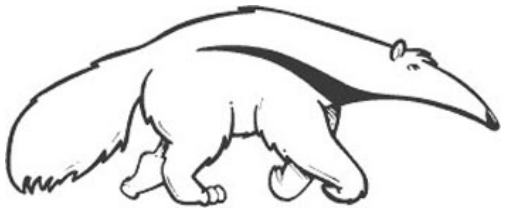
Algorithms for Causal Probabilistic Graphical Models

Class 1:
Introduction and Inference

Athens Summer School on AI
July 2024



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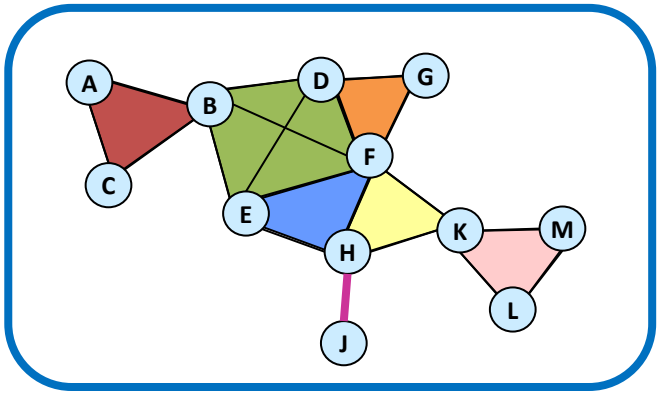
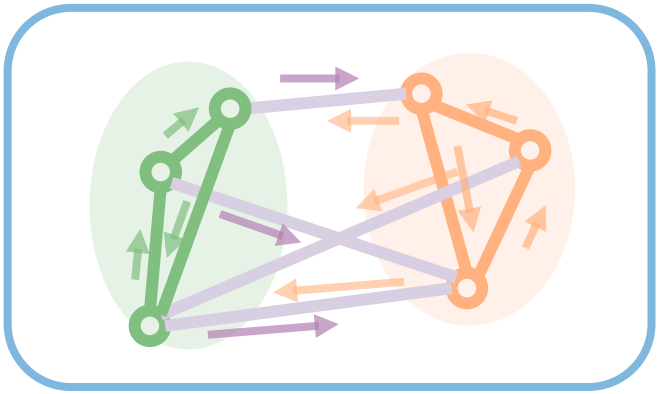
Outline of Lectures

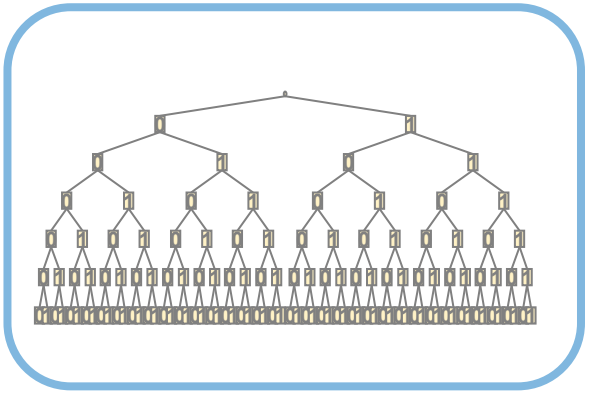
Class 1: Introduction & Inference



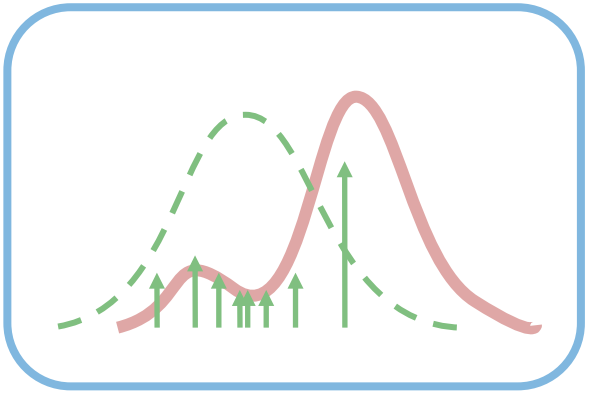
Class 2: Bounds & Variational Methods



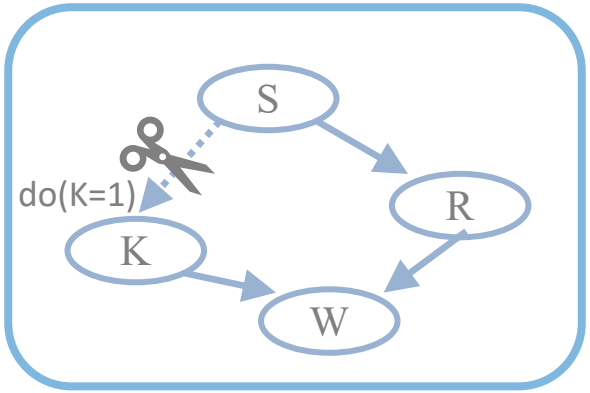
Class 3: Search Methods



Class 4: Monte Carlo Methods



Class 5: Causal Reasoning



Outline

- Graphical Models
- Inference Tasks
- Variable Elimination
- Tree Decomposition
- Variable Orderings
- Learning from Data

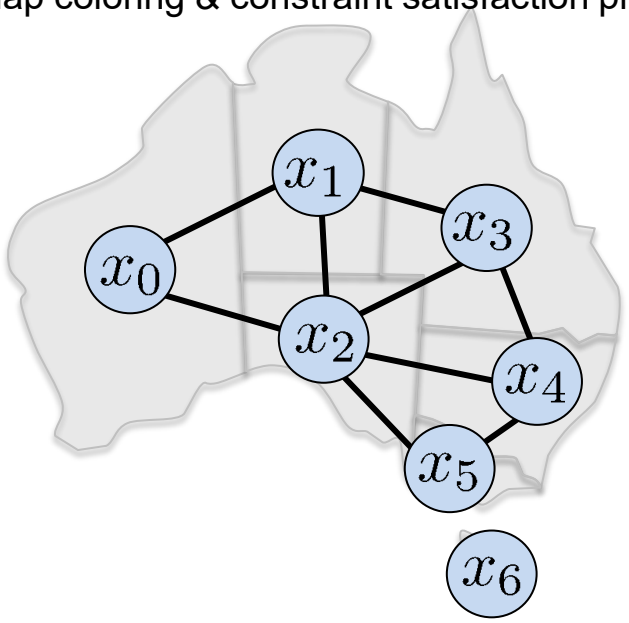
Graphical Models

Describe structure and interdependence in a model of the world

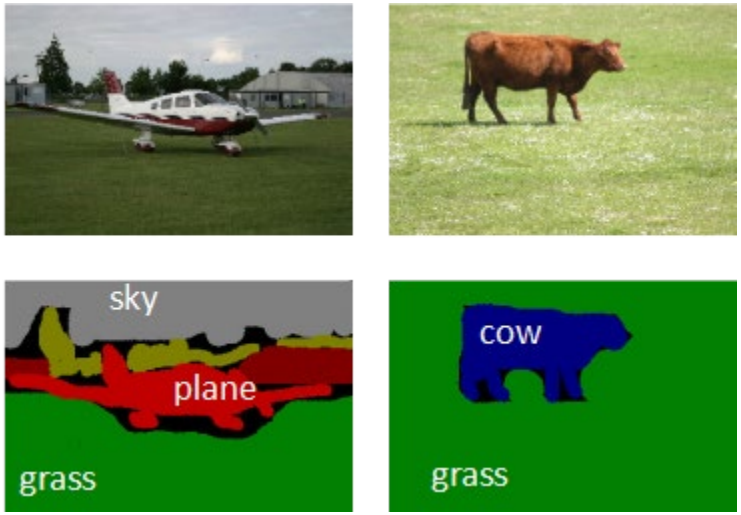
Examples:

- Markov Random Fields: correlations

Map coloring & constraint satisfaction problems



Semantic segmentation: fine-grain object recognition



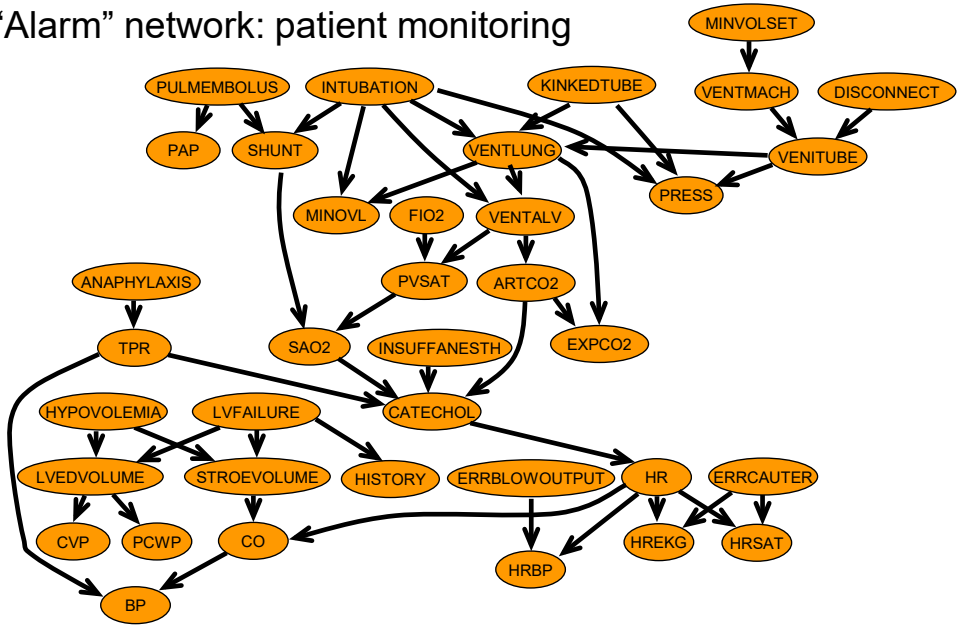
Graphical Models

Describe structure and interdependence in a model of the world

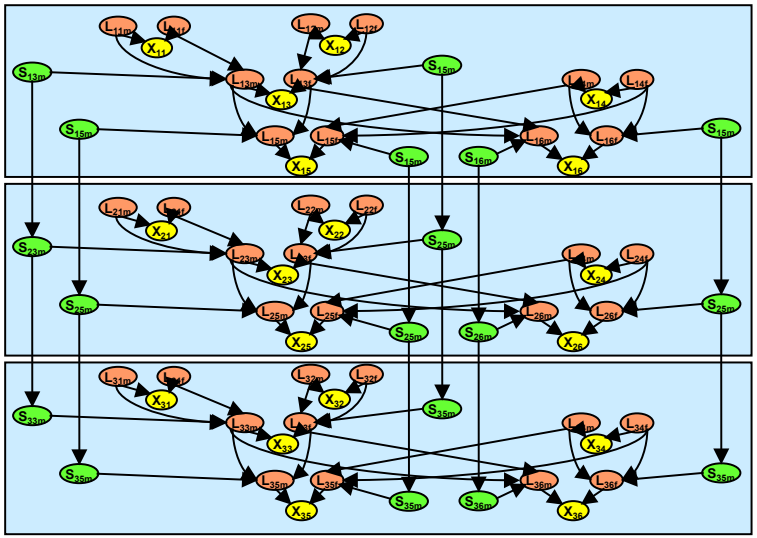
Examples:

- Markov Random Fields: correlations
- Bayesian Networks: conditional dependence

"Alarm" network: patient monitoring



Pedigree network: genetic inheritance



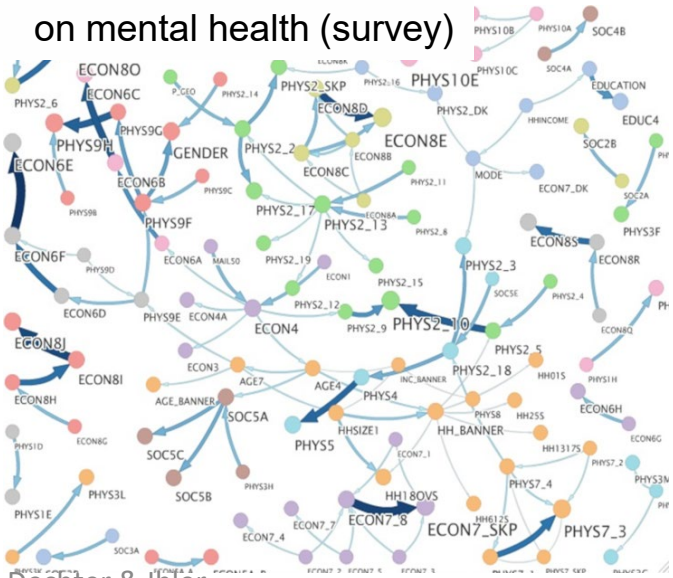
Graphical Models

Describe structure and interdependence in a model of the world

Examples:

- Markov Random Fields: correlations
- Bayesian Networks: conditional dependence
- Causal Networks: effect of intervention – what would happen if?

Impact of COVID & assistance on mental health (survey)



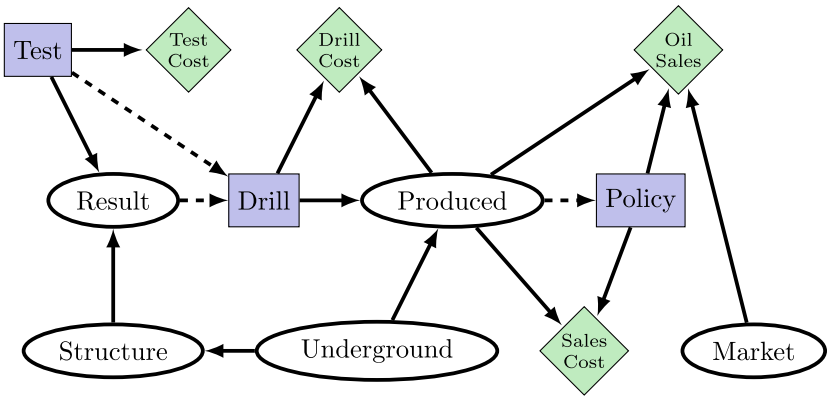
Graphical Models

Describe structure and interdependence in a model of the world

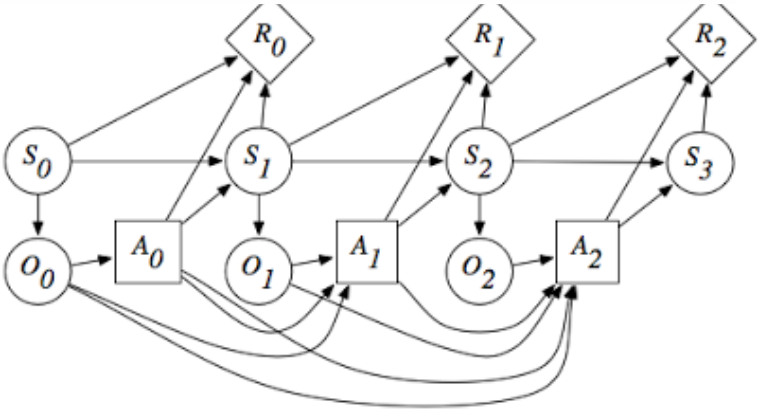
Examples:

- Markov Random Fields: correlations
- Bayesian Networks: conditional dependence
- Causal Networks: effect of intervention – what would happen if?
- Influence Diagrams: actions and rewards – what should we do if?

"Oil Wildcatter" Decision Network



(Partially Observable) Markov Decision Process
(Planning, Reinforcement Learning)



Bayesian networks

Use **independence** and **conditional independence** to simplify a **joint probability**

- Joint probability, p(X=x,Y=y,Z=z)
  - The probability that event (x,y,z) happens.

- Conditional probability
  - The chain rule of probability tells us

    $p(X=x,Y=y,Z=z) = p(X=x)\ \ p(Y=y \mid X=x)\ \ p(Z=z \mid X=x,Y=y)$

    (x,y,z all happen) (x happens) (y happens given x happened) (z happens given x,y happened)

  - Can use any order, e.g. (Z,X,Y):

    $p(X=x,Y=y,Z=z) = p(Z=z)\ \ p(X=x \mid Z=z)\ \ p(Y=y \mid X=x,Z=z)$

Independence

- X, Y independent:
  - $p(X=x,Y=y) = p(X=x)\ p(Y=y)$ for all x,y
  - Shorthand: $p(X,Y) = P(X)\ P(Y)$
  - Equivalent: $p(X|Y) = p(X)$ or $p(Y|X) = p(Y)$ (if $p(Y), p(X) > 0$)
  - Intuition: knowing X has no information about Y (or vice versa)

Independent probability distributions:

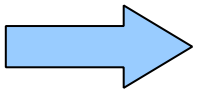
A	P(A)
0	0.4
1	0.6

B	P(B)
0	0.7
1	0.3

C	P(C)
0	0.1
1	0.9

This reduces representation size!

Joint:



A	B	C	P(A,B,C)
0	0	0	.4 * .7 * .1
0	0	1	.4 * .7 * .9
0	1	0	.4 * .3 * .1
0	1	1	…
1	0	0	
1	0	1	
1	1	0	
1	1	1	

Independence

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  - Shorthand: $p(X,Y) = P(X)\ P(Y)$
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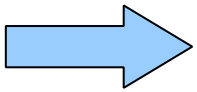
Joint:



A	B	C	P(A,B,C)
0	0	0	0.028
0	0	1	0.252
0	1	0	0.012
0	1	1	0.108
1	0	0	0.042
1	0	1	0.378
1	1	0	0.018
1	1	1	0.162

This reduces representation size!

Note: it is hard to "read" independence from the joint distribution.
We can "test" for it, however.

Conditional Independence

- X, Y independent given Z
  - $p(X=x,Y=y|Z=z) = p(X=x|Z=z)\, p(Y=y|Z=z)$ for all x,y,z
  - Equivalent: $p(X|Y,Z) = p(X|Z)$ or $p(Y|X,Z) = p(Y|Z)$ (if all > 0)
  - Intuition: X has no additional info about Y beyond Z's

- Example

  X = height $p(\text{height}|\text{reading, age}) = p(\text{height}|\text{age})$

  Y = reading ability $p(\text{reading}|\text{height, age}) = p(\text{reading}|\text{age})$

  Z = age

  Height and reading ability are dependent (not independent), but are conditionally independent given age

Conditional Independence

- X, Y independent given Z
  - p(X=x,Y=y|Z=z) = p(X=x|Z=z) p(Y=y|Z=z) for all x,y,z
  - Equivalent: p(X|Y,Z) = p(X|Z) or p(Y|X,Z) = p(Y|Z)
  - Intuition: X has no additional info about Y beyond Z's

- Example: Dentist

$(T \perp\!\!\!\perp D \mid C)?$

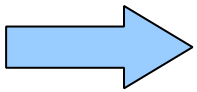
Is T conditionally independent of C given D?

Again, hard to "read" from the joint probabilities; only from the conditional probabilities.

Like independence, reduces representation size!

Joint prob:

T	D	C	P(T,D,C)
0	0	0	0.576
0	0	1	0.008
0	1	0	0.144
0	1	1	0.072
1	0	0	0.064
1	0	1	0.012
1	1	0	0.016
1	1	1	0.108



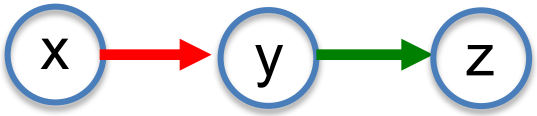
Conditional prob:

T	D	C	P(T|D,C)
0	0	0	0.90
0	0	1	0.40
0	1	0	0.90
0	1	1	0.40
1	0	0	0.10
1	0	1	0.60
1	1	0	0.10
1	1	1	0.60

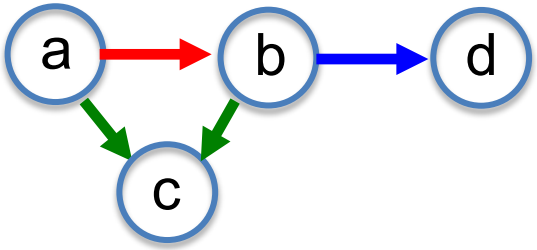
Bayesian networks

- Directed graphical model
- Nodes associated with variables
- "Draw" independence in conditional probability expansion
  - Parents in graph are the RHS of conditional

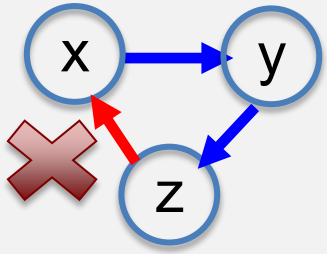
- Ex: $p(x, y, z) = p(x)\ p(y \mid x)\ p(z \mid y)$



- Ex $p(a, b, c, d) = p(a)\ p(b \mid a)\ p(c \mid a, b)\ p(d \mid b)$



*Graph must be **acyclic***



Corresponds to an order over the variables (chain rule)

Example adapted from Pearl

Example

- Consider the following 5 binary variables:
  - B = a burglary occurs at your house
  - E = an earthquake occurs at your house
  - A = the alarm goes off
  - W = Watson calls to report the alarm
  - H = Mrs. Hudson calls to report the alarm

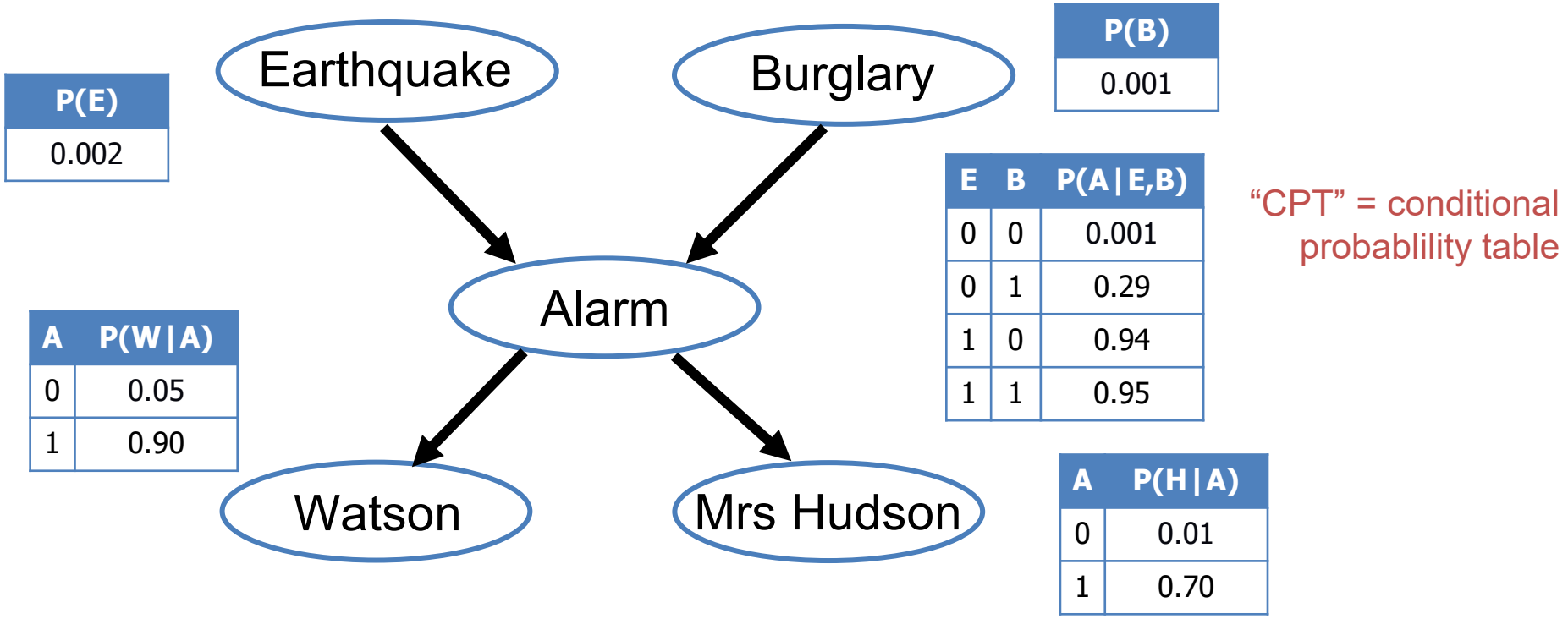
  - What is P(B | H=1, W=1) ? (for example)

  - We can use the full joint distribution to answer this question
    - Requires $2^5 = 32$ probabilities

    - Can we use prior domain knowledge to come up with a Bayesian network that requires fewer probabilities?

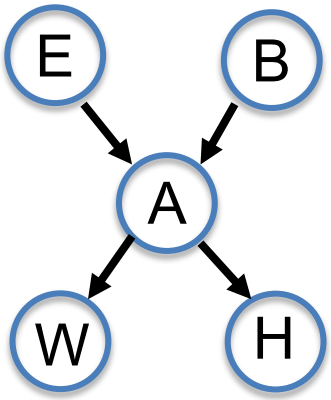
Constructing a Bayesian network

- Given $p(W, H, A, E, B) = p(E)\ p(B)\ p(A|E, B)\ p(W|A)\ p(H|A)$
- Define probabilities: 1 + 1 + 4 + 2 + 2
- Where do these come from?
  - Expert knowledge; estimate from data; some combination



Constructing a Bayesian network

- Joint distribution



Full joint distribution:
$2^5 = 32$ probabilities

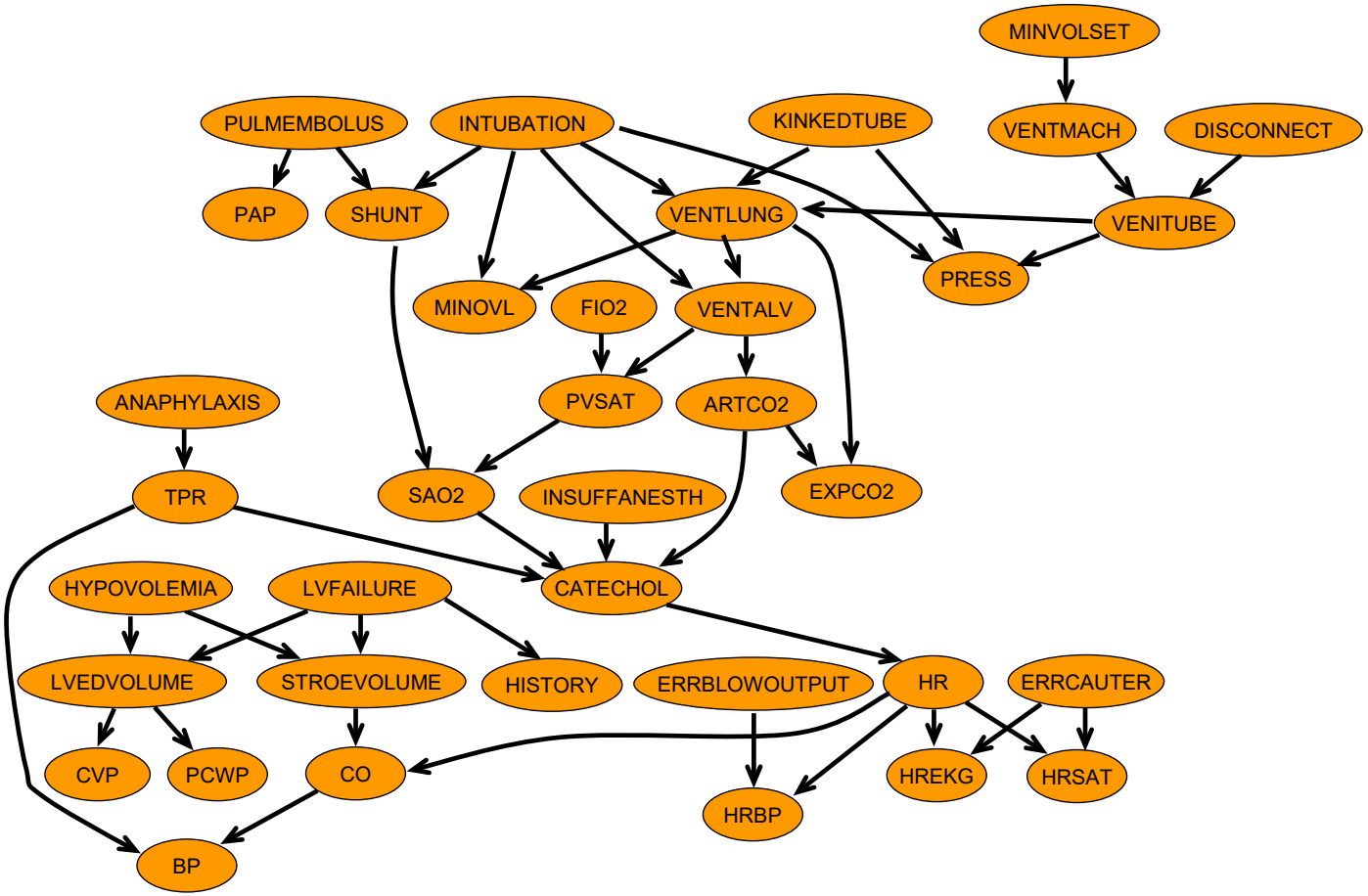
Structured distribution:
specify 10 parameters

E	B	A	W	H	P(…)
0	0	0	0	0	.93674
0	0	0	0	1	.00133
0	0	0	1	0	.00005
0	0	0	1	1	.00000
0	0	1	0	0	.00003
0	0	1	0	1	.00002
0	0	1	1	0	.00003
0	0	1	1	1	.00000
0	1	0	0	0	.04930
0	1	0	0	1	.00007
0	1	0	1	0	.00000
0	1	0	1	1	.00000
0	1	1	0	0	.00027
0	1	1	0	1	.00016
0	1	1	1	0	.00025
0	1	1	1	1	.00000

E	B	A	W	H	P(…)
1	0	0	0	0	.00946
1	0	0	0	1	.00001
1	0	0	1	0	.00000
1	0	0	1	1	.00000
1	0	1	0	0	.00007
1	0	1	0	1	.00004
1	0	1	1	0	.00007
1	0	1	1	1	.00000
1	1	0	0	0	.00050
1	1	0	0	1	.00000
1	1	0	1	0	.00000
1	1	0	1	1	.00000
1	1	1	0	0	.00063
1	1	1	0	1	.00037
1	1	1	1	0	.00059
1	1	1	1	1	.00000

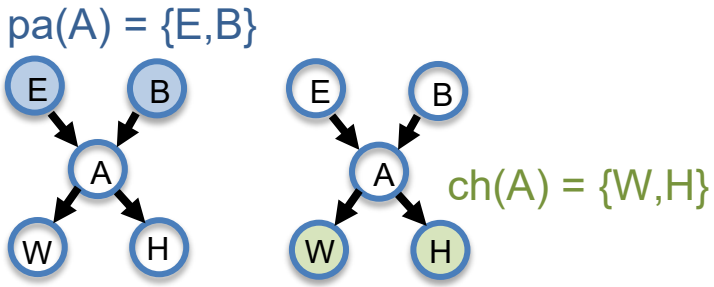
Alarm network [Beinlich et al., 1989]

The “alarm” network: 37 variables, 509 parameters (rather than $2^{37} = 10^{11}$!)

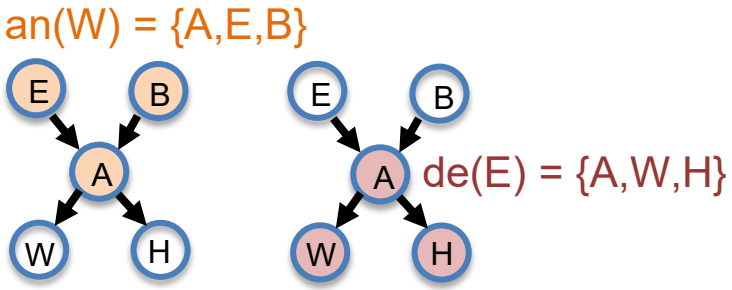


Some terminology

- Parents & Children
  - Parents pa(A) = {E,B}
  - Children ch(A) = {W,H}



- Ancestors & Descendants
  - Ancestors an(W) = {A,E,B}
  - Descendants de(E) = {A,W,H}



- Roots & Leaves
- Paths
  - Directed paths, undirected paths

Graphical models

A *graphical model* consists of:

$X = \{X_1, \ldots, X_n\}$ -- variables

$D = \{D_1, \ldots, D_n\}$ -- domains (we'll assume discrete)

$F = \{f_{\alpha_1}, \ldots, f_{\alpha_m}\}$ -- functions or "factors"

and a *combination operator*

Example:

$A \in \{0, 1\}$

$B \in \{0, 1\}$

$C \in \{0, 1\}$

$f_{AB}(A, B), \quad f_{BC}(B, C)$

The *combination operator* defines an overall function from the individual factors,

e.g., "*" : $F(A, B, C) = f_{AB}(A, B) \cdot f_{BC}(B, C)$

Notation:

Discrete X_i : values called "states"

"Tuple" or "configuration": states taken by a set of variables

"Scope" of f: set of variables that are arguments to a factor f

often index factors by their scope, e.g., $f_\alpha(X_\alpha), \quad X_\alpha \subseteq X$

Canonical forms

A *graphical model* consists of:

$X = \{X_1, \ldots, X_n\}$ -- variables

$D = \{D_1, \ldots, D_n\}$ -- domains

$F = \{f_{\alpha_1}, \ldots, f_{\alpha_m}\}$ -- functions or "factors"

and a *combination operator*

Typically either multiplication or summation; mostly equivalent:

$$f_\alpha(X_\alpha) \geq 0$$

$$F(X) = \prod_\alpha f_\alpha(X_\alpha)$$

Product of nonnegative factors
(probabilities, 0/1, etc.)

log / exp

$$\theta_\alpha(X_\alpha) = \log f_\alpha(X_\alpha) \in \mathbb{R}$$

$$\theta(X) = \log F(x) = \sum_\alpha \theta_\alpha(X_\alpha)$$

Sum of factors
(costs, utilities, etc.)

Graphical visualization

A *graphical model* consists of:

$X = \{X_1, \ldots, X_n\}$ -- variables

$D = \{D_1, \ldots, D_n\}$ -- domains

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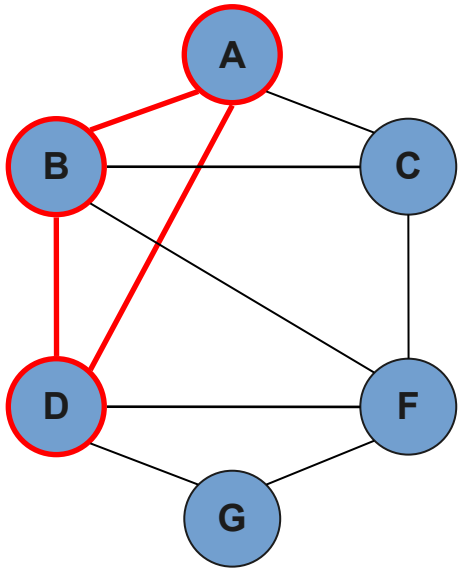
Primal graph:

variables ⟷ nodes

factors ⟷ cliques

$$p(A, B, C, D, F, G) = f_1(A, B, D) \cdot f_2(D, F, G) \cdot f_3(B, C, F) \cdot f_4(A, C)$$



Outline

- Graphical Models
- **Inference Tasks**
- Variable Elimination
- Tree Decomposition
- Variable Orderings
- Learning from Data

Inference

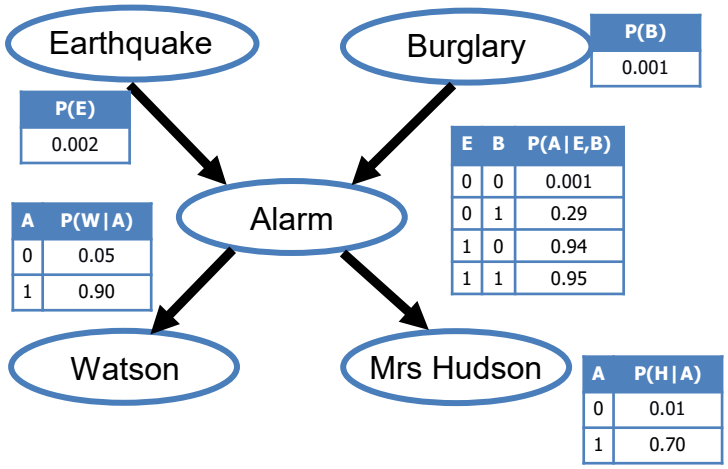
Enable us to answer **queries** about our model

- Some probabilities are directly accessible
- Some are only **implicit**, and require computation

p(B=1) = .001
Explicitly in model parameters

p(A=1) = ?
Implicit only:
p(A=1|E=0,B=0) p(E=0) p(B=0) +
p(A=1|E=1,B=0) p(E=1) p(B=0) + …

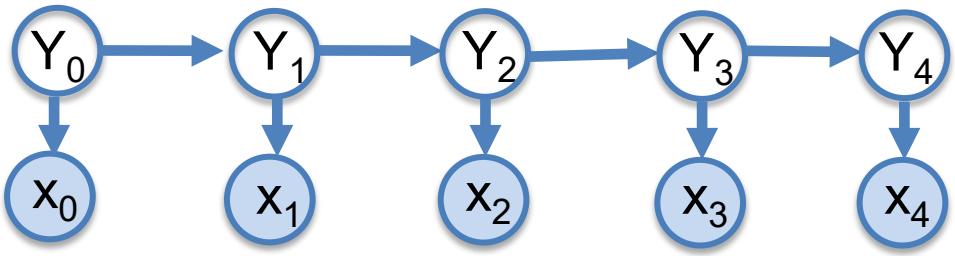
p(W=1) = ?
Implicit:
p(W=1|A=0) p(A=0) + p(W=1|A=1) p(A=1)
p(A) =? (may need to compute recursively!)



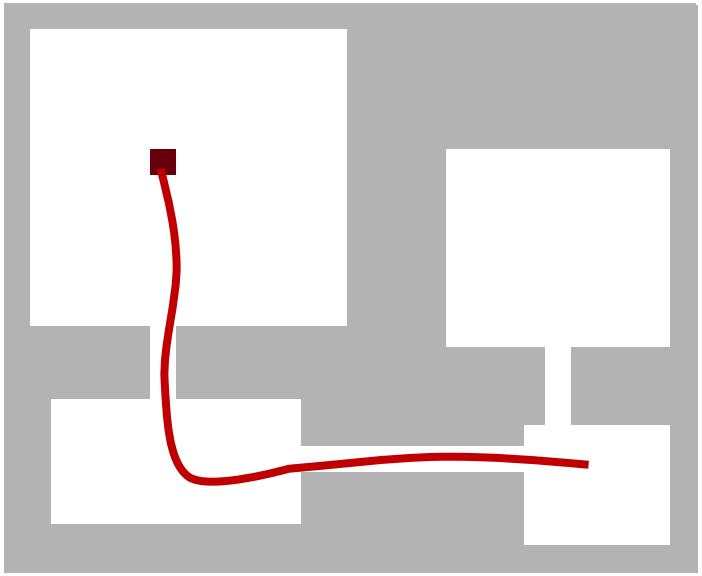
Types of queries

Ex: Robot position over time

Y_t : robot location at time t



x_t : noisy observations



Summation Query (marginal probailitiies, probability of evidence):

$$p(Y_t|x_0 \dots x_t) \propto \sum_{y_{t-1}} \dots \sum_{y_0} p(Y_t, x_t, y_{t-1}, \dots, x_0)$$

What do my model and observations tell me about my uncertainty?

Maximization Query (MAP: maximum a posteriori estmation):

$$\mathbf{y}^* = \arg \max_{y_0,\dots,y_t} p(y_t, x_t, y_{t-1}, \dots, x_0)$$

What is the most probable value of the unobserved variables?

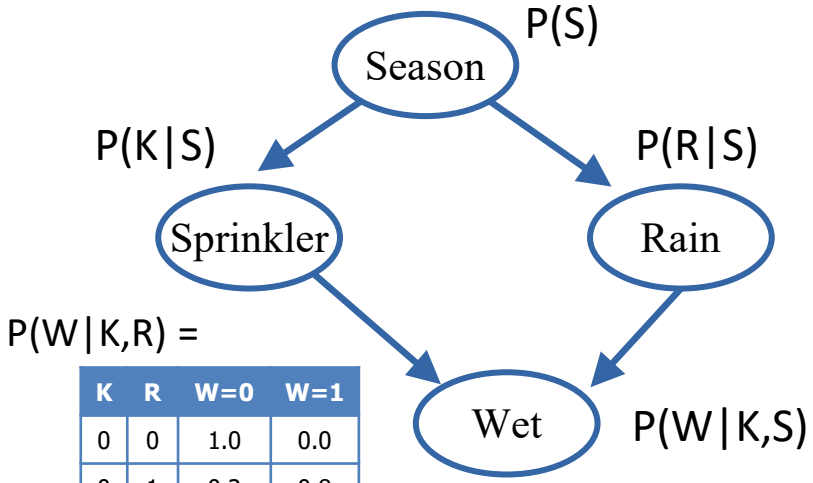
Causal Bayesian networks

- Typical BNs capture conditional independence
- May not correspond to causation; but if so:

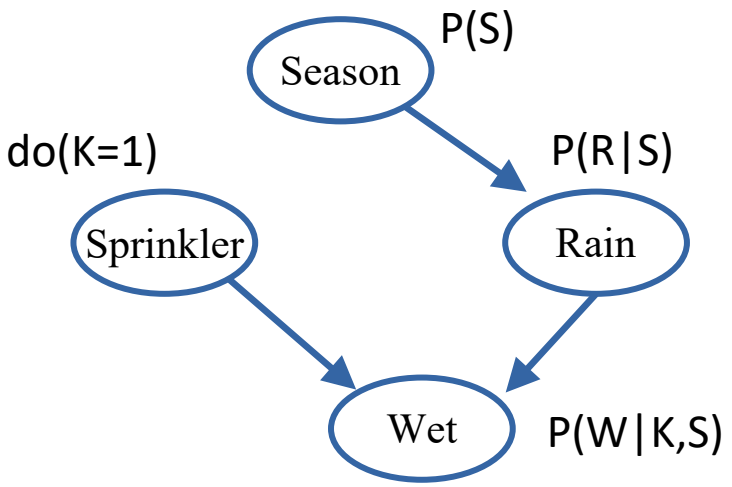
Causal Effect Query ("Intervention"):

$$p(W|\mathrm{do}(K=1))$$

What is the probability when we intervene to turn on the sprinkler?



K	R	W=0	W=1
0	0	1.0	0.0
0	1	0.2	0.8
1	0	0.1	0.9
1	1	0.01	0.99



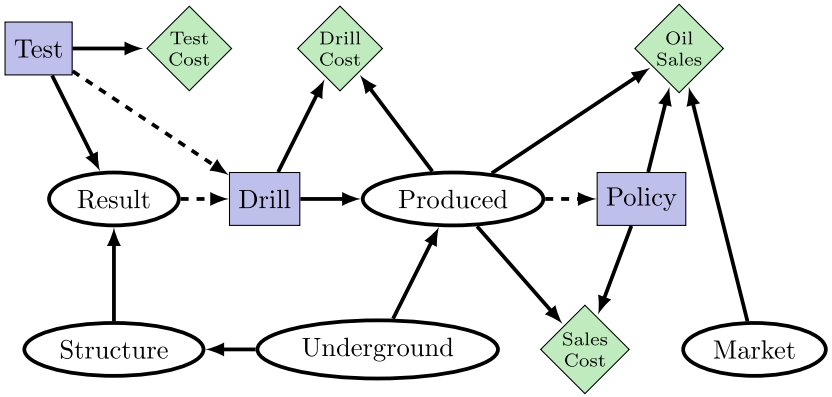
Influence diagrams

Random variables, plus **actions** (policy) and **utilities** (outcome values)

Maximum Expected Utility Query:

What actions should I take in a given situation?
What is the expected value of my policy over the actions?

The "oil wildcatter" problem:



e.g., [Raiffa 1968; Shachter 1986]

Chance variables: $X = x_1, \ldots, x_n$

Decision variables: $D = d_1, \ldots d_m$

CPDs for chance variables: $P_i = P(x_i | x_{\mathrm{pa}_i})$,

Reward components: $r = \{r_1, \ldots, r_j\}$

Utility function: $u(X) = \sum_i r_i(X)$

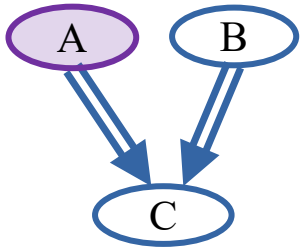
Structural Causal Models

Deterministic mechanisms involving (random) underlying causes

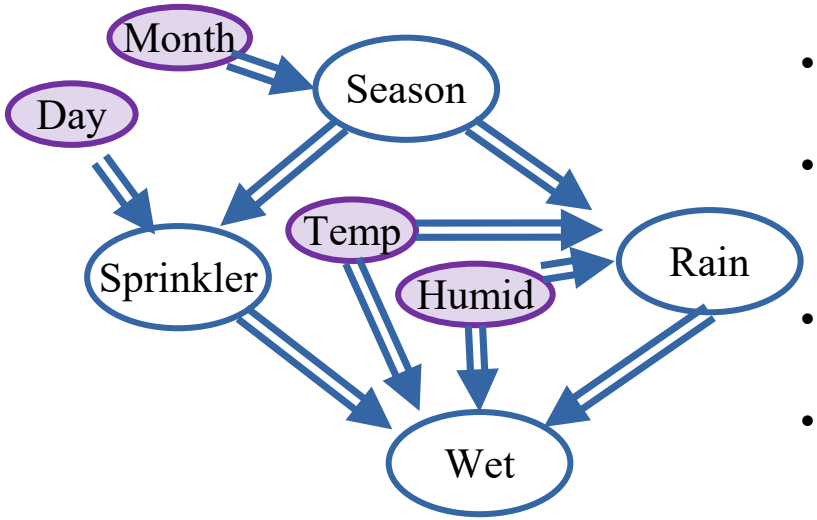
Unobservable random variables: {A}

Observable variables: {B,C}

Deterministic mechanism: ⟹ C = f(A,B)



Ex: Sprinkler



- p(S): season a function of (unobserved) month
- p(K|S): sprinkler on due to watering schedule: randomness in K due to (unobserved) day of week
- p(R|S) caused by humidity and temperature
- p(W|R,K) also caused by humidity and temperature (effects of evaporation, etc.)

Structural Causal Models

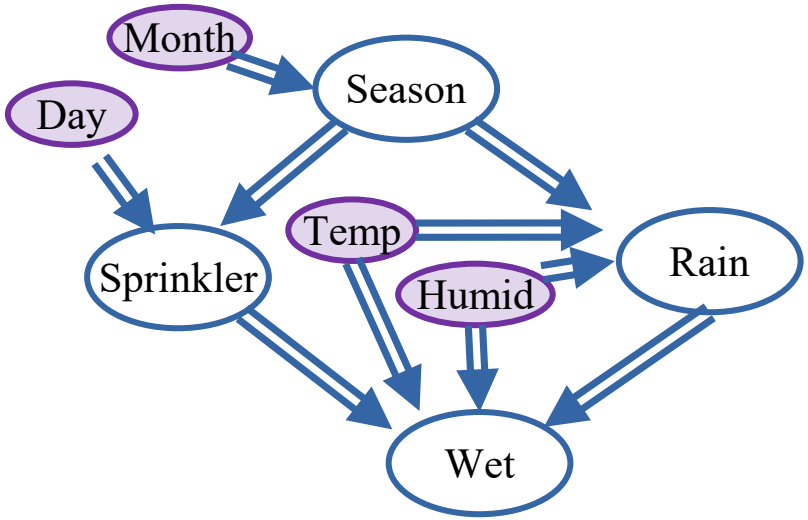
Deterministic mechanisms involving (random) underlying causes

Counterfactual Query:

Probability of an event in contradiction with the observations
*What **would have happened** if the sprinkler had been turned off?*

Requires that we transfer information about random outcomes that happened, to a different setting

Ex: Sprinkler



Observe the sprinkler is on & grass is wet: (K=1,W=1)

What is the probability it would still be wet if we had turned the sprinkler off?

Observing K=1 tells us it is more likely to be summer;
Observing K=1,W=1 tells us it is not too hot & dry.

Then, apply this knowledge to compute the counterfactual:

$$p(W_{K=0} \mid K = 1, W = 1)$$

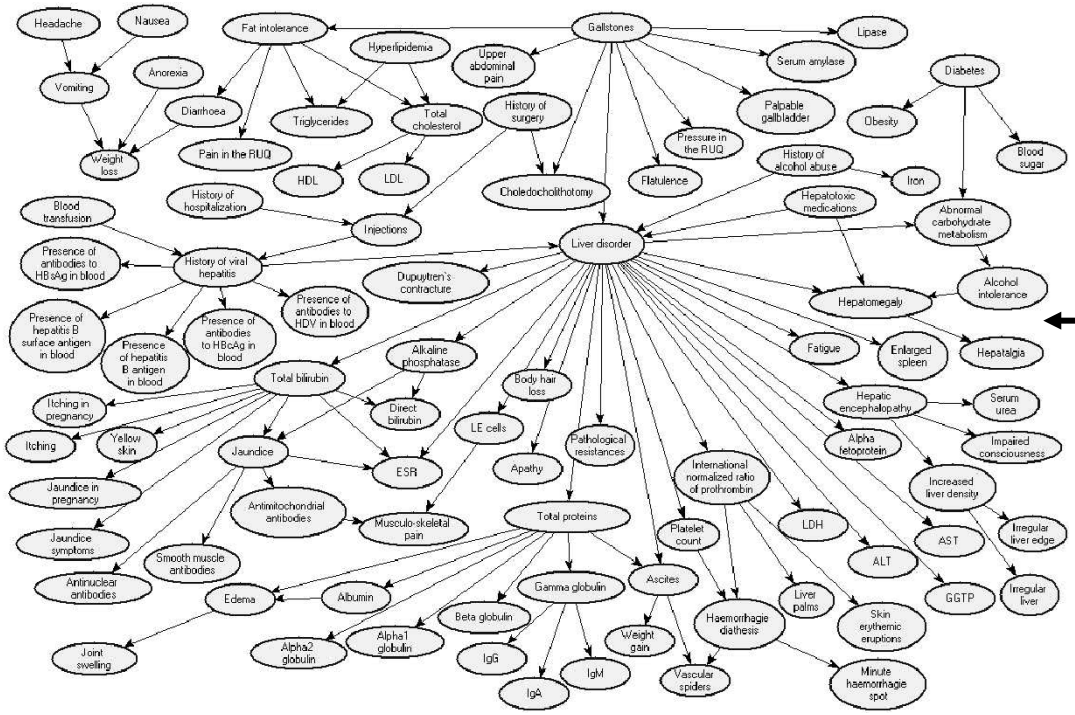
Why graphical models?

Combine domain knowledge with learning and data

- Domain knowledge
  - Problem structure: potential causation or interactions
  - Model parameters: known dependency mechanisms, probabilities
- Learning and data
  - Identify (in)dependence from data
  - Estimate model parameters to explain observations
- Scalable and Composable
  - Models over large systems may be composed of smaller parts
  - Efficient representation allows learning from relatively few data

Ex: Medical diagnosis

Diagnosing liver disease [Onisko et al., 1999]



Queries:

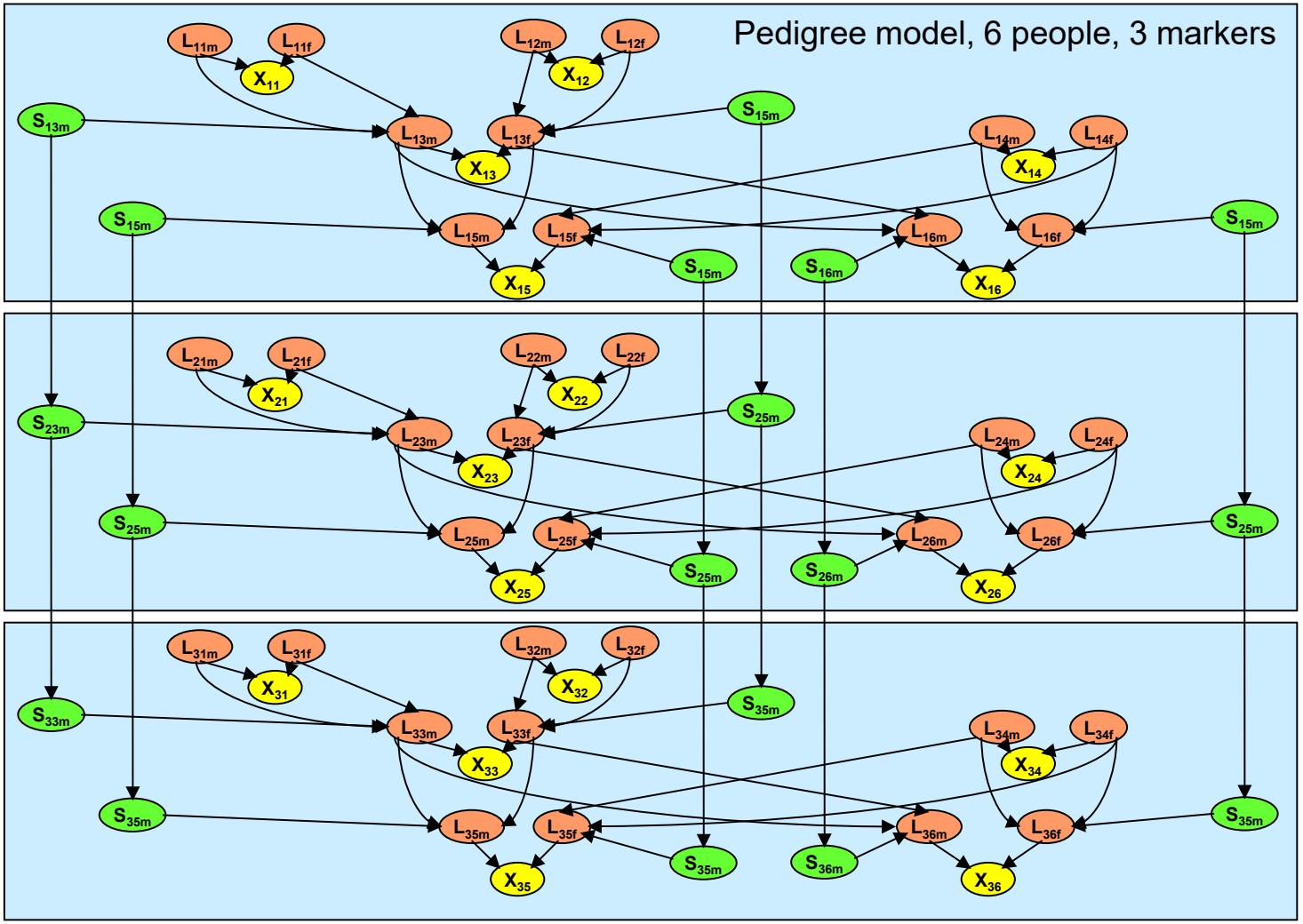
- Prediction
- Diagnosis, explanation
- Situation assessment
- Planning, decision making
- Counterfactual reasoning

Automated Reasoning:

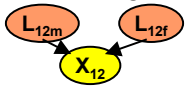
- Develop methods to answer these questions
- Learning models from experts and data

Ex: Model composability

Large models may be defined by many repeated, interrelated structures

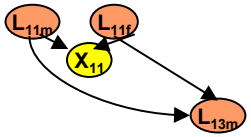


Individual's genotype



determines phenotype

Each parent



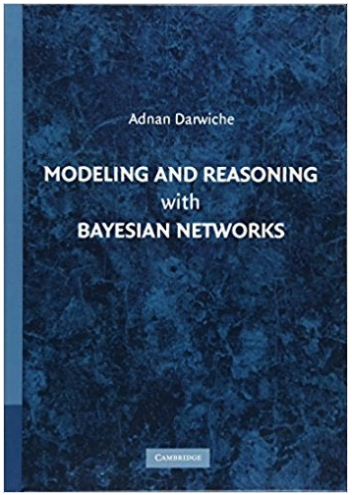
passes one gene copy to their child

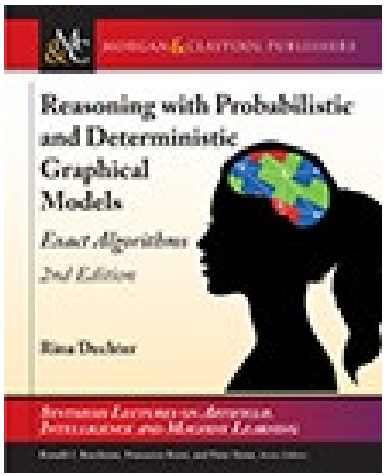
Gene position correlates which copy is inherited over several genes

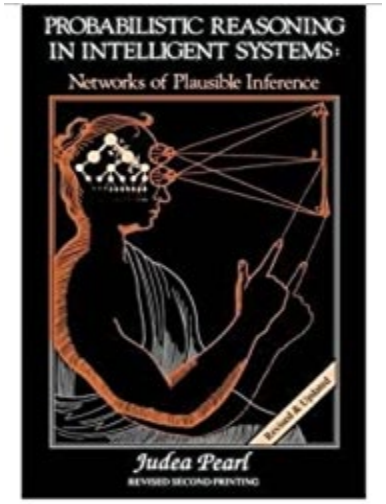
Domains for graphical models

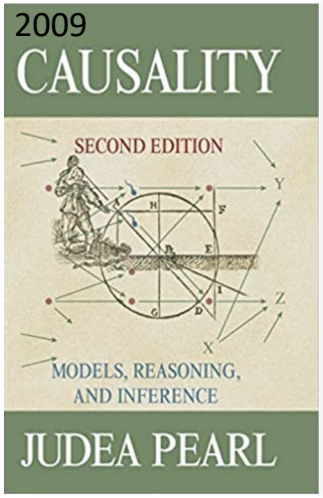
- Natural Language processing
  - Information extraction, semantic parsing, translation, topic models, …
- Computer vision
  - Object recognition, scene analysis, segmentation, tracking, …
- Computational biology
  - Pedigree analysis, protein folding and binding, sequence matching, …
- Networks
  - Webpage link analysis, social networks, communications, citations, ….
- Robotics
  - Planning & decision making

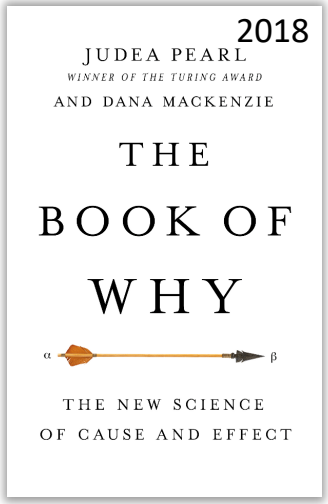
Books on Graphical Models & Causality



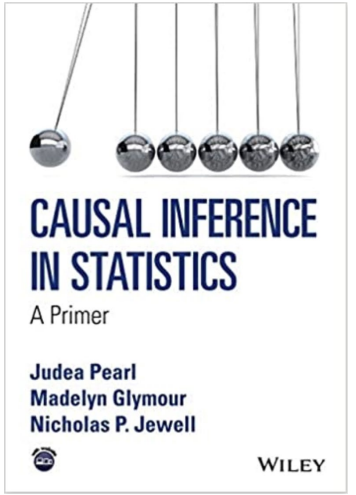






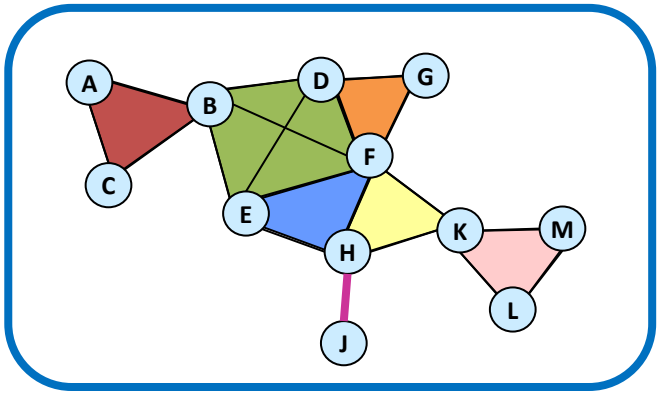


(intervention & counterfactuals)

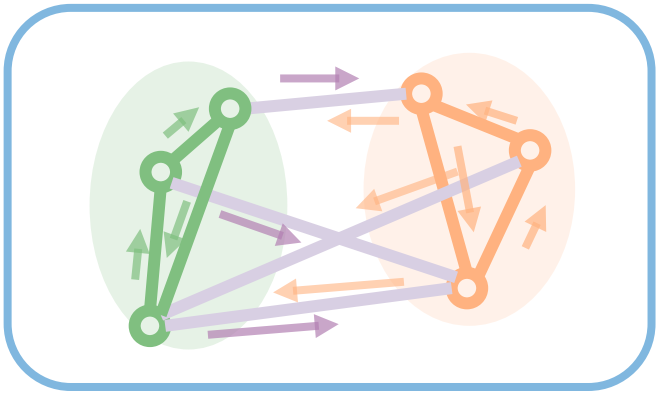


Outline of Lectures

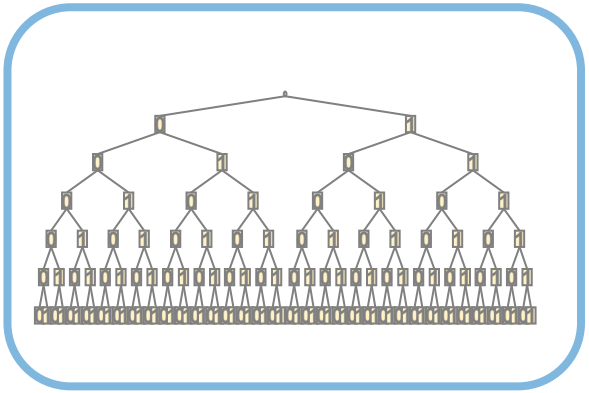
Class 1: Introduction & Inference



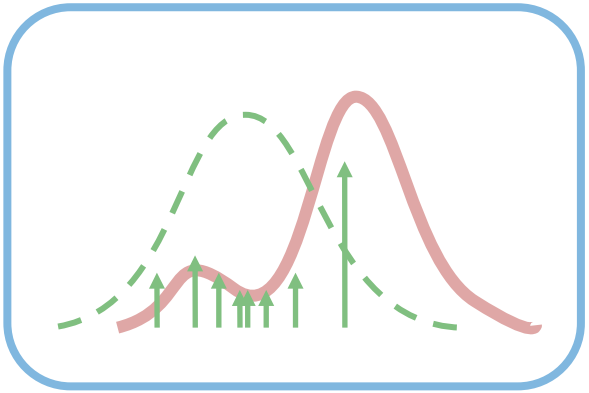
Class 2: Bounds & Variational Methods



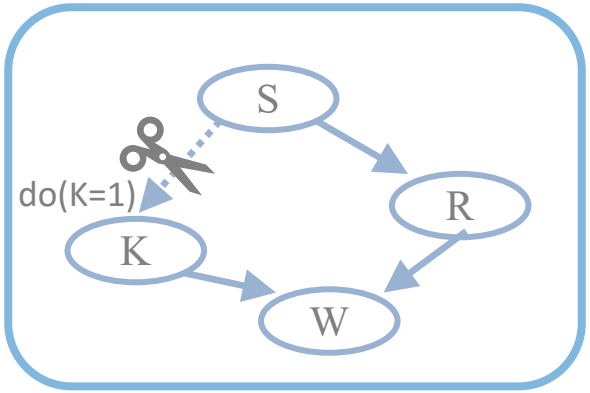
Class 3: Search Methods



Class 4: Monte Carlo Methods



Class 5: Causal Reasoning



Outline

- Graphical Models
- Inference Tasks
- **Variable Elimination**
- Tree Decomposition
- Variable Orderings
- Learning from Data

Inference

- Take information (model, observations)
  - Implicitly defines a joint / conditional joint distribution
- Inference: what does that information mean?
  - How do other probabilities change? (Conditional) marginals
  - How likely was our observation? Probabiliity of evidence
  - Predict the value of the other variables? MPE / MAP estimates
- Tasks

"summation"

$$Z = \sum_{x} \prod_{\alpha} f_\alpha(x_\alpha)$$

$$p(X_i = x_i) = Z^{-1} \sum_{x \sim x_i} \prod_{\alpha} f_\alpha(x_\alpha)$$

"maximization"

$$x^* = \arg\max_{x} \prod_{\alpha} f_\alpha(x_\alpha)$$

$$f^* = f(x^*) = \max_{x} \prod_{\alpha} f_\alpha(x_\alpha)$$

A simple example

- Suppose we have two factors: $f(X) = f_{12}(X_1, X_2)\, f_{23}(X_2, X_3)$

- To compute the partition function (sum):

$$Z = \sum_{x_1,x_2,x_3} f(x_1, x_2, x_3) = f(0,0,0) + f(0,0,1) + f(0,0,2) + f(0,1,0) + \dots$$
$$+ f(1,0,0) + f(1,0,1) + f(1,0,2) + f(1,1,0) + \dots$$

  - Use the factorization of f(x):

$$Z = f_{12}(0,0)\, f_{23}(0,0) + f_{12}(0,0)\, f_{23}(0,1) + f_{12}(0,0)\, f_{23}(0,2) + f_{12}(0,1)\, f_{23}(1,0) + \dots$$
$$+ f_{12}(1,0)\, f_{23}(0,0) + f_{12}(1,0)\, f_{23}(0,1) + f_{12}(1,0)\, f_{23}(0,2) + f_{12}(1,1)\, f_{23}(1,0) + \dots$$

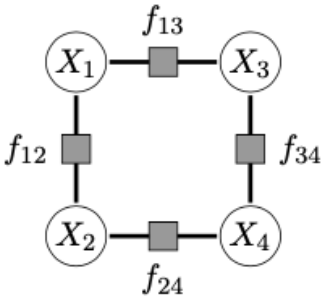
    and apply the distributive rule:

$$= f_{12}(0,0)\left(f_{23}(0,0) + f_{23}(0,1) + f_{23}(0,2)\right) + f_{12}(0,1)\left(f_{23}(1,0) + \dots\right.$$
$$+ f_{12}(1,0)\left(f_{23}(0,0) + f_{23}(0,1) + f_{23}(0,2)\right) + f_{12}(1,1)\left(f_{23}(1,0) + \dots\right.$$

We can pre-compute and re-use these terms in the sum!

$$\lambda(x_2) = \left(\sum_{x_3} f_{23}(x_2, x_3)\right) \qquad Z = \sum_{x_1,x_2} f_{12}(x_1, x_2)\, \lambda(x_2)$$

Variable Elimination



Product of factors:

$$p(X_1, X_2, X_3, X_4) = \frac{1}{Z} f_{12}(X_1, X_2) f_{13}(X_1, X_3) f_{24}(X_2, X_4) f_{34}(X_3, X_4).$$

Compute:

$$Z = \sum_{x_4} \sum_{x_3} \sum_{x_2} \sum_{x_1} f_{34}(x_3, x_4) f_{24}(x_2, x_4) f_{12}(x_1, x_2) f_{13}(x_1, x_3),$$

Collect terms involving x_1, then x_2, and so on:

$$Z = \sum_{x_4} \sum_{x_3} f_{34}(x_3, x_4) \sum_{x_2} f_{24}(x_2, x_4) \sum_{x_1} f_{12}(x_1, x_2) f_{13}(x_1, x_3),$$

"Bucket elimination":

$$\lambda_1(x_2, x_3) = \sum_{x_1} f_{12}(x_1, x_2) f_{13}(x_1, x_3),$$

Collect all factors with x_1 in a "bucket"

$$\lambda_2(x_3, x_4) = \sum_{x_2} f_{24}(x_2, x_4) \lambda_1(x_2, x_3),$$

Collect all remaining factors with x_2

$$\lambda_3(x_4) = \sum_{x_3} f_{34}(x_3, x_4) \lambda_2(x_3, x_4),$$

Place intermediate calculations in bucket of their earliest argument

$$Z = \sum_{x_4} \lambda_3(x_4),$$

Combination of factors

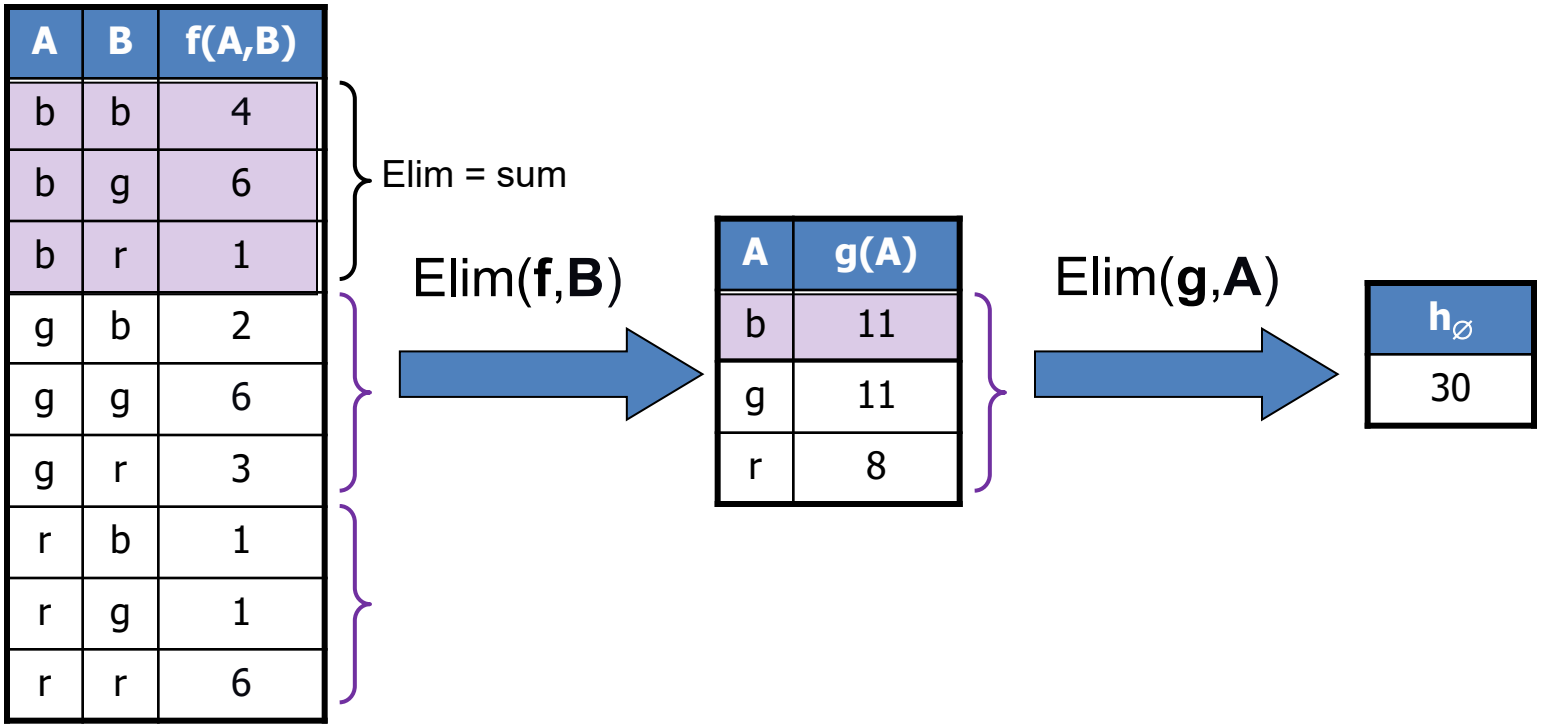
A	B	f(A,B)
b	b	0.4
b	g	0.1
g	b	0
g	g	0.5

B	C	f(B,C)
b	b	0.2
b	g	0
g	b	0
g	g	0.8

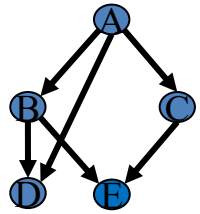
A	B	C	f(A,B,C)
b	b	b	0.1
b	b	g	0
b	g	b	0
b	g	g	0.08
g	b	b	0
g	b	g	0
g	g	b	0
g	g	g	0.4

= 0.1 x 0.8

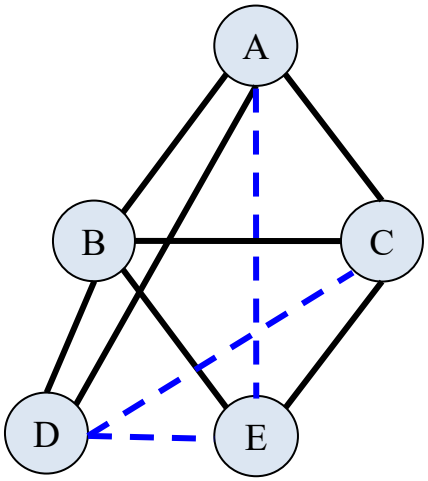
Elimination in a factor



Belief updating



- p(X | Evidence) = ?



"primal" graph

$$p(A|E=0)$$
$$\propto p(A, E=0)$$
$$= \sum_{e,d,c,b} p(A)\, p(b|A)\, p(c|A)\, p(d|b,A)\, p(e|b,c)\, \mathbb{1}[e=0]$$

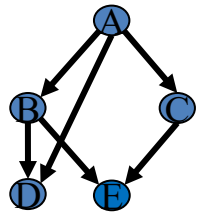
$$p(A) \sum_e \sum_d \sum_c p(c|A)\, \mathbb{1}[e=0] \sum_b p(b|A)\, p(d|b,A)\, p(e|b,c)$$

$$\lambda_{B\to C}(a,d,c,e)$$

Variable Elimination

Bucket elimination

Algorithm *BE-bel* [Dechter 1996]



$$p(A|E=0) = \alpha \sum_{e,d,c,b} p(A)\, p(b|A)\, p(c|A)\, p(d|A,b)\, p(e|b,c)\, \mathbb{1}[e=0]$$

$\sum_b \prod$ ← Elimination & combination operators

bucket B: $p(b|A)\ p(d|b,A)\ p(e|b,c)$

bucket C: $p(c|A)$ $\lambda_{B\to C}(A,d,c,e)$

bucket D: $\lambda_{C\to D}(A,d,e)$

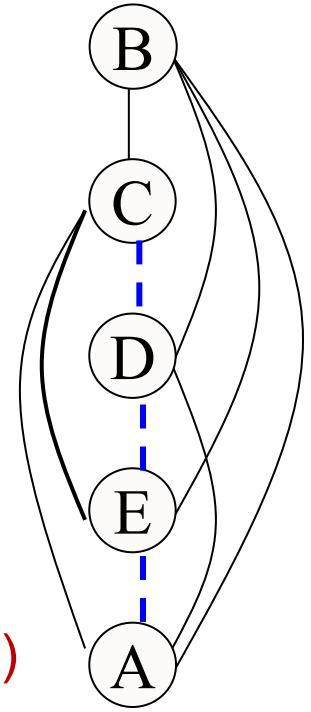
bucket E: $\mathbb{1}[E=0]\ \lambda_{D\to E}(A,e)$

bucket A: $p(A)$ $\lambda_{E\to A}(A)$

$p(E=0)$

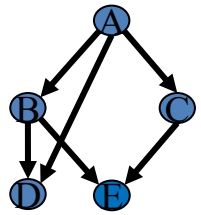
$p(A|E=0) = p(A,E=0)\,/\,p(E=0)$

W*=4
"induced width"
(max clique size)



Bucket elimination

Algorithm *BE-bel* [Dechter 1996]



$$p(A|E=0) = \alpha \sum_{e,d,c,b} p(A)\, p(b|A)\, p(c|A)\, p(d|A,b)\, p(e|b,c)\, \mathbb{1}[e=0]$$

$\sum \prod$ ⟵ Elimination & combination operators

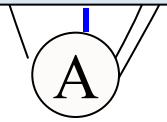
Time and space exponential in the induced-width / treewidth

bucket A: $p(A)$ $\lambda_{E\to A}(A)$

$p(E=0)$

$p(A|E=0) = p(A, E=0) \,/\, p(E=0)$

induced width (max clique size)

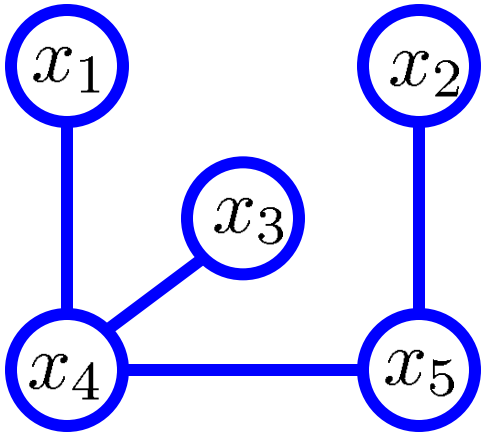


Variable elimination in trees

(Use distributive rule to calculate efficiently:)

$$\max_{x_1 \dots x_5} f_{14}\ f_{25}\ f_{34}\ f_{45}$$

$$= \max_{x_2 \dots x_5} f_{25}\ f_{34}\ f_{45} \Big[\max_{x_1} f_{14} \Big]$$



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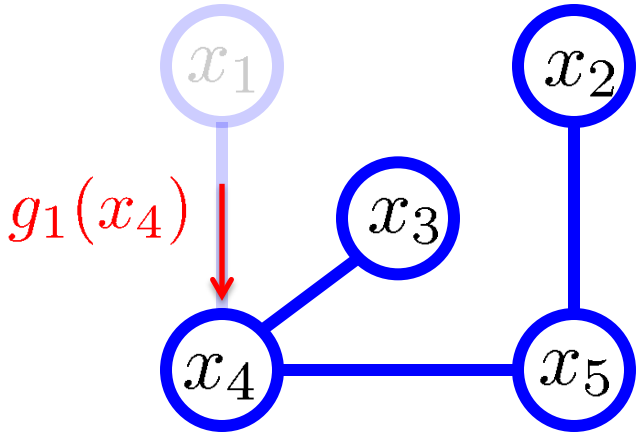
$$= \max_{x_2 \dots x_5} f_{25}\ f_{34}\ f_{45} \left[\max_{x_1} f_{14} \right]$$

$$= \max_{x_3 \dots x_5} f_{34}\ f_{45}\ g_1(x_4)\ \left[\max_{x_2} f_{25} \right]$$



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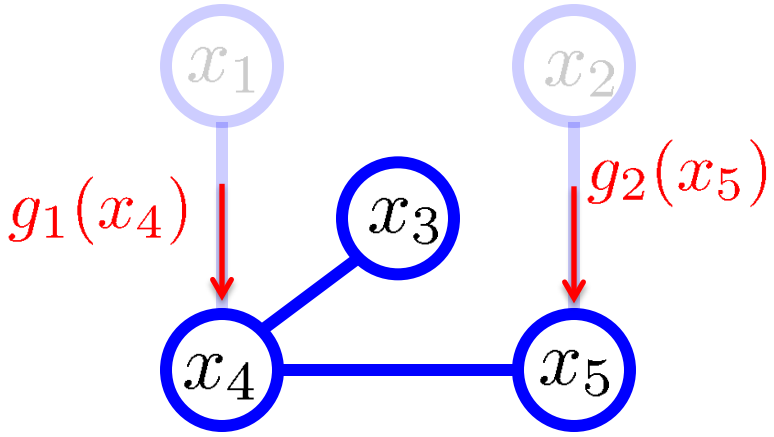
$$= \max_{x_3 \dots x_5} f_{34}\ f_{45}\ g_1(x_4)\ \left[\max_{x_2} f_{25} \right]$$

$$= \max_{x_4 \dots x_5} f_{45}\ g_1(x_4)\ g_2(x_5)\ \left[\max_{x_3} f_{34} \right]$$



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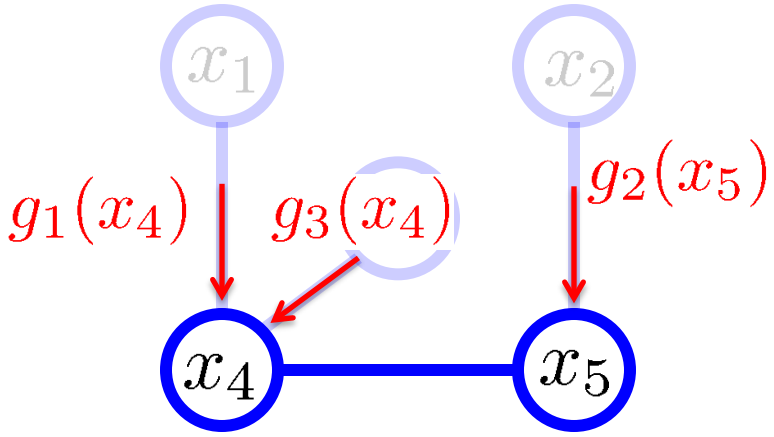
$$= \max_{x_3 \dots x_5} f_{34}\ f_{45}\ g_1(x_4) \left[\max_{x_2} f_{25} \right]$$

$$= \max_{x_4 \dots x_5} f_{45}\ g_1(x_4)\ g_2(x_5) \left[\max_{x_3} f_{34} \right]$$

$$= \max_{x_5} g_2(x_5) \left[\max_{x_4} f_{45}\ g_1(x_4)\ g_3(x_4) \right]$$



Variable elimination in trees

(Use distributive rule to calculate efficiently:)

$$\max_{x_1 \dots x_5} f_{14}\ f_{25}\ f_{34}\ f_{45}$$

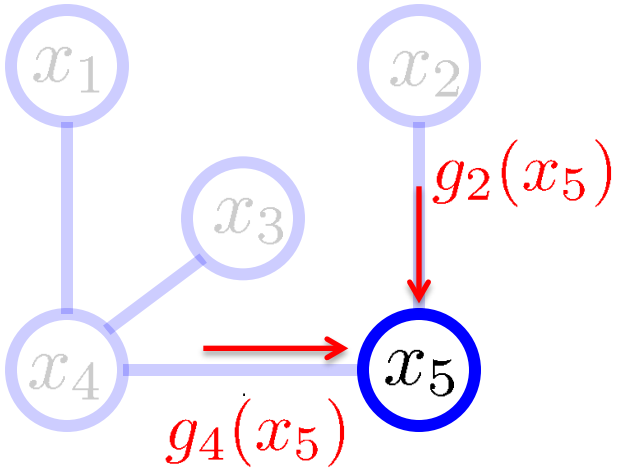
$$= \max_{x_2 \dots x_5} f_{25}\ f_{34}\ f_{45} \left[\max_{x_1} f_{14} \right]$$

$$= \max_{x_3 \dots x_5} f_{34}\ f_{45}\ g_1(x_4)\ \left[\max_{x_2} f_{25} \right]$$

$$= \max_{x_4 \dots x_5} f_{45}\ g_1(x_4)\ g_2(x_5)\ \left[\max_{x_3} f_{34} \right]$$

$$= \max_{x_5} g_2(x_5)\ \left[\max_{x_4} f_{45}\ g_1(x_4)\ g_3(x_4) \right]$$

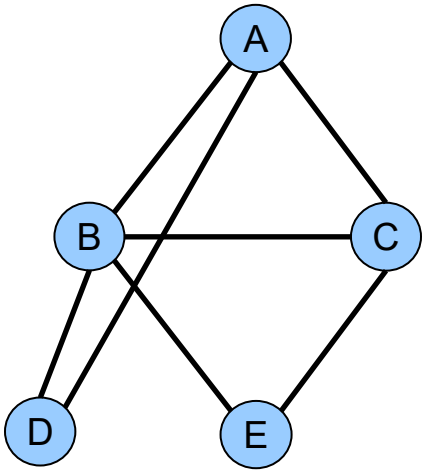
$$= \max_{x_5} g_2(x_5)\ g_4(x_5)$$



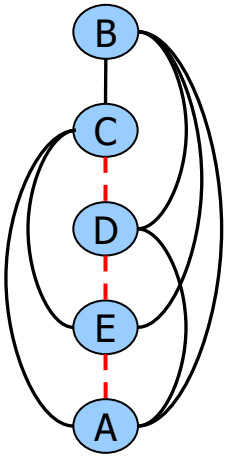
For trees:
Efficient elimination order (leaves to root);
computational complexity same as model size

Induced Width

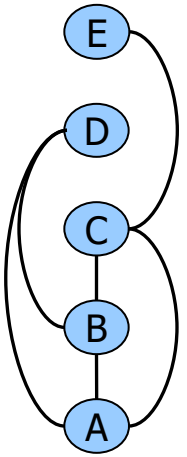
- Width is the max number of parents in the ordered graph
- Induced-width is the width of the induced ordered graph: recursively connecting parents going from last node to first.
- Induced-width w*(d) is the max induced-width over all nodes in ordering d
- Induced-width of a graph, w* is the min w*(d) over all orderings d



primal graph



$w^*(d_1) = 4$



$w^*(d_2) = 2$

Complexity of Bucket Elimination

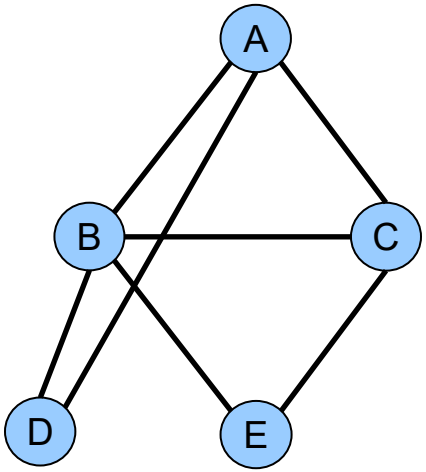
Bucket-Elimination is **time** and **space**

$$O\left(r \exp(w_d^*) \right)$$

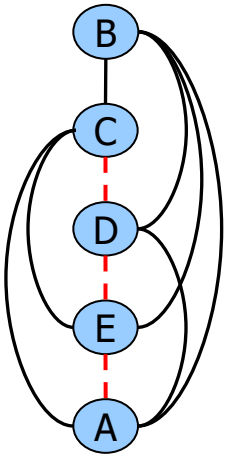
w_d^* : the induced width of the primal graph along ordering d

r = number of functions

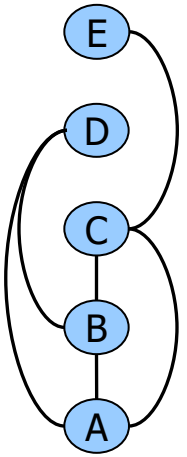
The effect of the ordering:



primal graph



$w^*(d_1) = 4$

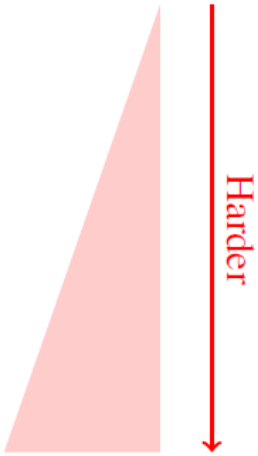


$w^*(d_2) = 2$

Finding smallest induced-width is hard!

Types of queries

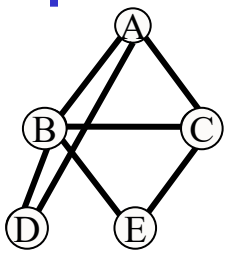
Max-Inference:	$f(x^*) = \max_x \prod_\alpha f_\alpha(x_\alpha)$
Sum-Inference: (e.g., causal effects)	$Z = \sum_x \prod_\alpha f_\alpha(x_\alpha)$
Mixed-Inference (MMAP): (optimal prediction)	$f_M(x_M^*) = \max_{x_M} \sum_{x_S} \prod_\alpha f_\alpha(x_\alpha)$
Mixed-Inference (MEU): (e.g., decisions & planning)	$\text{MEU} = \max_{D_1,\ldots,D_m} \sum_{X_1,\ldots X_n} (\prod_{P_i \in P} P_i) \times (\sum_{r_i \in R} r_i)$



- **NP-hard**: exponentially many terms
- Difficulty (in part) due to restricted elimination orderings
- We will focus on **approximation** algorithms
  - **Anytime**: very fast & very approximate ! Slower & more accurate

Finding MPE/MAP

Algorithm BE-mpe (Dechter 1996, Bertele and Briochi,



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

$$= \max_b p(b|a) \cdot p(d|b,a) \cdot p(e|b,c)$$

$$\max_x \prod$$

bucket B: $p(b|a)\ p(d|b,a)\ p(e|b,c)$

bucket C: $p(c|a)\quad \lambda_{B\to C}(a,d,c,e)$

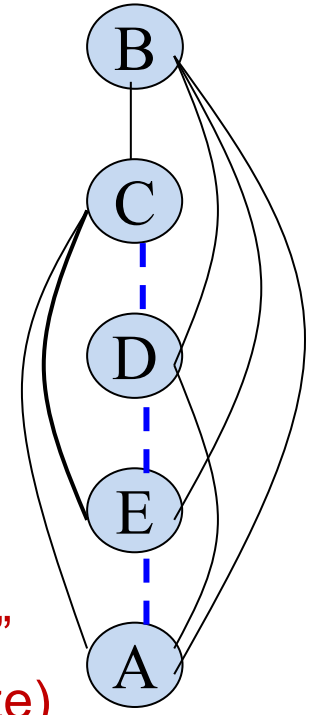
bucket D: $\lambda_{C\to D}(a,d,e)$

bucket E: $\mathbb{1}[e=0]\quad \lambda_{D\to E}(a,e)$

bucket A: $p(a)\quad \lambda_{E\to A}(a)$

OPT

W*=4
"induced width"
(max clique size)



Generating the optimal assignment

- Given BE messages, select optimum config in reverse order

$$\mathbf{b}^* = \arg\max_b \; p(b|a^*)\, p(d^*|b,a^*)\, p(e^*|b,c^*)$$

$$\mathbf{c}^* = \arg\max_c \; p(c|a^*)\, \lambda_{B\to C}(a^*,c,d^*,e^*)$$

$$\mathbf{d}^* = \arg\max_d \; \lambda_{C\to D}(a^*,d,e^*)$$

$$\mathbf{e}^* = \arg\max_e \; \mathbb{1}[e=0]\, \lambda_{D\to E}(a^*,e)$$

$$\mathbf{a}^* = \arg\max_a \; p(a)\cdot \lambda_{E\to A}(a)$$

Return optimal configuration (a*,b*,c*,d*,e*)

B: $p(b|a)\; p(d|b,a)\; p(e|b,c)$

C: $p(c|a) \qquad \lambda_{B\to C}(a,c,d,e)$

D: $\lambda_{C\to D}(a,d,e)$

E: $\mathbb{1}[e=0] \quad \lambda_{D\to E}(a,e)$

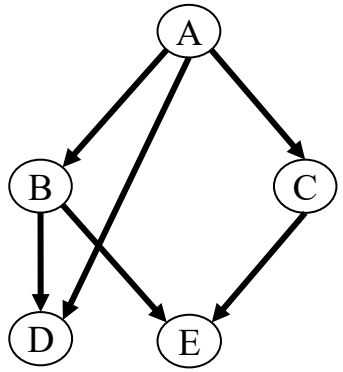
A: $p(a)\; \lambda_{E\to A}(a)$

OPT = optimal value

Outline

- Graphical Models
- Inference Tasks
- Variable Elimination
- **Tree Decompositions**
- Variable Orderings
- Learning from Data

Bucket Tree Elimination



$$p(A|E=0) = \alpha \sum_{e,d,c,b} p(A)\, p(b|A)\, p(c|A)\, p(d|A,b)\, p(e|b,c)\, \mathbb{1}[e=0]$$

E: $p(E|B,C)\mathbb{1}[E=0]$

D: $p(D|A,B)$

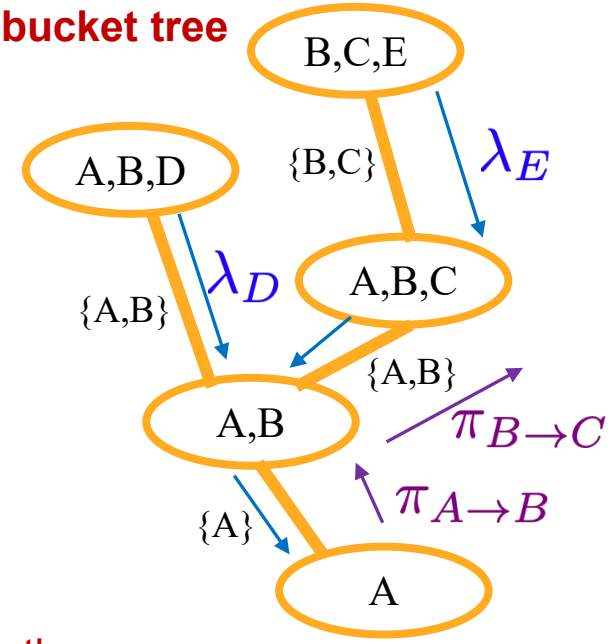
C: $p(C|A)$ $\lambda_E(B,C)$

B: $\lambda_D(A,B)$ $p(B|A)$ $\lambda_C(A,B)$

A: $p(A)$ $\lambda_B(A)$

Z = p(E=0)

View elimination as messages on a **bucket tree**



Can pass messages both ways:

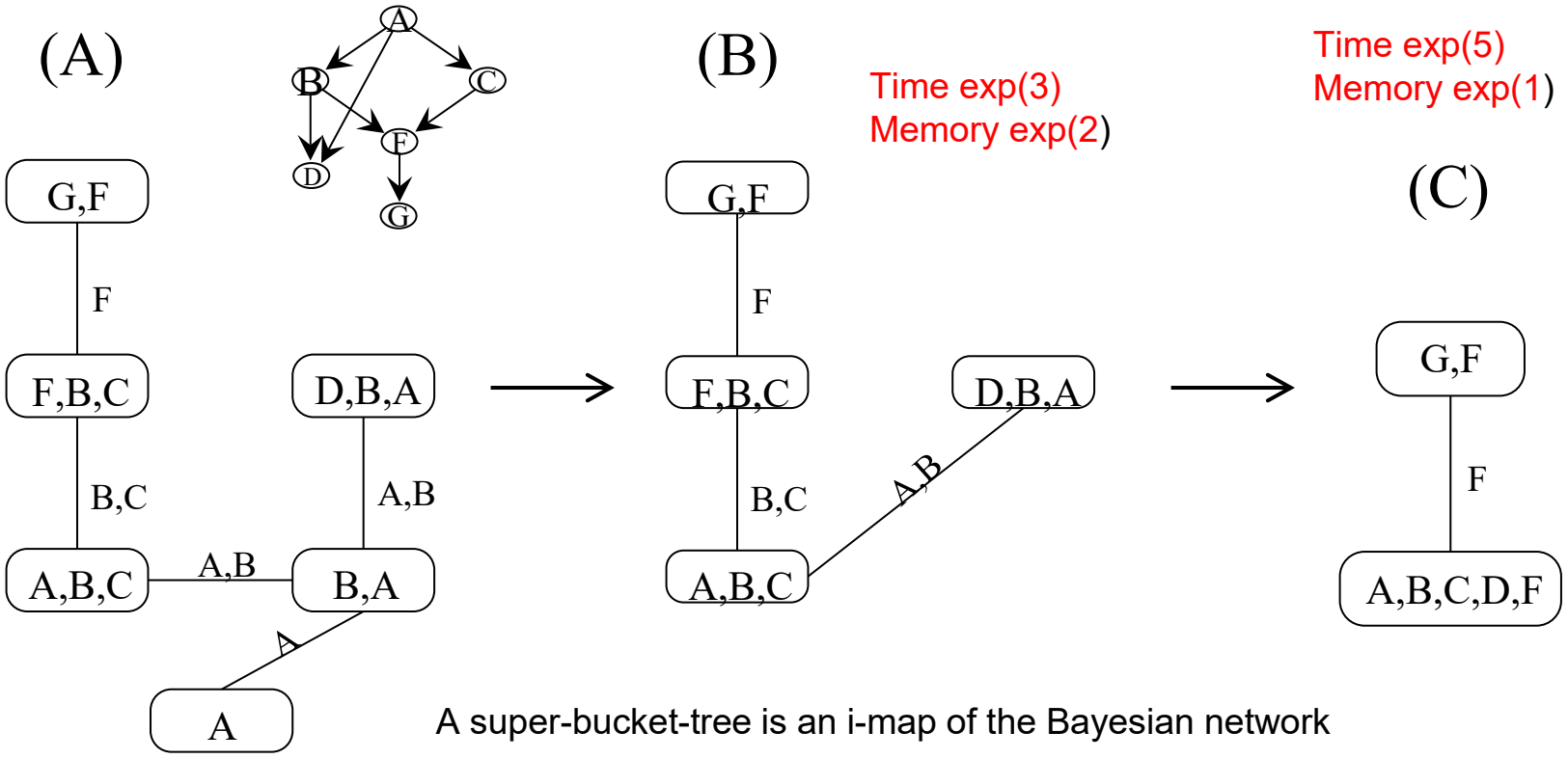
$$p(C|E=0) \propto p(C|A)\ \lambda_E(B,C)\ \pi_{B\to C}(A,B)$$

$$\pi_{B\to C}(A,B) = \lambda_D(A,B)\ p(B|A)\ \pi_{A\to B}(A)$$

$$\pi_{A\to B}(A) = p(A)$$

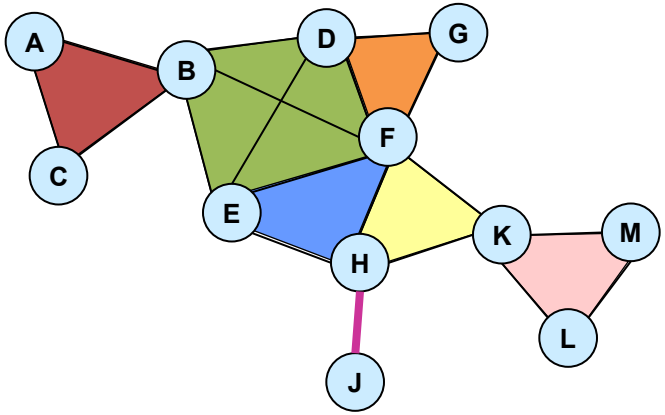
From Buckets to Clusters

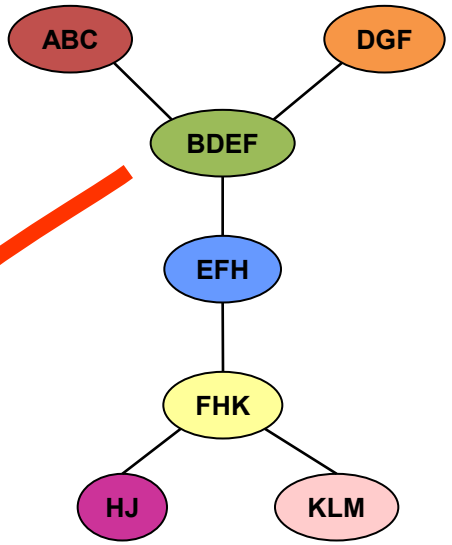
- Merge non-maximal buckets into maximal clusters.
- Connect clusters into a tree: each cluster to one with which it shares a largest subset of variables.
- Separators are variable- intersection on adjacent clusters.



A super-bucket-tree is an i-map of the Bayesian network

The General Tree-Decomposition





Inference algorithm:

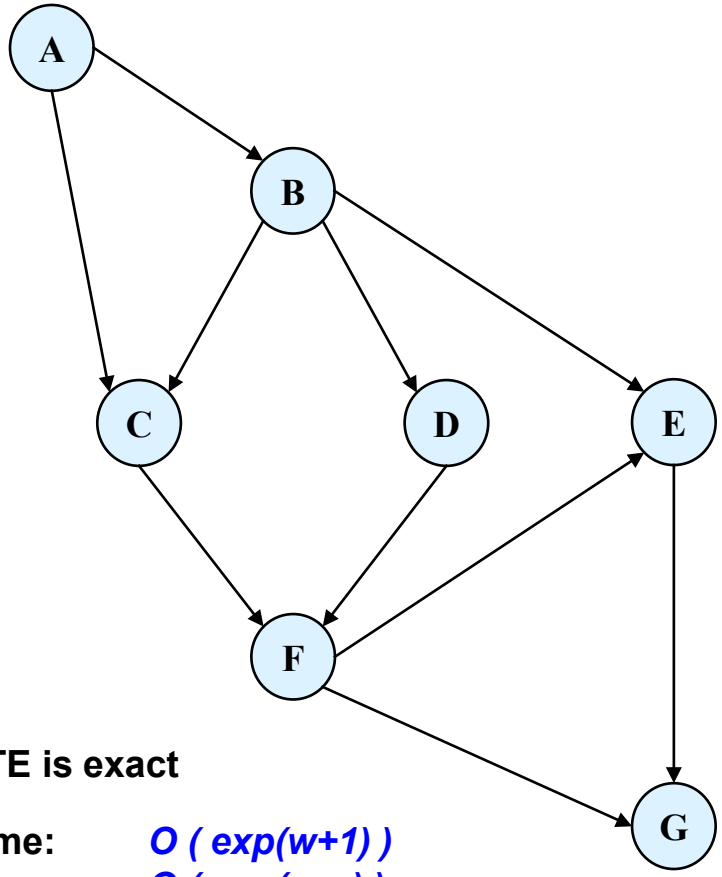
Time: exp(tree-width)

Space: exp(tree-width)

treewidth = 4 - 1 = 3

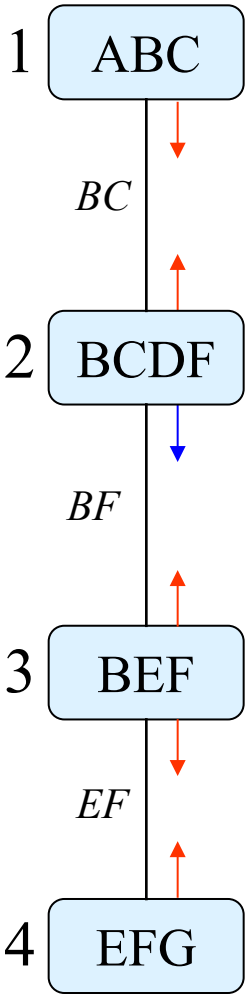
treewidth = (maximum cluster size) - 1

Cluster-Tree Elimination (CTE), or Join-tree message-passing



CTE is exact

Time: ***O (exp(w+1))***
Space: ***O (exp(sep))***



$$h_{(1,2)}(b,c) = \sum_{a} p(a) \cdot p(b \mid a) \cdot p(c \mid a,b)$$

$$h_{(2,1)}(b,c) = \sum_{d,f} p(d \mid b) \cdot p(f \mid c,d) \cdot h_{(3,2)}(b,f)$$

$$h_{(2,3)}(b,f) = \sum_{c,d} p(d \mid b) \cdot p(f \mid c,d) \cdot h_{(1,2)}(b,c)$$

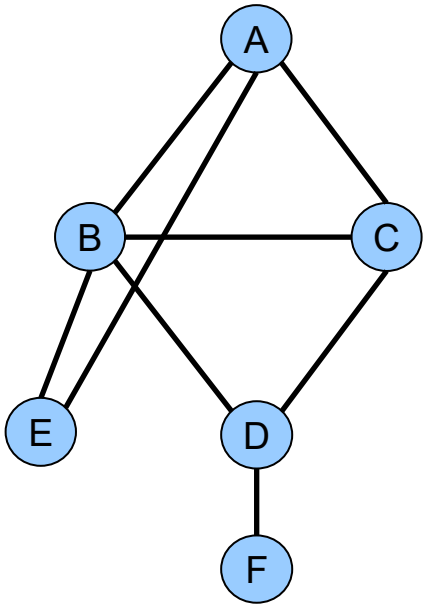
$$h_{(3,2)}(b,f) = \sum_{e} p(e \mid b,f) \cdot h_{(4,3)}(e,f)$$

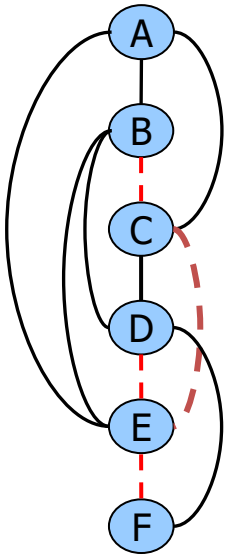
$$h_{(3,4)}(e,f) = \sum_{b} p(e \mid b,f) \cdot h_{(2,3)}(b,f)$$

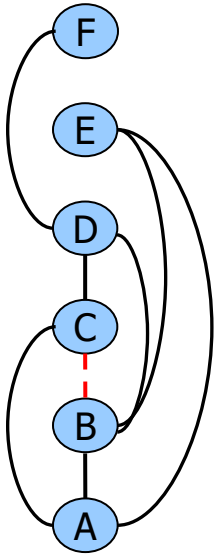
$$h_{(4,3)}(e,f) = p(G = g_e \mid e,f)$$

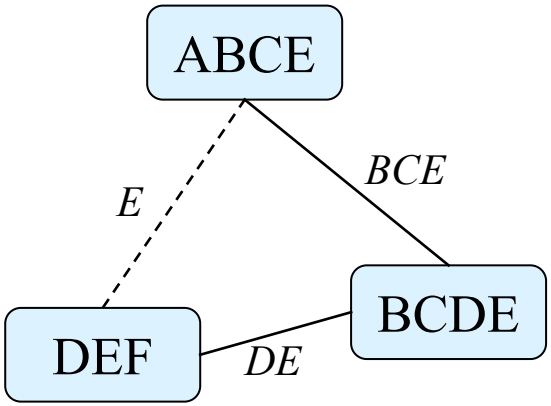
For each cluster P(X|e) is computed, also P(e)

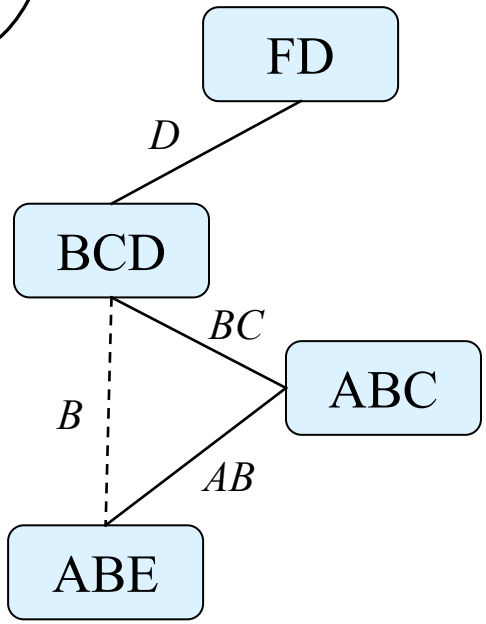
Examples of (Join)-Trees Construction









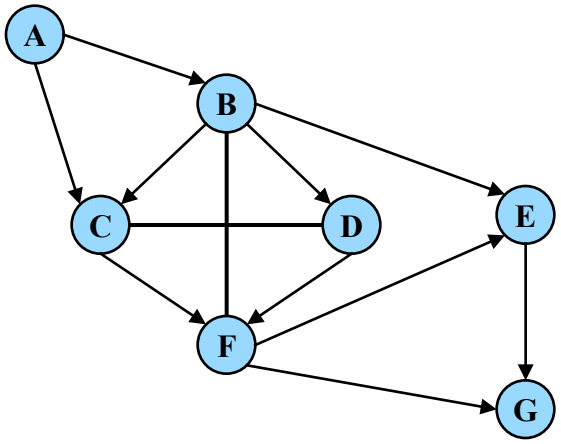


Tree and Hypertree Decompositions

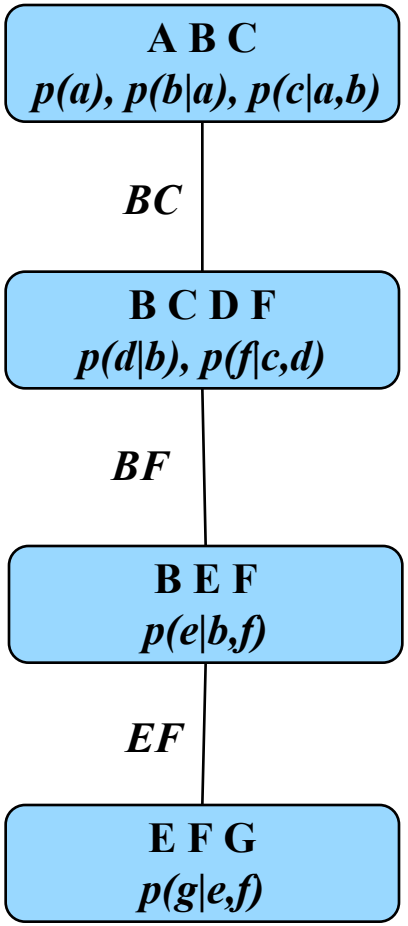
A *tree decomposition* for a belief network $BN =< X,D,G,P >$ is a triple $< T, \chi, \psi >$, where $T = (V,E)$ is a tree and χ and ψ are labeling functions, associating with each vertex $v \in V$ two sets, $\chi(v) \subseteq X$ and $\psi(v) \subseteq P$ satisfying :

1. For each function $p_i \in P$ there is exactly one vertex such that $p_i \in \psi(v)$ and $scope(p_i) \subseteq \chi(v)$
2. For each variable $X_i \in X$ the set $\{v \in V | X_i \in \chi(v)\}$ forms a connected subtree (running intersection property)

Connectedness, or
Running intersection property



Treewidth (w) = 3
Hyper tree-width (hw) =2



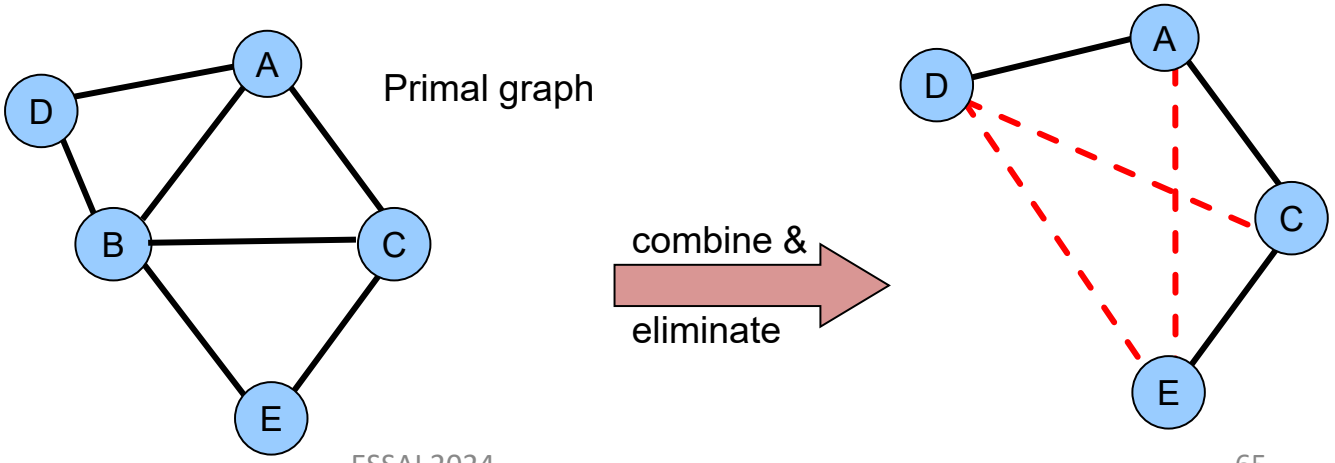
Tree decomposition

Outline

- Graphical Models
- Inference Tasks
- Variable Elimination
- Tree Decompositions
- **Variable Orderings**
- Learning from Data

Variable ordering heuristics

- What makes a good order?
  - Low induced width
  - Elimination creates a function over neighbors
- Finding the best order is hard (NP-complete!)
  - But we can do well with simple heuristics
    - Min-induced-width, Min-Fill, …
  - Anytime algorithms
    - Search-based [Gogate & Dechter 2003]
    - Stochastic (CVO) [Kask, Gelfand & Dechter 2010]

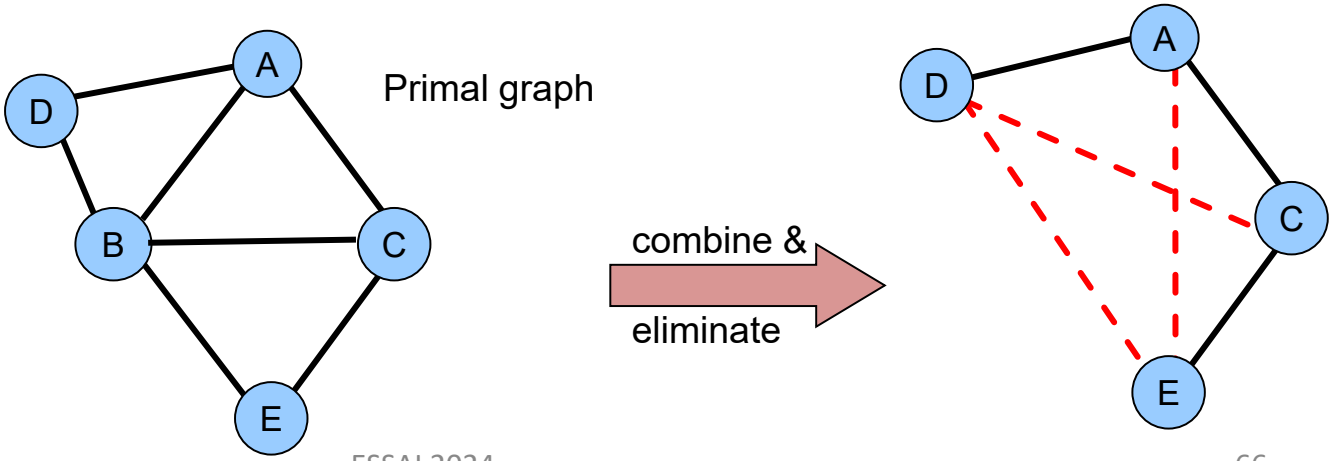


Variable ordering heuristics

- Min (induced) width heuristic

1. for i=1 to n (# of variables)
2. Select a node X_i with smallest degree as next eliminated
3. Connect Xi's neighbors:
4. E = E + { (X_i,X_k) : (X_i,X_j) and (X_i,X_k) in E }
5. Remove X_i from the graph: V = V – $\{X_i\}$
6. end

("Weighted" version: weight edges by domain size)

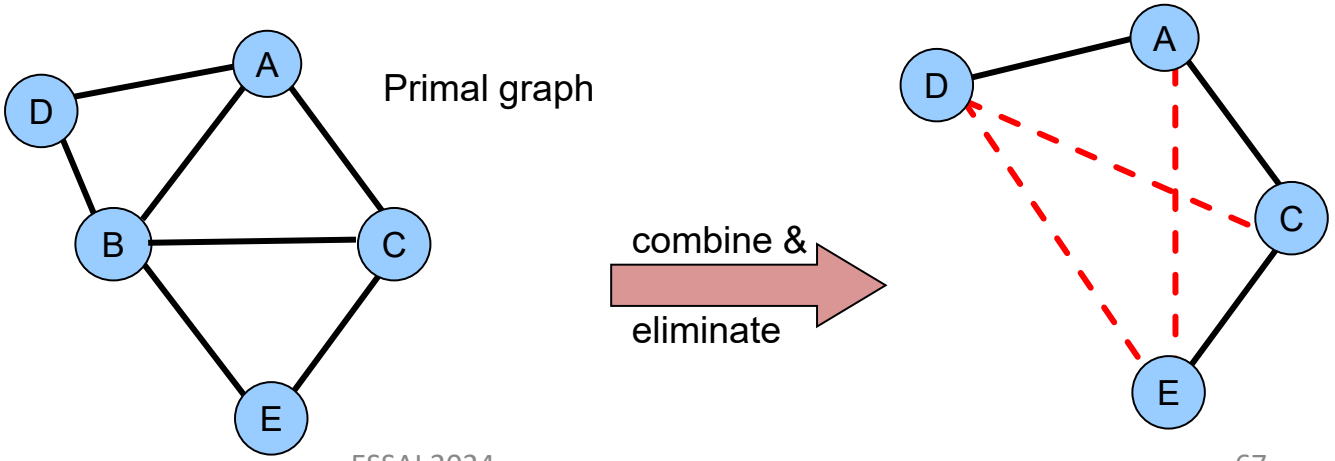


Variable ordering heuristics

- Min fill heuristic

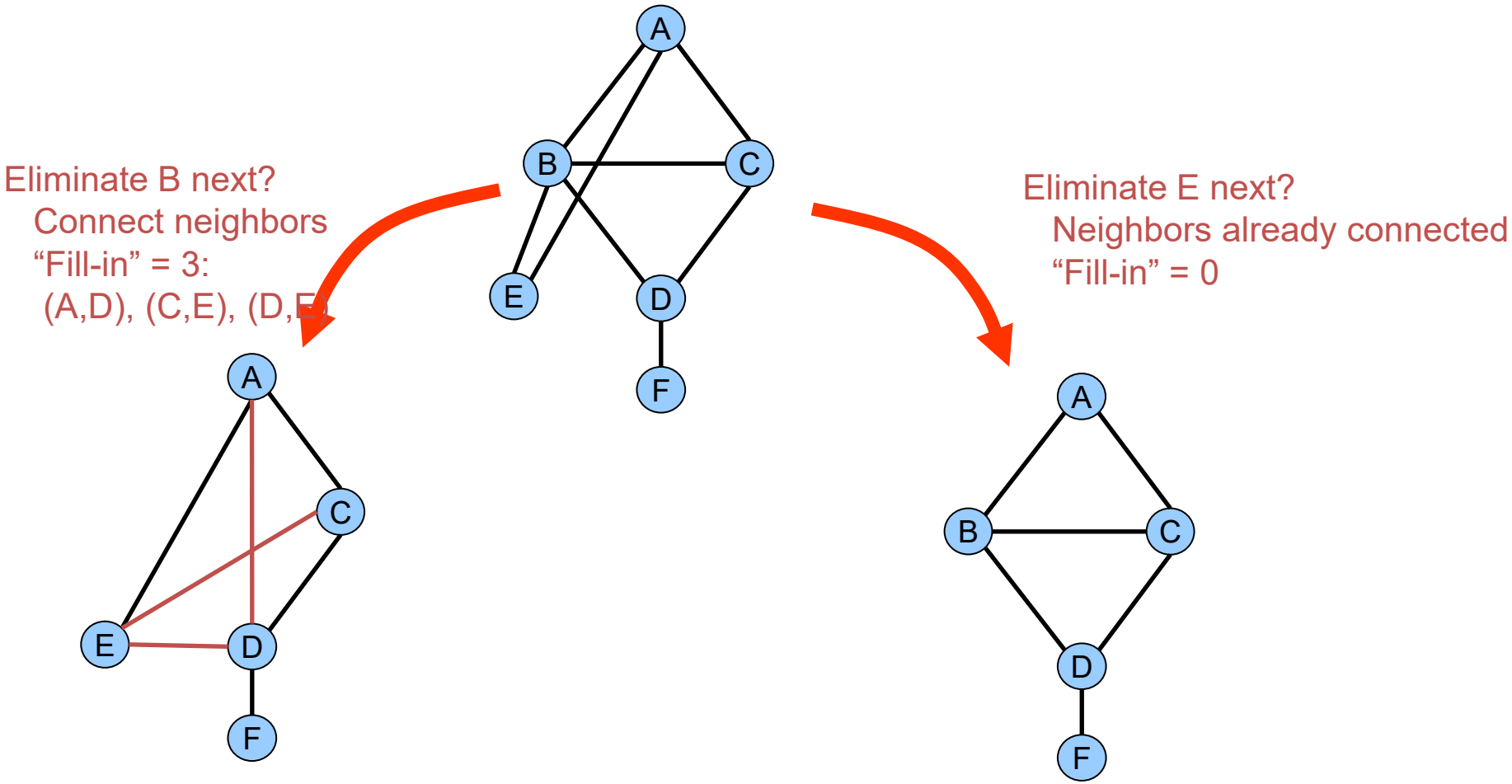
1. for i=1 to n (# of variables)
2. Select a node X_i with smallest "fill edges" as next eliminated
3. Connect Xi's neighbors:
4. E = E + { (X_j, X_k) : (X_i, X_j) and (X_i, X_k) in E }
5. Remove X_i from the graph: V = V – $\{X_i\}$
6. end

("Weighted" version: weight edges by domain size)



Min-Fill Heuristic

- Select the variable that creates the fewest “fill-in” edges



Outline

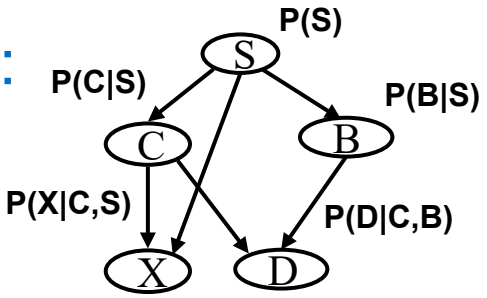
- Graphical Models
- Inference Tasks
- Variable Elimination
- Tree Decompositions
- Variable Orderings
- **Learning from Data**

Learning Bayesian networks

- Known graph? learn parameters:

  Complete data
  - parameter estimation (ML, MAP, …)

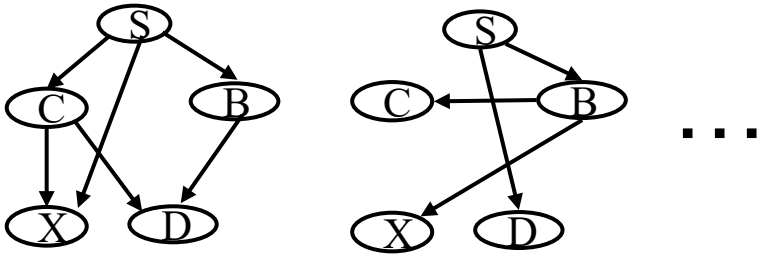
  Incomplete data
  - parameter optimization (gradient, EM, …)



- Unknown graph? learn graph and parameters

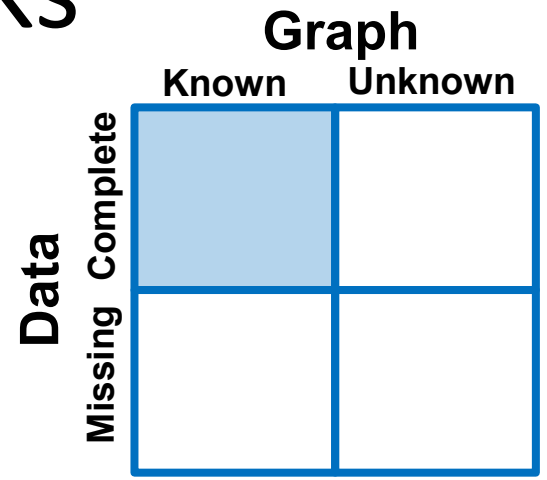
  Complete data
  - search over graphs (score-based, constraint-based)

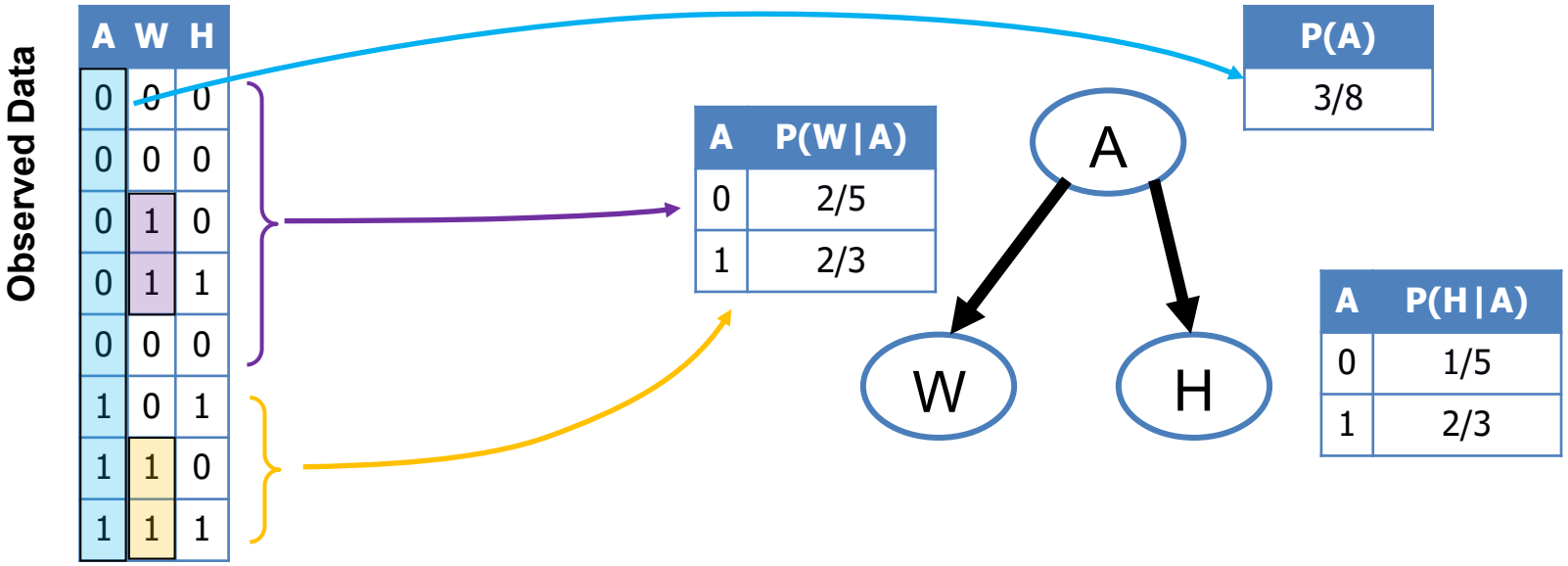
  Incomplete data
  - iterative optimization & search (structural EM, etc.)



Learning Bayesian networks

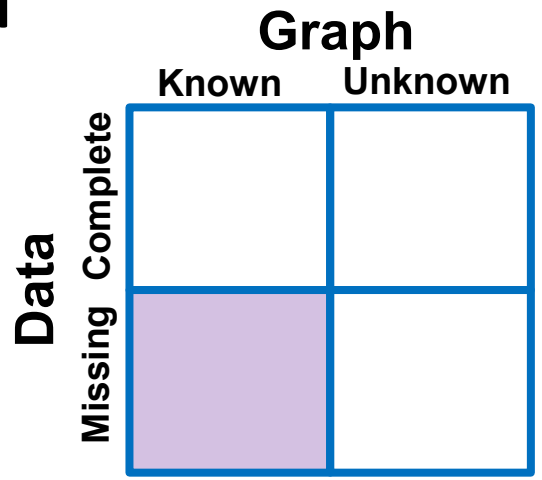
- Maximum Likelihood estimation
  - Select model that makes the data most probable
- For discrete X_i & no shared parameters
  - ML estimates are empirical probabilities





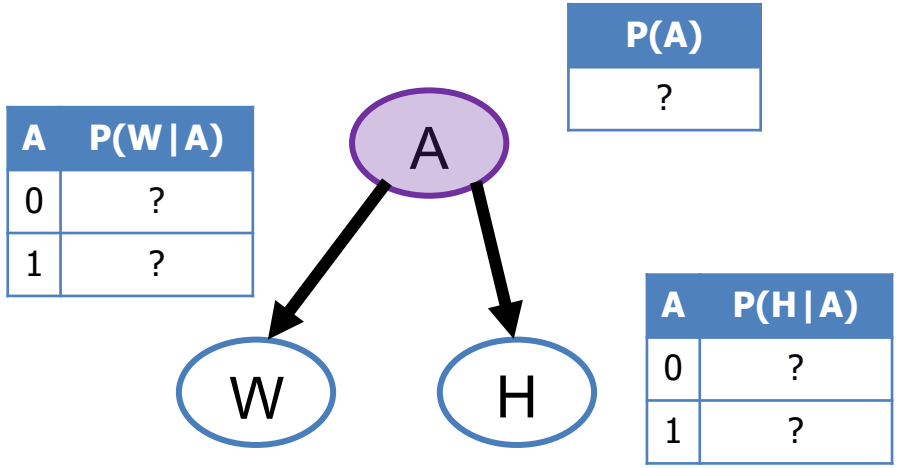
Learning with missing data

- Latent / hidden variables
  - Value is never observed
  - No unique model (e.g., symmetry)
  - No closed form solution; iterative ML
- More general missing values?
  - May depend on the reason for missingness!

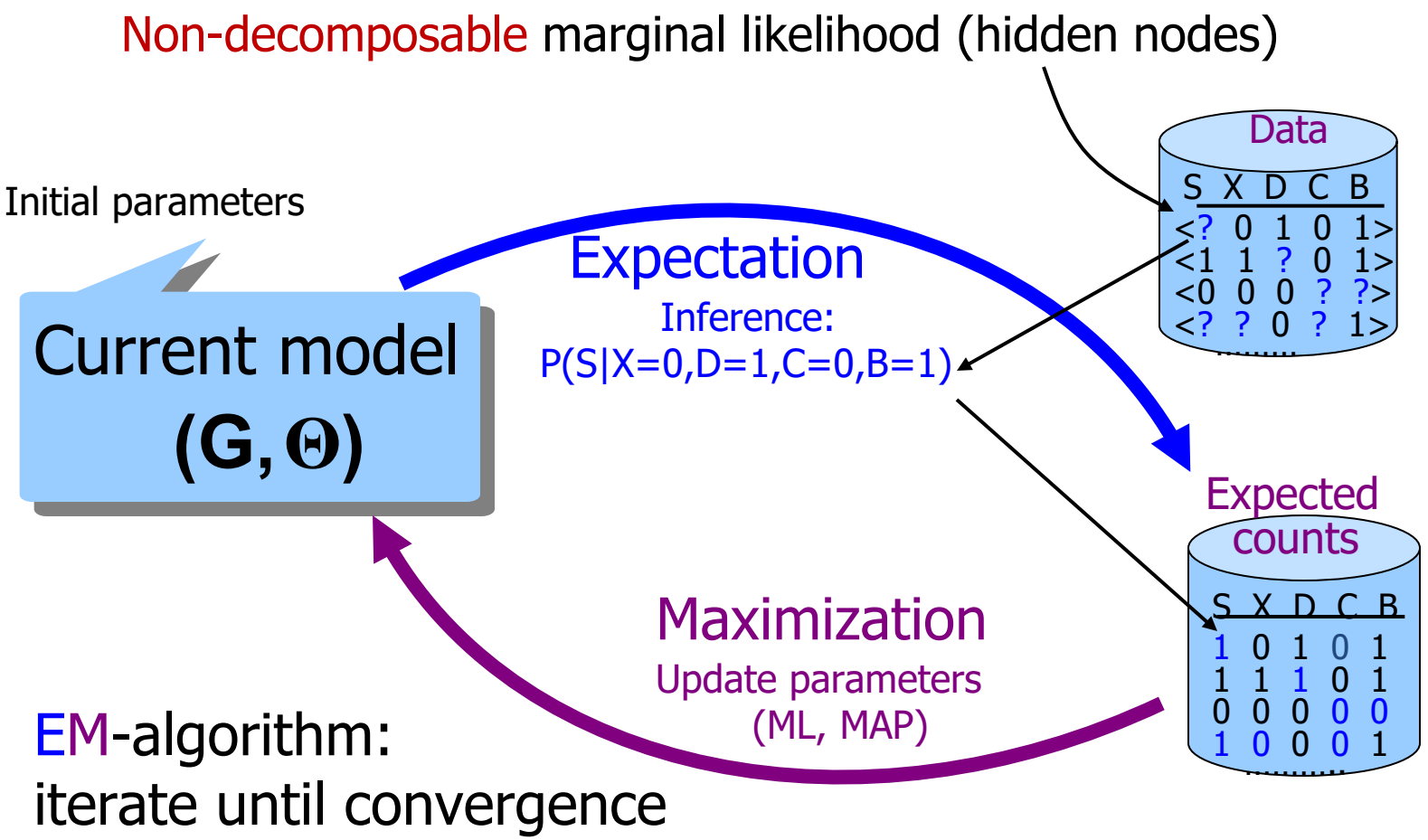


Observed Data

A	W	H
?	0	0
?	0	0
?	1	0
?	1	1
?	0	0
?	0	1
?	1	0
?	1	1



Learning with missing data

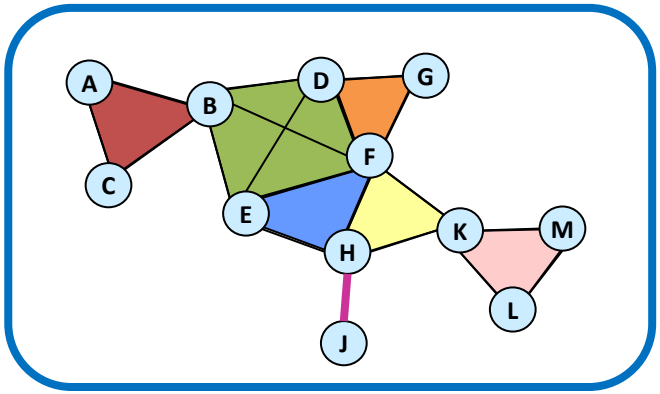


Summary

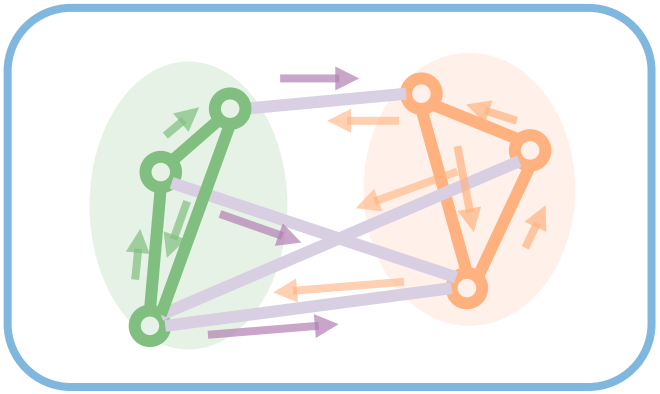
- Graphical Models
- Inference Tasks
- Variable Elimination
- Tree Decomposition
- Variable Orderings
- Learning from Data

Outline of Lectures

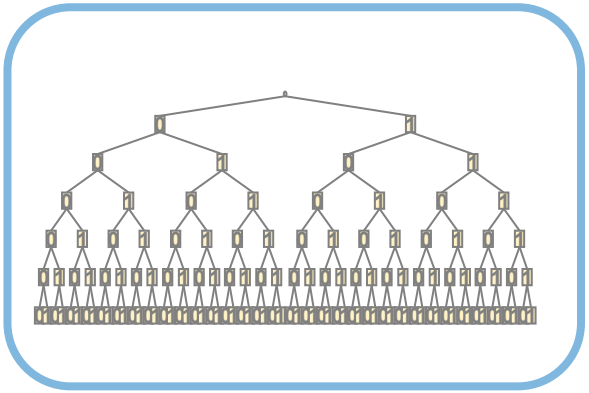
Class 1: Introduction & Inference



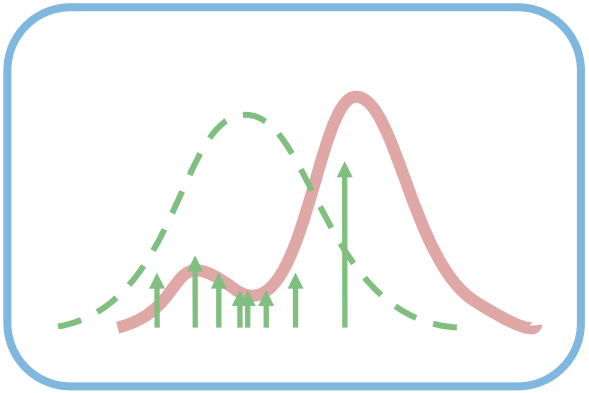
Class 2: Bounds & Variational Methods



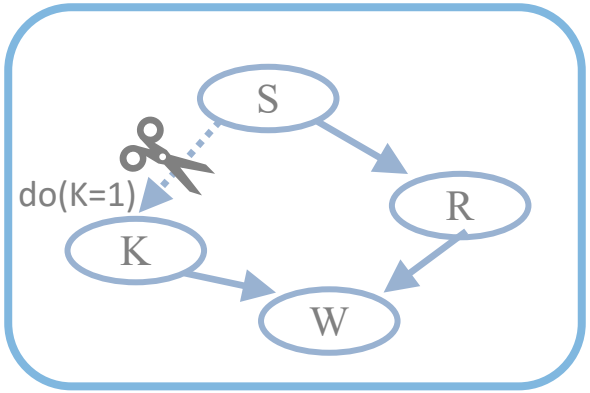
Class 3: Search Methods



Class 4: Monte Carlo Methods



Class 5: Causal Reasoning



Summary

- Formalisms for describing probabilistic & causal models
  - Bayesian networks, Influence Diagrams, Structural Causal Models
- Reasoning & Inference Queries
- Exact inference
  - Bucket elimination: time & memory exponential in the induced width.
  - Tree decomposition: organize computation into message-passing
  - Finding optimal induced width is hard, but greedy schemes work well
  - Inference task may restrict elimination orderings & increase width
- Learning from Data
  - Maximum likelihood learning
  - Easy case: match empirical statistics of the data