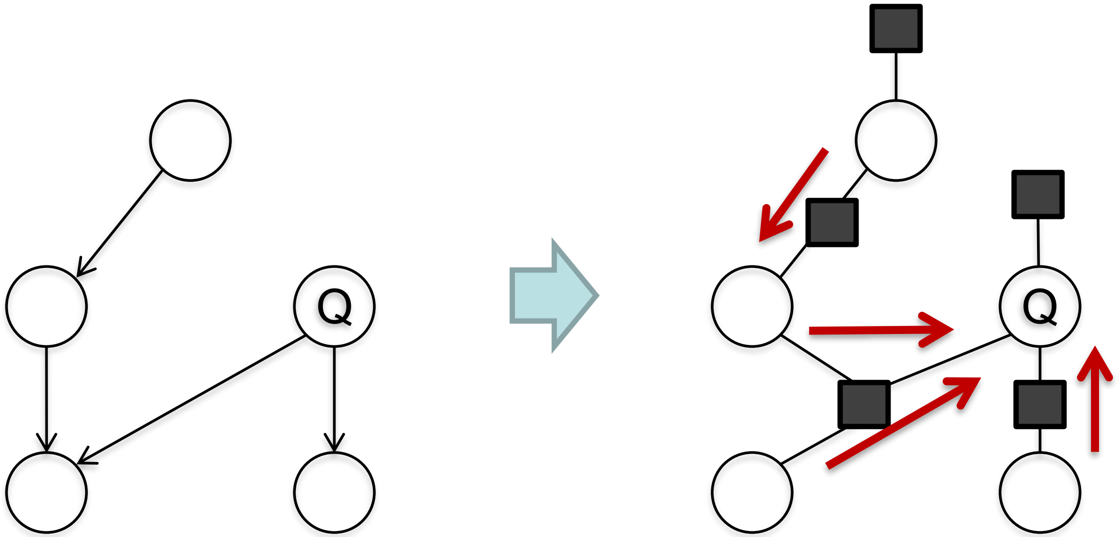






Variable Elimination on Polytrees

- For poly-tree BNs, the complexity of VE is ***linear in the BN size*** (number of CPT entries) with the following elimination ordering:
  - Convert to a factor graph
  - Take Q as the root
  - Eliminate from the leaves towards the root

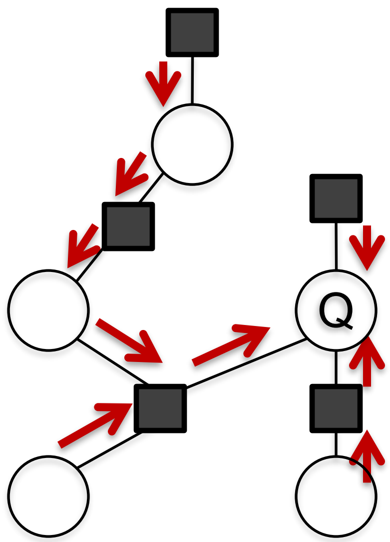


Bayesian Network

Factor Graph

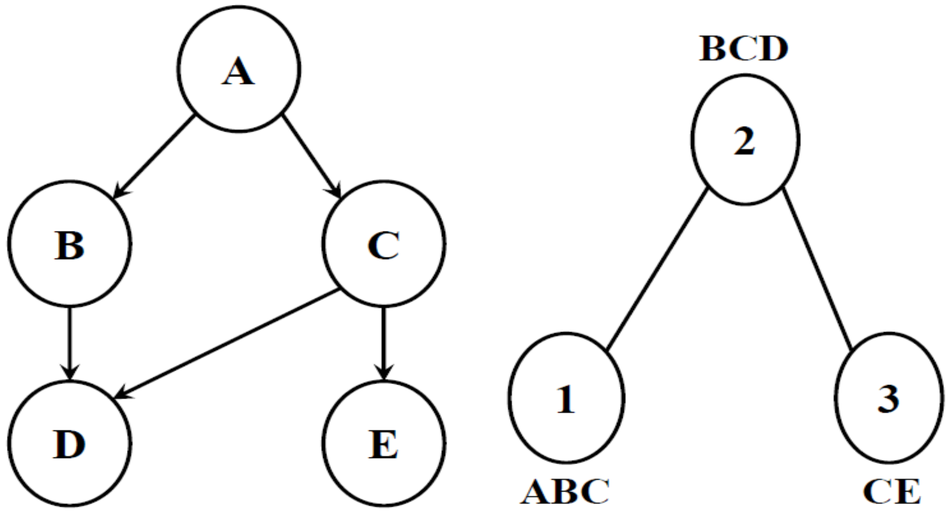
Variable Elimination on Polytrees

- VE for poly-tree BNs is equivalent to
  - Sum-product message passing algorithm or belief propagation algorithm (i.e., passing messages/beliefs from leaf nodes to the root node)
  - “Messages” are just 1d factors resulted from joining/elimination



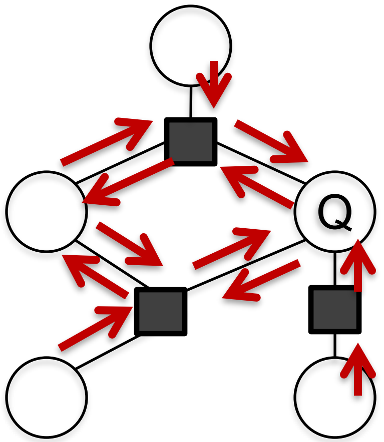
Message Passing on General Graphs

- Exact inference: Junction Tree Algorithm
  - Group individual nodes to form cluster nodes in such a way that the resulting network is a polytree (called a junction tree or join tree)
  - Run a sum-product-like algorithm on the junction tree.
  - *Intractable* on graphs with large cluster nodes (i.e., large tree-width).



Message Passing on General Graphs

- Approximate inference: Loopy Belief Propagation
  - Simply pass the messages on the general graph
    - Will not terminate with loops
    - Run until convergence (not guaranteed!)
  - *Approximate* but *tractable* for large graphs.
  - Sometime works well, sometimes not at all.



Summary

- Exact inference of Bayesian networks
  - Enumeration
    - exponential complexity
  - Variable Eliminating
    - worst-case exponential complexity, often better
  - VE on polytrees
    - linear complexity
    - = message passing
  - Message passing on general graphs
    - Junction Tree Algorithm
    - Loopy Belief Propagation: no longer exact