A Primer on Graphical Models

Almost completely built from materials of Prof Noah Smith (CMU) Prof David Sontag (NYU) Prof Eric Xing (CMU)

General ML Strategy

- **Represent** the world as a collection of random variables X_1, \ldots, X_n with joint distribution $p(X_1, \ldots, X_n)$
- 2 Learn the distribution from data
- OPERFORM "inference" (compute conditional distributions $p(X_i \mid X_1 = x_1, \dots, X_m = x_m)$)
- Ompute "**Likelihood**" of observed data/variables $p(X_{i_1},...,X_{i_k})$

Example:

Consider three binary-valued random variables

$$X_1, X_2, X_3$$
 $Val(X_i) = \{0, 1\}$

• Let outcome space Ω be the cross-product of their states:

$$\Omega = \operatorname{Val}(X_1) \times \operatorname{Val}(X_2) \times \operatorname{Val}(X_3)$$

- $X_i(\omega)$ is the value for X_i in the assignment $\omega \in \Omega$
- Specify $p(\omega)$ for each outcome $\omega \in \Omega$ by a big table:

• How many parameters do we need to specify?

$$2^3 - 1$$

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Marginalization

• Suppose X and Y are random variables with distribution p(X, Y)

X: Intelligence, $Val(X) = \{ \text{"Very High"}, \text{"High"} \}$

Y: Grade, $Val(Y) = \{ \text{"a", "b"} \}$

Joint distribution specified by:

- p(Y = a) = ?= 0.85
- More generally, suppose we have a joint distribution $p(X_1, ..., X_n)$. Then,

$$p(X_i = x_i) = \sum_{x_1} \sum_{x_2} \cdots \sum_{x_{i-1}} \sum_{x_{i+1}} \cdots \sum_{x_n} p(x_1, \dots, x_n)$$

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Conditioning

• Suppose X and Y are random variables with distribution p(X, Y)

X: Intelligence, $Val(X) = \{ \text{"Very High"}, \text{"High"} \}$

 $Y: Grade, Val(Y) = \{ \text{"a", "b"} \}$

Can compute the conditional probability

$$p(Y = a \mid X = vh) = \frac{p(Y = a, X = vh)}{p(X = vh)}$$

$$= \frac{p(Y = a, X = vh)}{p(Y = a, X = vh) + p(Y = b, X = vh)}$$

$$= \frac{0.7}{0.7 + 0.1} = 0.875.$$

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Example: Medical Diagonsis

- Variable for each symptom (e.g. "fever", "cough", "fast breathing", "shaking", "nausea", "vomiting")
- Variable for each disease (e.g. "pneumonia", "flu", "common cold", "bronchitis", "tuberculosis")
- Diagnosis is performed by **inference** in the model:

$$p(\text{pneumonia} = 1 \mid \text{cough} = 1, \text{fever} = 1, \text{vomiting} = 0)$$

 One famous model, Quick Medical Reference (QMR-DT), has 600 diseases and 4000 findings

Representing the distribution

- Naively, could represent multivariate distributions with table of probabilities for each outcome (assignment)
- How many outcomes are there in QMR-DT? 2^{4600}
- Estimation of joint distribution would require a huge amount of data
- Inference of conditional probabilities, e.g.

$$p(\text{pneumonia} = 1 \mid \text{cough} = 1, \text{fever} = 1, \text{vomiting} = 0)$$

would require summing over exponentially many variables' values

Structure through independence

• If X_1, \ldots, X_n are independent, then

$$p(x_1,\ldots,x_n)=p(x_1)p(x_2)\cdots p(x_n)$$

- 2^n entries can be described by just n numbers (if $|Val(X_i)| = 2$)!
- However, this is not a very useful model observing a variable X_i cannot influence our predictions of X_i
- If X_1, \ldots, X_n are conditionally independent given Y, denoted as $X_i \perp \mathbf{X}_{-i} \mid Y$, then

$$p(y, x_1, ..., x_n) = p(y)p(x_1 | y) \prod_{i=2}^n p(x_i | x_1, ..., x_{i-1}, y)$$

$$= p(y)p(x_1 | y) \prod_{i=2}^n p(x_i | y).$$

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cture1.pdf

Revisit: naïve Bayes for spam

- Classify e-mails as spam (Y = 1) or not spam (Y = 0)
 - Let 1: n index the words in our vocabulary (e.g., English)
 - $X_i = 1$ if word i appears in an e-mail, and 0 otherwise
 - E-mails are drawn according to some distribution $p(Y, X_1, \dots, X_n)$
- \bullet Suppose that the words are conditionally independent given Y. Then,

$$p(y, x_1, ..., x_n) = p(y) \prod_{i=1}^{n} p(x_i \mid y)$$

Estimate the model with maximum likelihood. Predict with:

$$p(Y = 1 \mid x_1, \dots x_n) = \frac{p(Y = 1) \prod_{i=1}^n p(x_i \mid Y = 1)}{\sum_{y=\{0,1\}} p(Y = y) \prod_{i=1}^n p(x_i \mid Y = y)}$$

As an Aside

 Are the independence assumptions made here reasonable?

 Philosophy: Nearly all probabilistic models are "wrong", but many are nonetheless useful

Observation

Any probability distribution $p(X_1,...,X_n)$ can always be expressed as follows:

$$p(X_1, ..., X_n) = \prod_{i=1}^n p(X_i | X_{C_i})$$

for some set $C_i \subset [n]$.

We call this set parent of i and henceforth denote by pa_i .

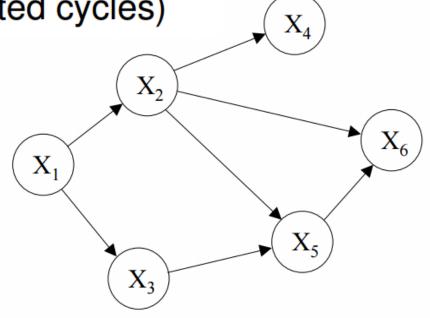
Visualization always helps!

Algebra is boring, so let's draw this

- Let's represent variables as circles
- Let's draw an arrow from j to i if $j \in pa_i$
- The resulting drawing will be a Directed Graph

Moreover it will be Acyclic (no directed cycles)

Llatent variable / latent parameter	var
Observed variable	obs
Constant / hyper parameter	const



Bayesian Network

- A **Bayesian network** is specified by a directed *acyclic* graph G = (V, E) with:
 - ① One node $i \in V$ for each random variable X_i
 - ② One conditional probability distribution (CPD) per node, $p(x_i \mid \mathbf{x}_{Pa(i)})$, specifying the variable's probability conditioned on its parents' values
- Corresponds 1-1 with a particular factorization of the joint distribution:

$$p(x_1,\ldots x_n)=\prod_{i\in V}p(x_i\mid \mathbf{x}_{\mathrm{Pa}(i)})$$

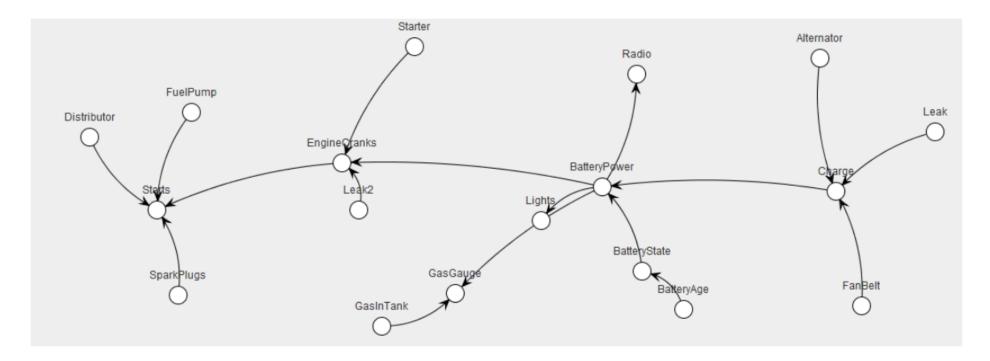
 Powerful framework for designing algorithms to perform probability computations

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Examples

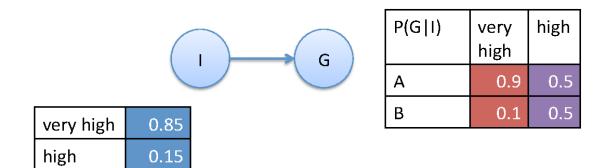
$$p(x_1,\ldots x_n)=\prod_{i\in V}p(x_i\mid \mathbf{x}_{\mathrm{Pa}(i)})$$

Will my car start this morning?



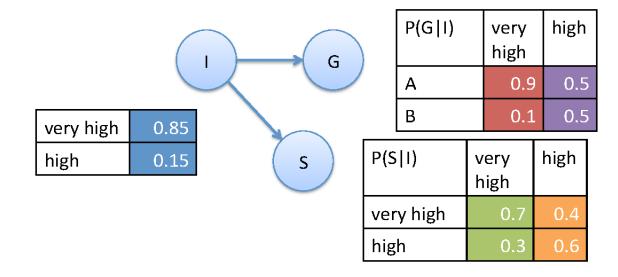
Conditional Parameterization

Grade is determined by Intelligence.



Conditional Parameterization

• Grade and SAT score are determined by Intelligence: $G \perp S \mid I$



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More drawing skills

- Drawing these figures can get messy for large models!
- How do we compactly represent repeated structure?

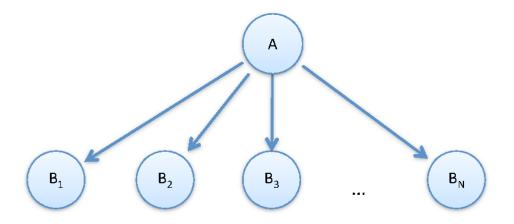
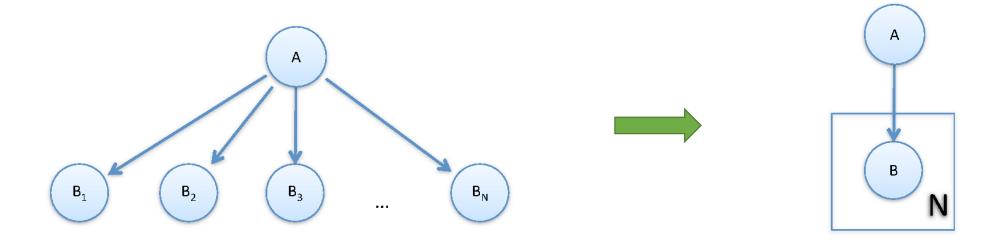
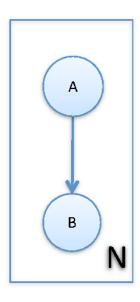


Plate Model



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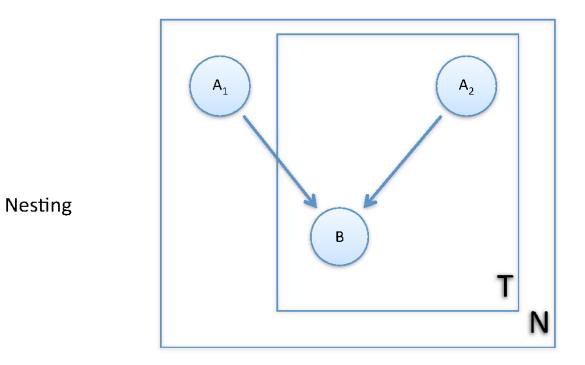
Students and their Grades



Example: A = student, B = grade

Student, Course, Grade, Difficulty

Each student takes only one course

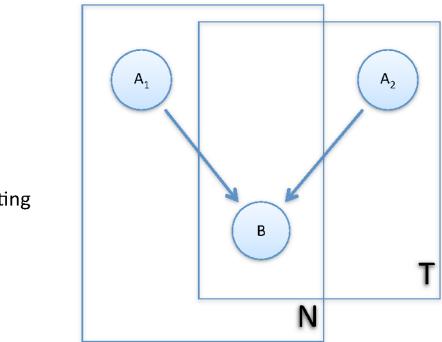


Example: A_1 = course difficulty, A_2 = student aptitude for the area, B = grade

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Student, Course, Grade, Difficulty

Multiple courses per student



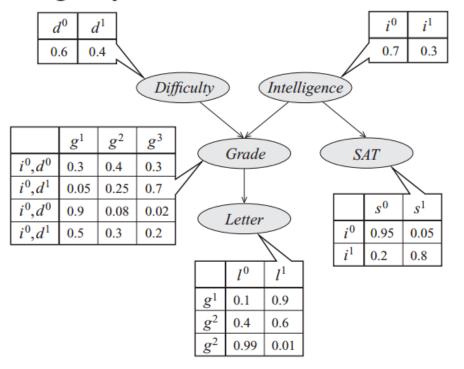
Intersecting

Example: A_1 = assignment difficulty, A_2 = intelligence, B = grade

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Detailed Example

Consider the following Bayesian network:



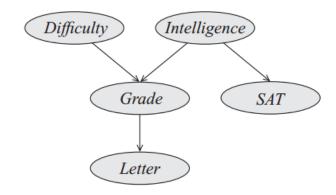
• What is its joint distribution?

$$p(x_1, \dots x_n) = \prod_{i \in V} p(x_i \mid \mathbf{x}_{Pa(i)})$$

$$p(d, i, g, s, l) = p(d)p(i)p(g \mid i, d)p(s \mid i)p(l \mid g)$$

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Independencies



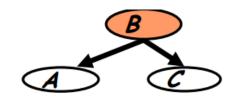
- The joint distribution corresponding to the above BN factors as $p(d, i, g, s, l) = p(d)p(i)p(g \mid i, d)p(s \mid i)p(l \mid g)$
- However, by the chain rule, any distribution can be written as $p(d, i, g, s, l) = p(d)p(i \mid d)p(g \mid i, d)p(s \mid i, d, g)p(l \mid g, d, i, g, s)$
- Thus, we are assuming the following additional independencies: $D \perp I$, $S \perp \{D, G\} \mid I$, $L \perp \{I, D, S\} \mid G$. What else?

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Generalizing

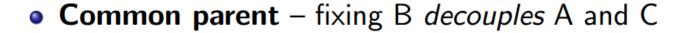
 Generalizing the above arguments, we obtain that a variable is independent from its non-descendants given its parents

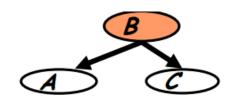
• Common parent – fixing B decouples A and C



Generalizing

 Generalizing the above arguments, we obtain that a variable is independent from its non-descendants given its parents





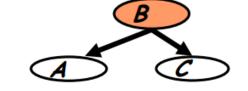
Proof: From the graph we have p(A, B, C) = p(B)p(A|B)p(C|B). Now we can evaluate using Bayes rule as:

$$p(A, C|B) = \frac{p(A, B, C)}{p(B)}$$
$$= \frac{p(B)p(A|B)p(C|B)}{p(B)}$$
$$= p(A|B)p(C|B)$$

Thus showing the conditional independence.

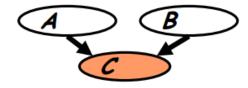
Generalizing

 Generalizing the above arguments, we obtain that a variable is independent from its non-descendants given its parents



- Common parent fixing B decouples A and C
- Cascade knowing B decouples A and C

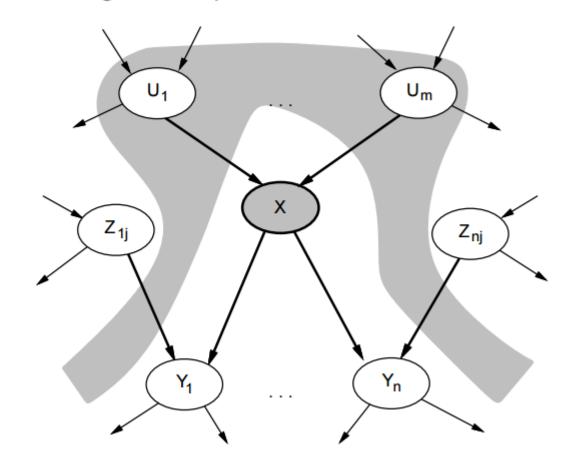




- **V-structure** Knowing C *couples* A and B
 - This important phenomona is called explaining away and is what makes Bayesian networks so powerful

More properties

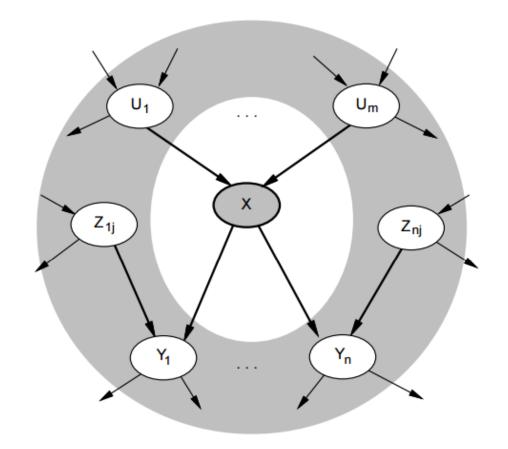
Local semantics: each node is conditionally independent of its nondescendants given its parents



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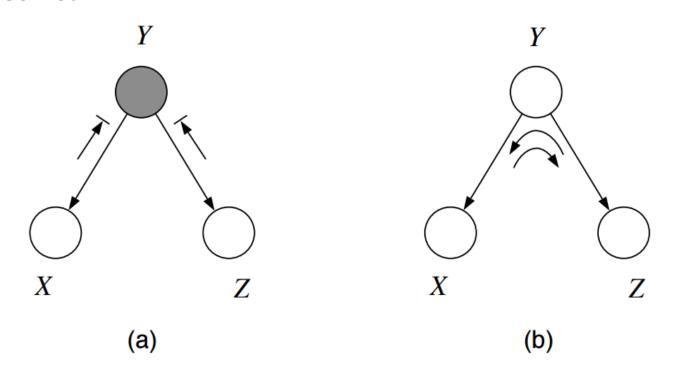
More Properties

Each node is conditionally independent of all others given its Markov blanket: parents + children + children's parents



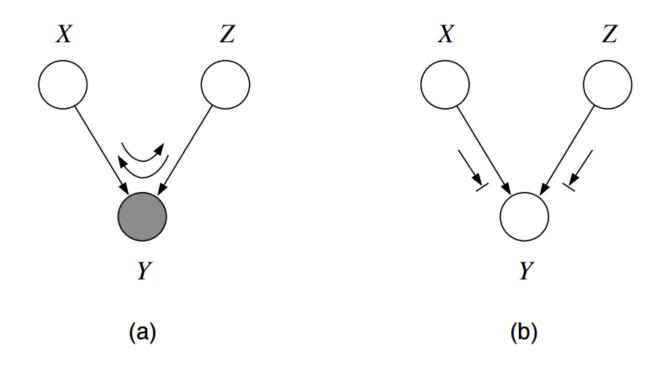
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- Algorithm to calculate whether $X \perp Z \mid \mathbf{Y}$ by looking at graph separation
- Look to see if there is active path between X and Z when variables
 Y are observed:



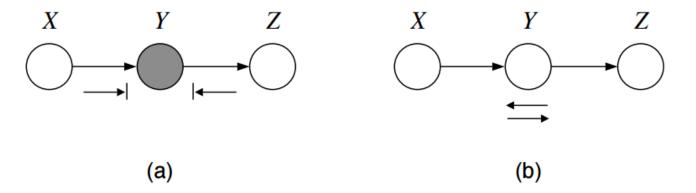
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- Algorithm to calculate whether $X \perp Z \mid \mathbf{Y}$ by looking at graph separation
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- Algorithm to calculate whether $X \perp Z \mid \mathbf{Y}$ by looking at graph separation
- Look to see if there is active path between X and Z when variables
 Y are observed:



• If no such path, then X and Z are conditionally independent given Y

 This reduces statistical independencies (hard) queries to connectivity in graphs (easy)

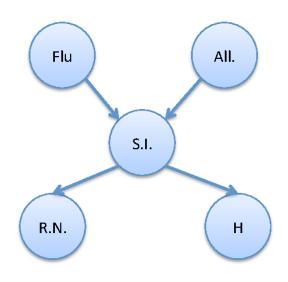
 Important because it allows us to quickly prune the Bayesian network, finding just the relevant variables for answering a query

Causal Structure

- The flu causes sinus inflammation
- Allergies also cause sinus inflammation
- Sinus inflammation causes a runny nose
- Sinus inflammation causes headaches

Causal Structure

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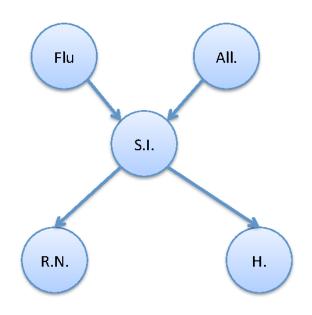


Querying the Model

 Inference (e.g., do you have allergies?)

What's the best explanation?

 Active data collection (what is the next best r.v. to observe?)

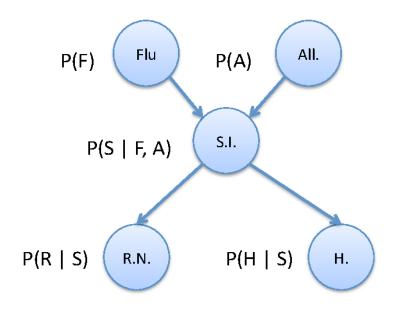


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Factored Joint Distribution

Want:

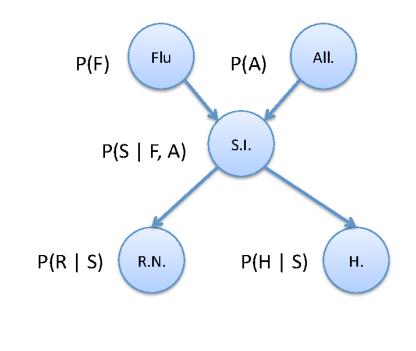
 P(F, A, S, R, H)
 = P(F)
 P(A)
 P(S | F, A)
 P(R | S)
 P(H | S)



Factored Joint Distribution

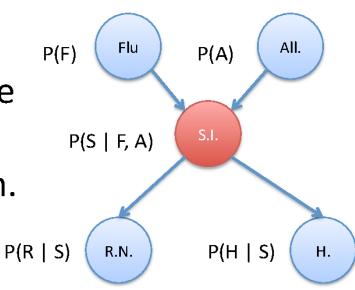
Want:

 P(F, A, S, R, H)
 = P(F)
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 P(H | S)



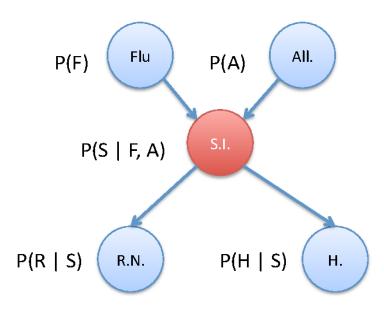
How many parameters?

 Notice: knowing the value of S separates the other variables from each other in the graph.



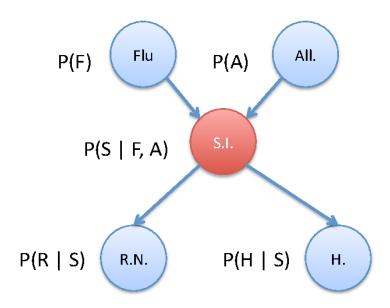
• In this model, ¬ R ⊥ H

1



- In this model, ¬ R ⊥ H
- But: R ⊥ H | S



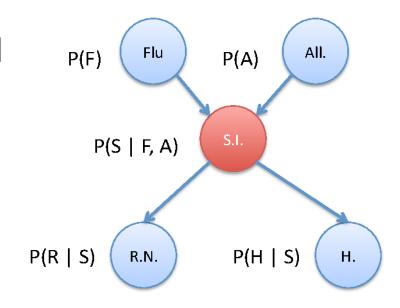


• In this model, ¬ R ⊥ H

• But: R ⊥ H | S

• Also: ¬ A ⊥ H

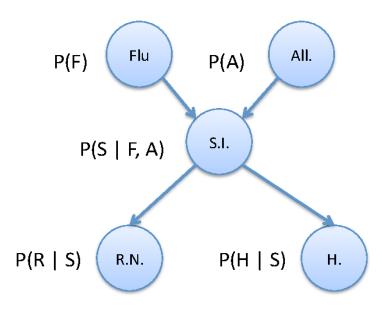
But: A ⊥ H | S



Marginal Independence

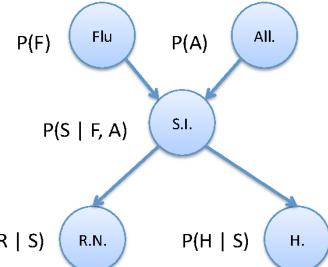
- In this model, $F \perp A$
- P(F, A) = P(F) P(A)

3



Marginal Independence

- In this model, F ⊥ A
- P(F, A) = P(F) P(A)



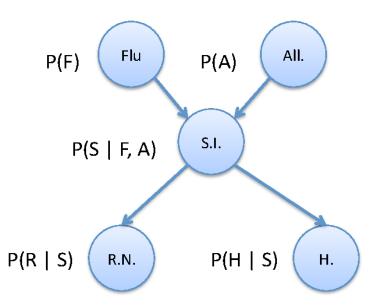
Marginal independence of a set:

$$\forall Y \subseteq X, Z \subseteq X, Y \perp Z$$

• Let **X** = {A, F}

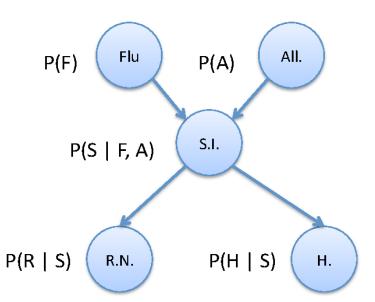
Conditional Independence

- In this model, ¬ F ⊥ H
- P(F, H) = P(F | H) P(H)
 ≠ P(F) P(H), in general



Conditional Independence

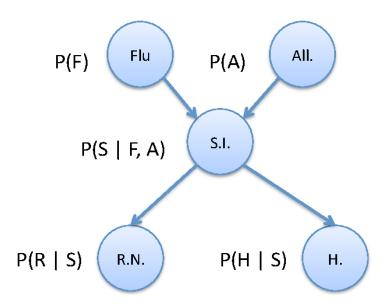
- In this model, ¬ F ⊥ H
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 ≠ P(F) P(H), in general



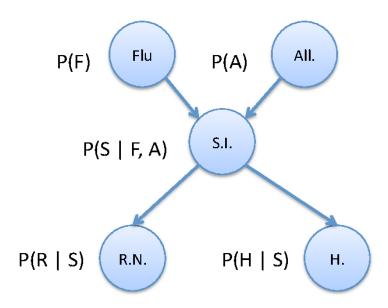
Given S, however ...

- F⊥H | S
- P(F, H | S) = P(F | S) P(H | S)
 - How do we know this?

• F⊥A | ∅

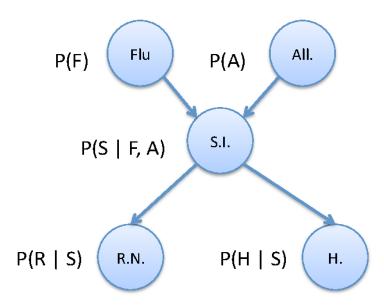


- F⊥A | ∅
- A ⊥ F | ∅



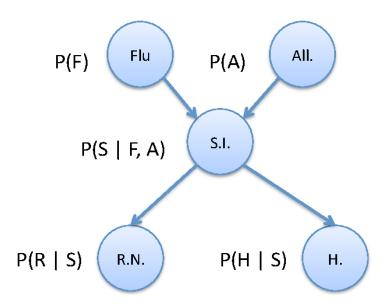
- F⊥A | ∅
- A ⊥ F | Ø

• R ⊥ {F, A, H} | S



- F⊥A | ∅
- A ⊥ F | Ø

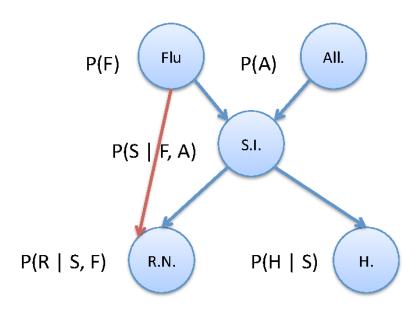
- R ⊥ {F, A, H} | S
- H ⊥ {F, A, R} | S



New Edge: What's Independent?

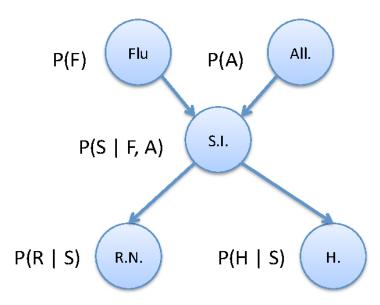
- F⊥A | ∅
- A ⊥ F | Ø

- R ⊥ {F, A, H} | S, F
- H ⊥ {F, A, R} | S



A Puzzle

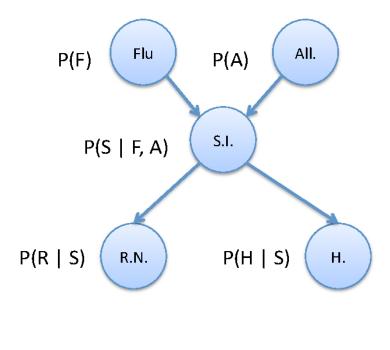
• F⊥A | S?

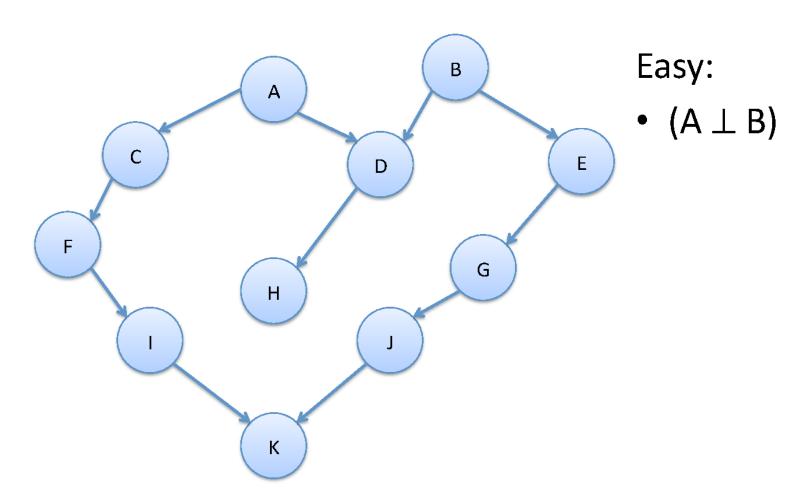


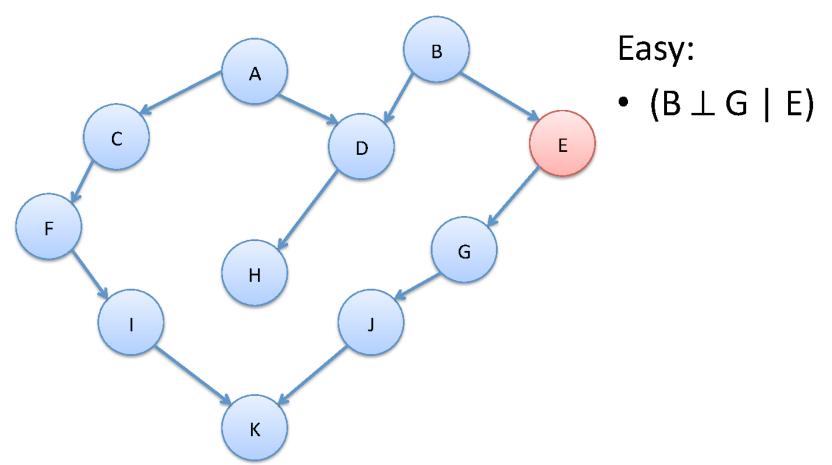
A Puzzle

• F⊥A | S?

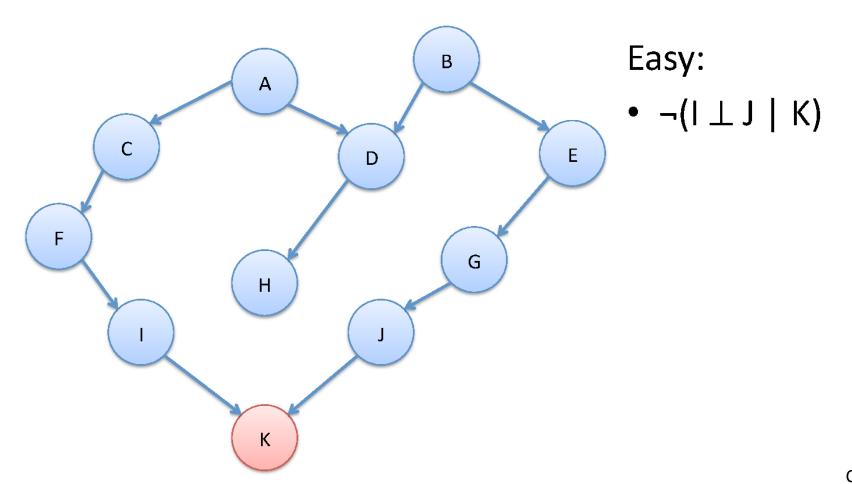
- In general, **no**.
 - This independence statement does not follow from the Local Markov assumption.
- ¬ (F ⊥ A | S)



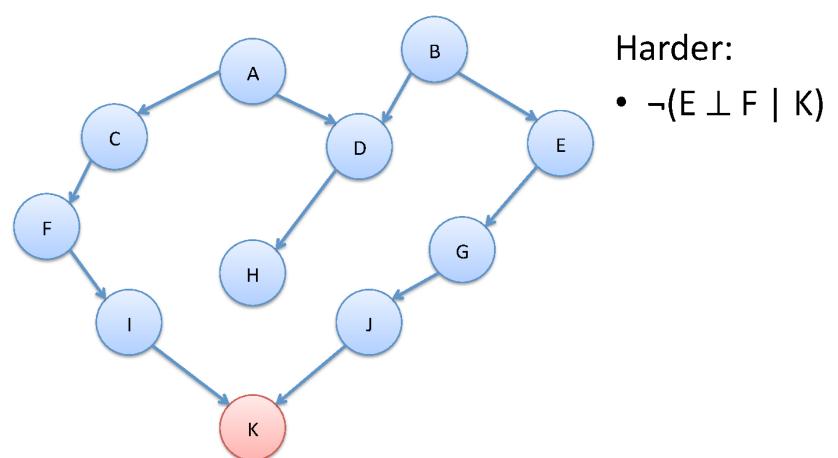




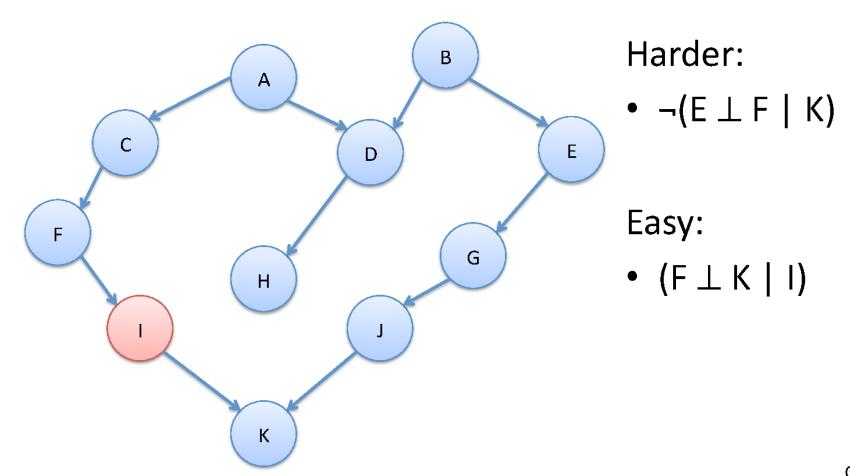
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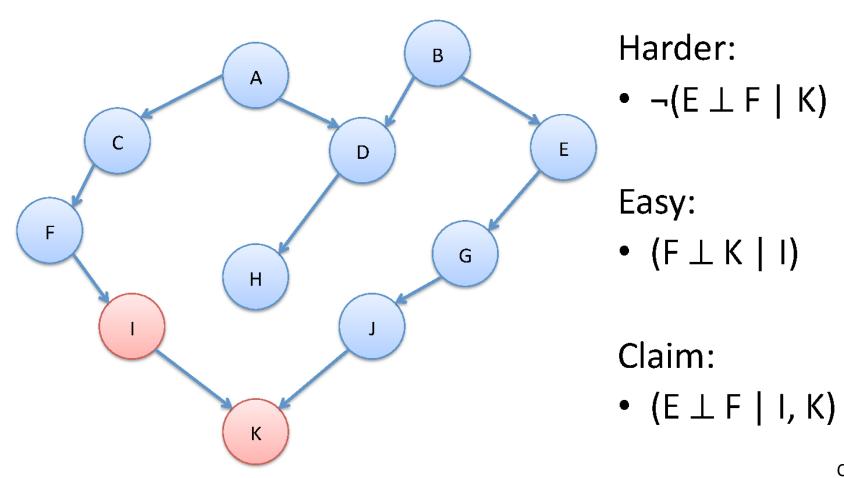
V-Structure!



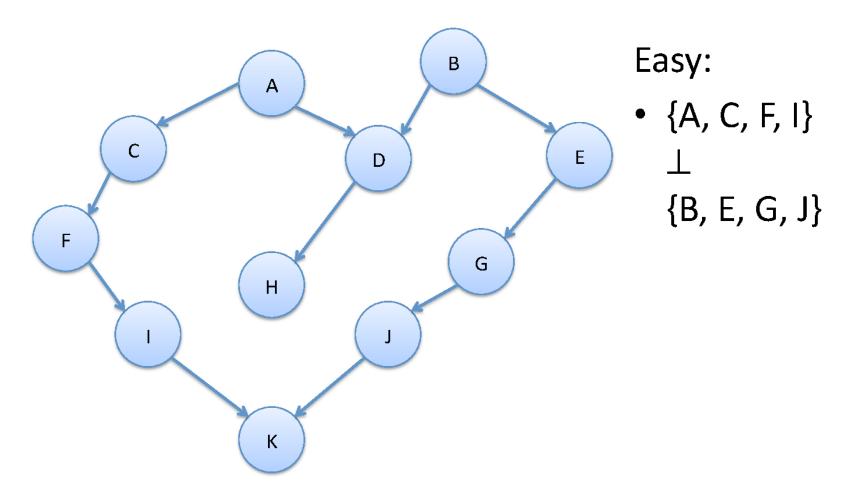
"Flow of influence" along chains



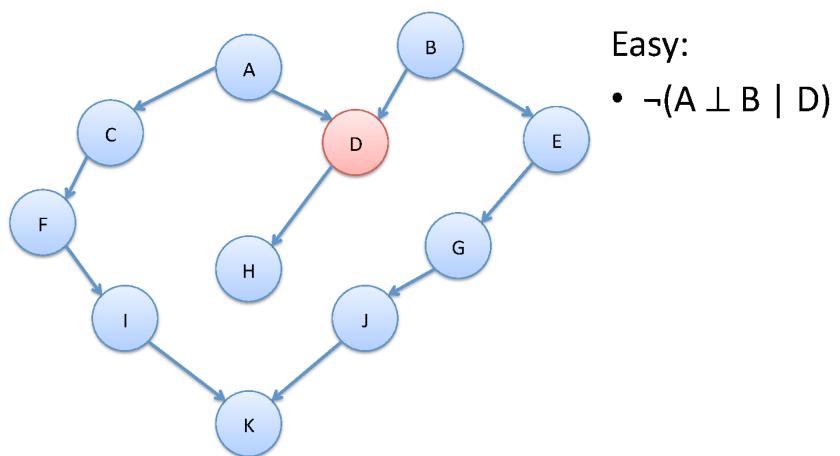
Local Markov Assumption for K!



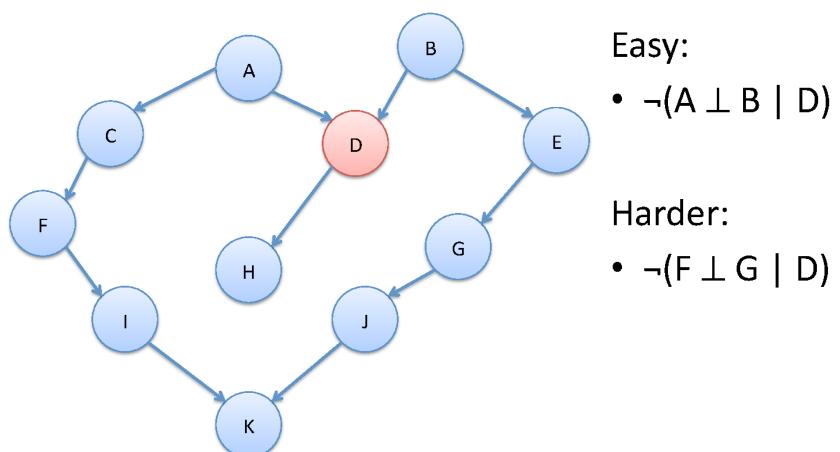
Interaction?



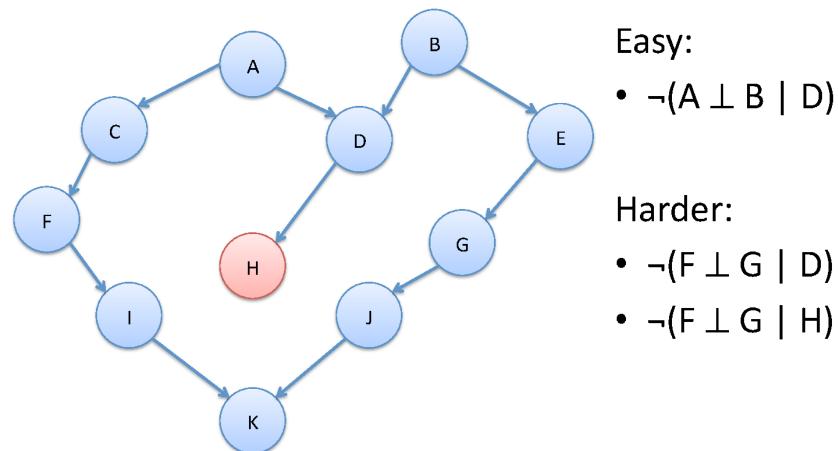
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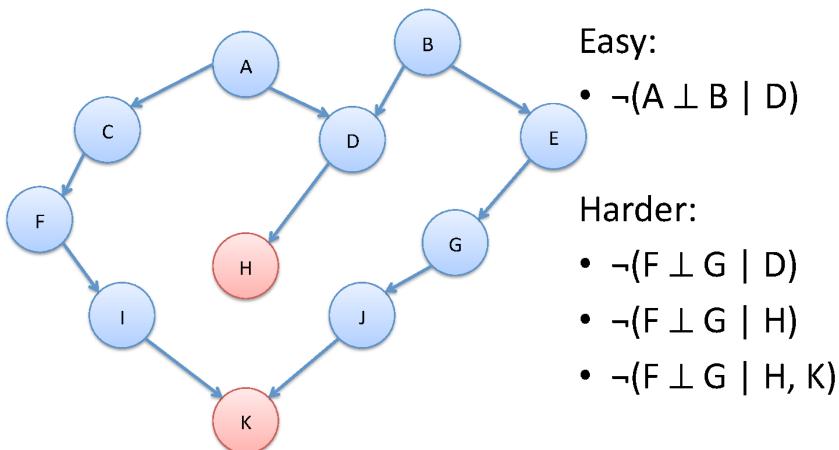
V-Structure!



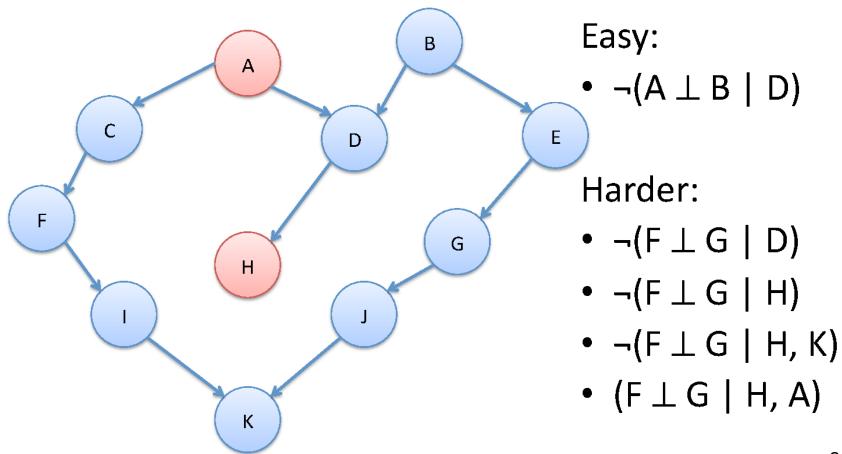
"Flow of influence" again.

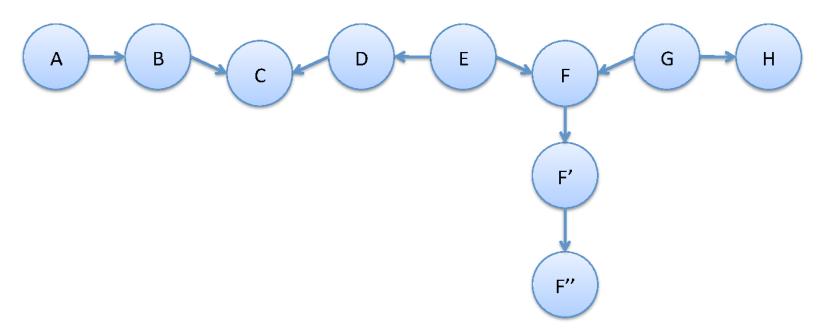


Flow of influence, again?

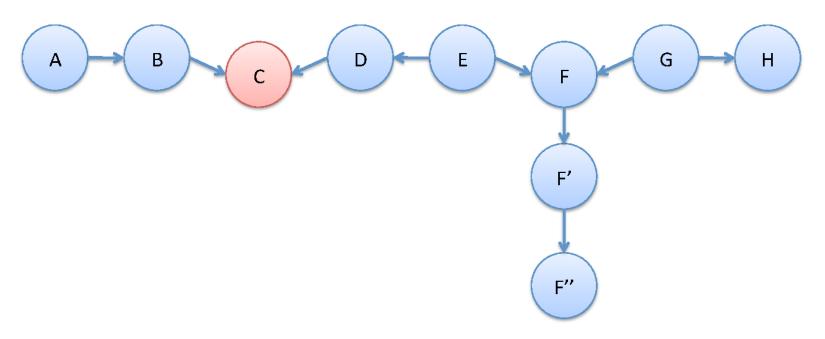


More flow of influence!

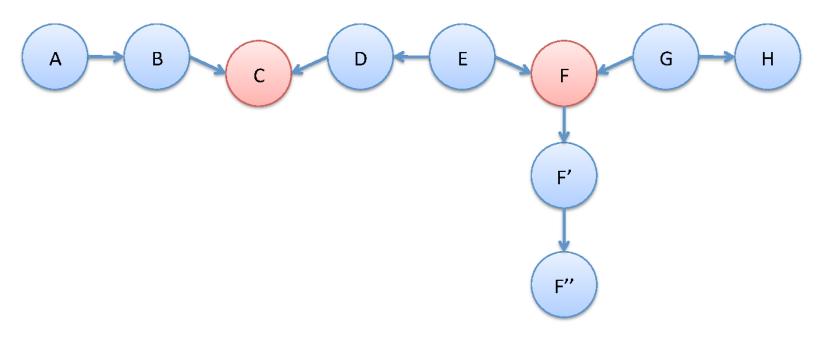




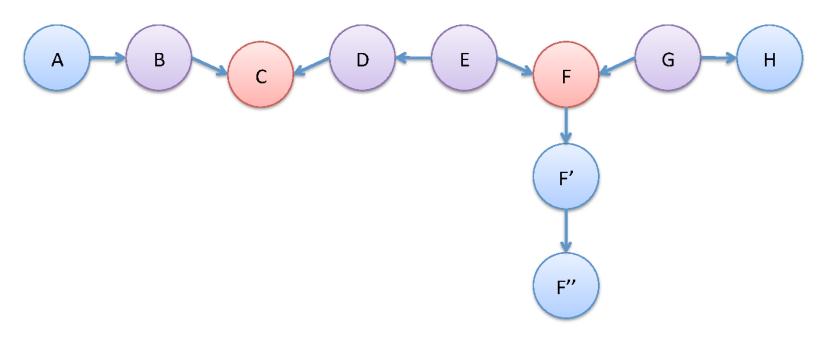
• If I observe nothing, then $A \perp H$.



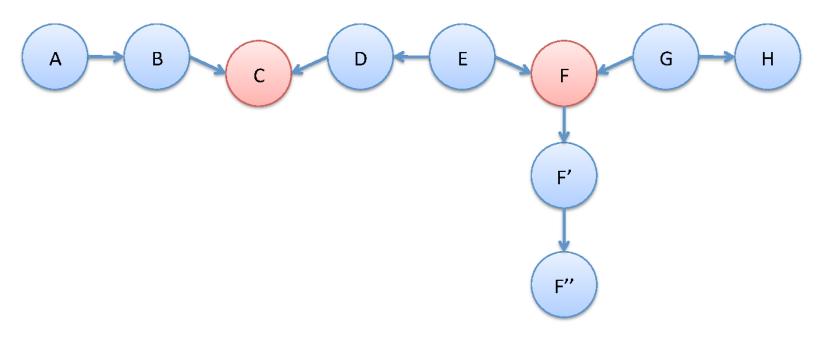
• If I observe C, then $A \perp H$.



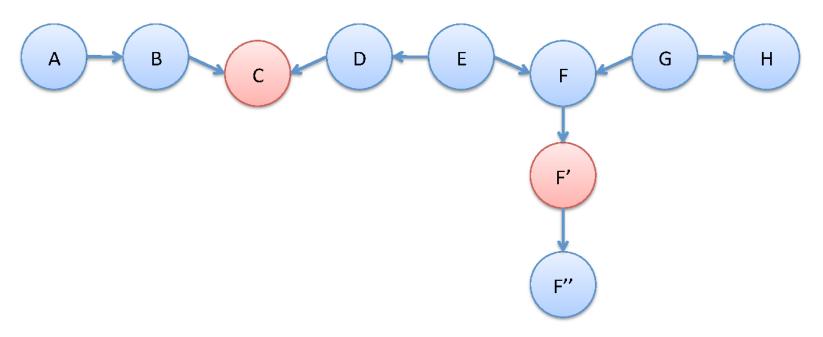
• If I observe C and F, then $\neg(A \perp H)$.



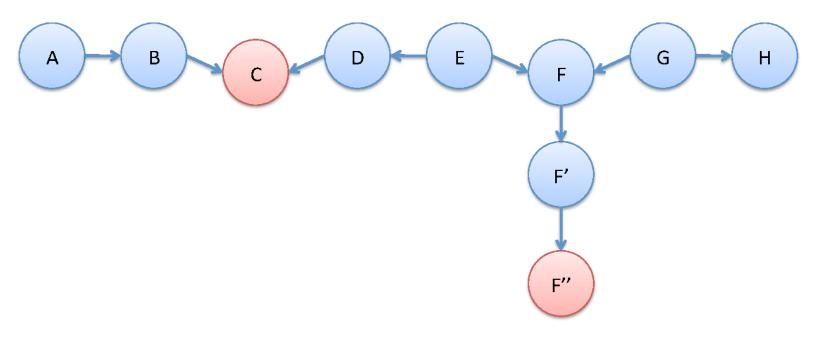
- If I observe C and F, then $\neg(A \perp H)$.
 - But if I observe B, D, E, and/or G, then A \perp H.



• If I observe C and F, then $\neg(A \perp H)$.



• If I observe C and F', then $\neg(A \perp H)$.



• If I observe C and F", then $\neg(A \perp H)$.

The Real Inference Problem

• Given a Bayesian network over X, and a value $x \in Val(X_i)$, compute $P(X_i = x)$.

$$P(X_i = x) = \sum_{x_{-i} \in Val(X_{-i})} P(X_1 = x_1, ..., X_i = x, ..., X_n = x_n)$$

- Assume we are given a graphical model.
- Want:

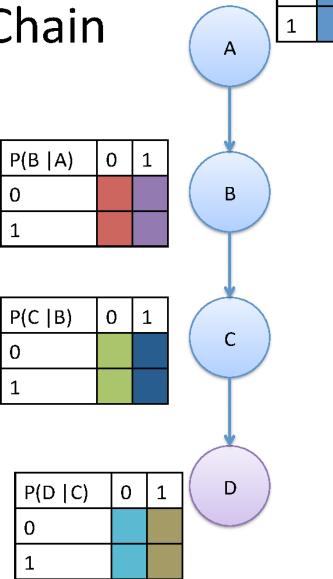
$$P(X \mid E = e) = \frac{P(X, E = e)}{P(E = e)}$$
 $\propto P(X, E = e)$
 $= \sum_{y \in Val(Y)} P(X, E = e, Y = y)$

Such exact inference is hopeless in general.

Let's just try it anyway.



• Let's calculate P(B) from things we have.

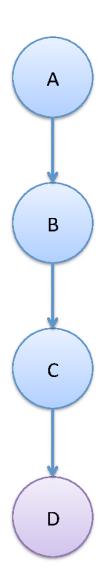


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 Let's calculate P(B) from things we have.

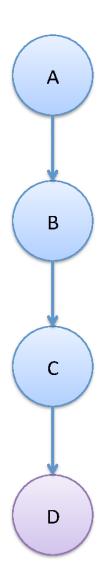
$$P(B) = \sum_{a \in Val(A)} P(A = a)P(B \mid A = a)$$



 Let's calculate P(B) from things we have.

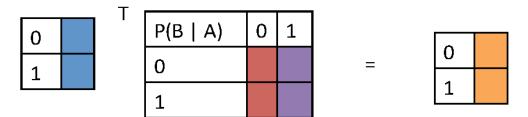
$$P(B) = \sum_{a \in Val(A)} P(A = a) P(B \mid A = a)$$

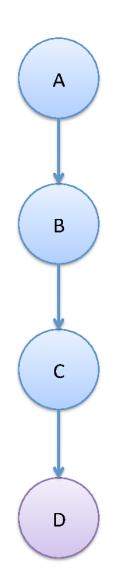
 Note that C and D do not matter.



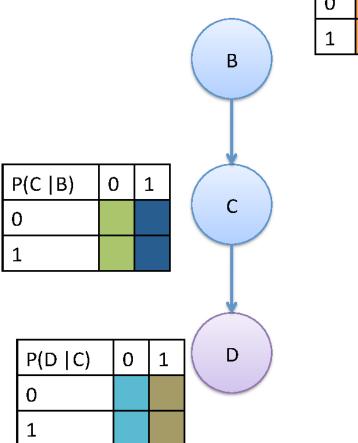
• Let's calculate P(B) from things we have.

$$P(B) = \sum_{a \in Val(A)} P(A = a)P(B \mid A = a)$$





 We now have a Bayesian network for the marginal distribution P(B, C, D).

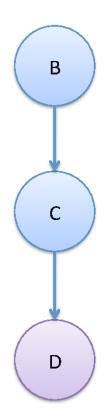


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 We can repeat the same process to calculate P(C).

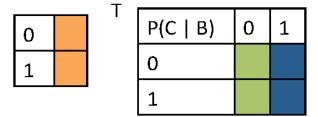
$$P(C) = \sum_{b \in Val(B)} P(B = b) P(C \mid B = b)$$

We already have P(B)!

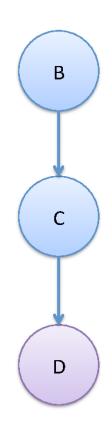


 We can repeat the same process to calculate P(C).

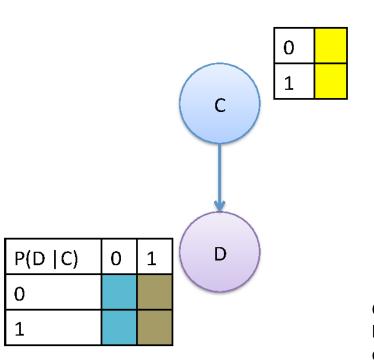
$$P(C) = \sum_{b \in Val(B)} P(B = b) P(C \mid B = b)$$





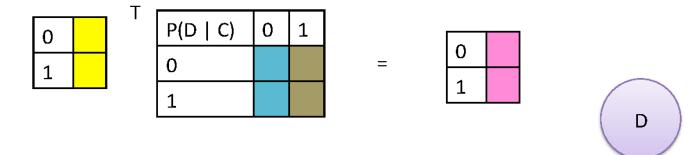


- We now have P(C, D).
- Marginalizing out A and B happened in two steps, and we seem to be exploiting the Bayesian network structure.



• Last step to get P(D):

$$P(D) = \sum_{c \in Val(C)} P(C = c)P(D \mid C = c)$$



- Notice that the same step happened for each random variable:
 - We created a new CPD over the variable and its "successor"
 - We summed out (marginalized) the variable.

$$P(D) = \sum_{a \in Val(A)} \sum_{b \in Val(B)} \sum_{c \in Val(C)} P(A = a) P(B = b \mid A = a) P(C = c \mid B = b) P(D \mid C = c)$$

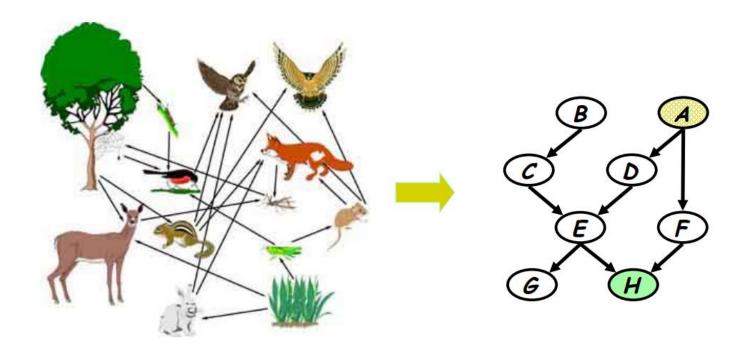
$$= \sum_{c \in Val(C)} P(D \mid C = c) \sum_{b \in Val(B)} P(C = c \mid B = b) \sum_{a \in Val(A)} P(A = a) P(B = b \mid A = a)$$

That Was Variable Elimination

- We reused computation from previous steps and avoided doing the same work more than once.
 - Dynamic programming!
- We exploited the Bayesian network structure (each subexpression only depends on a small number of variables).
- Exponential blowup avoided!
- But: is there a general technique for any graphical model?

A more complex example

A food web

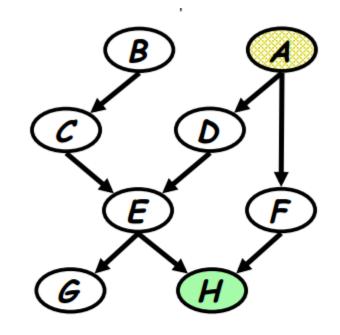


What is the probability that hawks are leaving given that the grass condition is poor?

- Query: P(A | h)
 - Need to eliminate: B,C,D,E,F,G,H
- Initial factors:

$$P(a)P(b)P(c|b)P(d|a)P(e|c,d)P(f|a)P(g|e)P(h|e,f)$$

Choose an elimination order: H,G,F,E,D,C,B

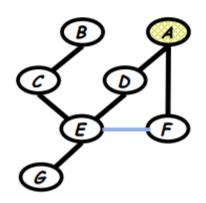


- Step 1:
 - Conditioning (fix the evidence node (i.e., h) on its observed value (i.e., h):

$$m_h(e, f) = p(h = \widetilde{h} \mid e, f)$$

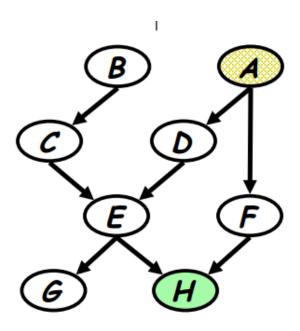
This step is isomorphic to a marginalization step:

$$m_h(e,f) = \sum_h p(h|e,f)\delta(h=\widetilde{h})$$



- Query: *P(B | h)*
 - Need to eliminate: B,C,D,E,F,G
- Initial factors:

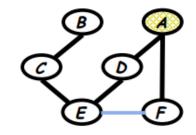
P(a)P(b)P(c|b)P(d|a)P(e|c,d)P(f|a)P(g|e)P(h|e,f) $\Rightarrow P(a)P(b)P(c|b)P(d|a)P(e|c,d)P(f|a)P(g|e)m_h(e,f)$



- Step 2: Eliminate G
- compute

$$m_g(e) = \sum_g p(g \mid e) = 1$$

- $\Rightarrow P(a)P(b)P(c|b)P(d|a)P(e|c,d)P(f|a)m_g(e)m_h(e,f)$
- $= P(a)P(b)P(c \mid b)P(d \mid a)P(e \mid c,d)P(f \mid a)\underline{m_h(e,f)}$



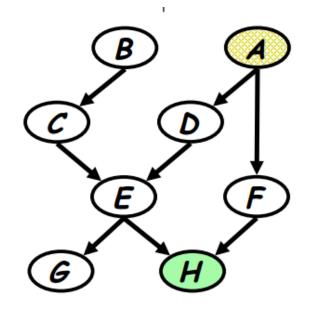
Keep eliminating F,E,D,C,B in order

- Query: P(B | h)
 - Need to eliminate: B

Initial factors:

$$P(a)P(b)P(c|d)P(d|a)P(e|c,d)P(f|a)P(g|e)P(h|e,f)$$

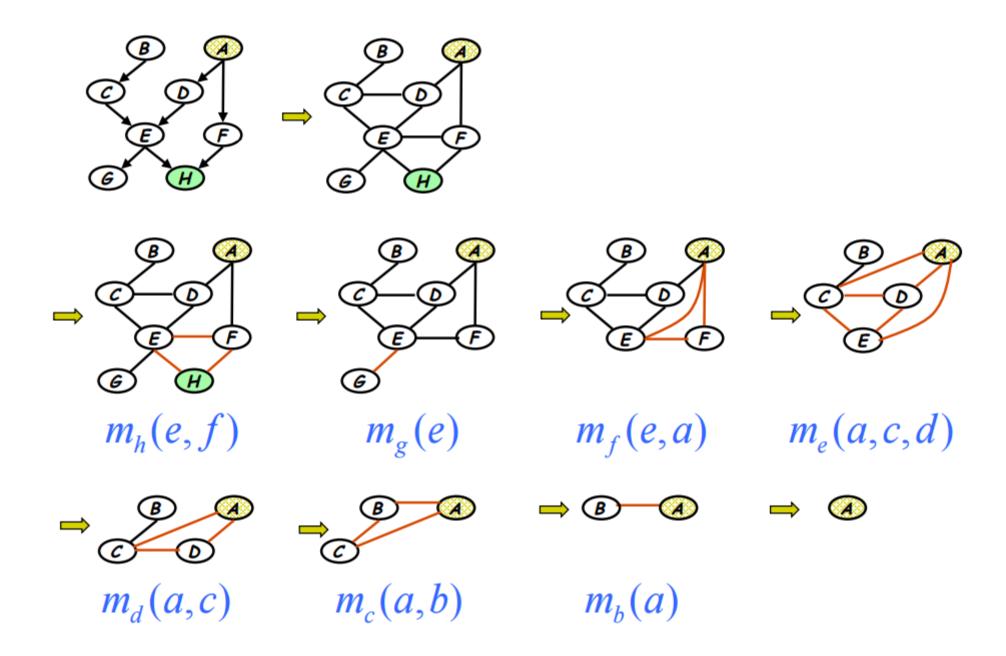
- $\Rightarrow P(a)P(b)P(c \mid d)P(d \mid a)P(e \mid c, d)P(f \mid a)P(g \mid e)m_h(e, f)$
- $\Rightarrow P(a)P(b)P(c|d)P(d|a)P(e|c,d)P(f|a)m_h(e,f)$
- $\Rightarrow P(a)P(b)P(c|d)P(d|a)P(e|c,d)m_f(a,e)$
- $\Rightarrow P(a)P(b)P(c \mid d)P(d \mid a)m_e(a,c,d)$
- $\Rightarrow P(a)P(b)P(c \mid d)m_d(a,c)$
- $\Rightarrow P(a)P(b)m_c(a,b)$
- $\Rightarrow P(a)m_b(a)$
- Final Step: Wrap-up $p(a, \widetilde{h}) = p(a)m_b(a)$, $p(\widetilde{h}) = \sum_a p(a)m_b(a)$ $\Rightarrow P(a \mid \widetilde{h}) = \frac{p(a)m_b(a)}{\sum_b p(a)m_b(a)}$

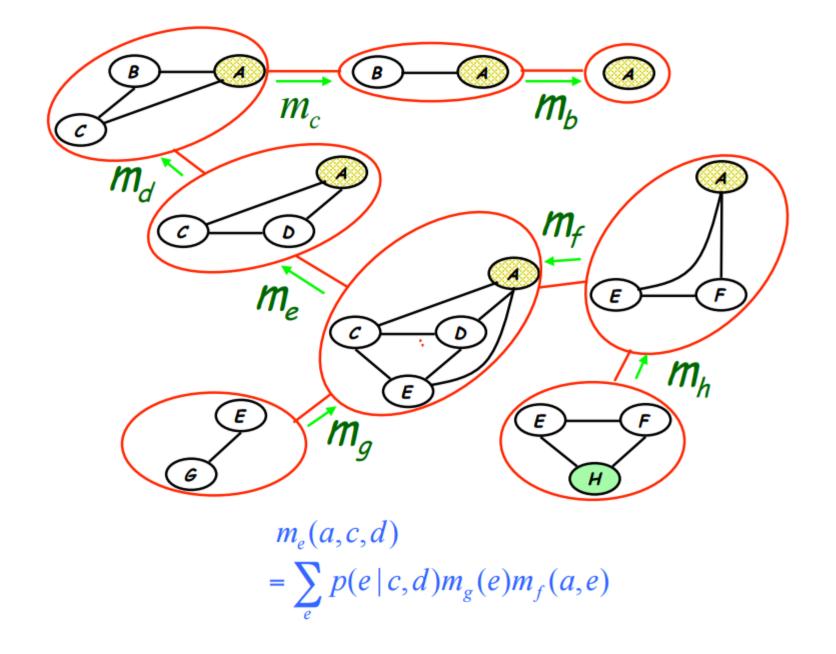


Cumbersome

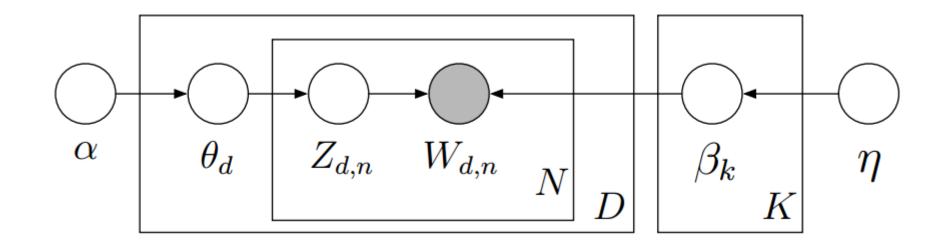
- Maybe graph way could be easier
- Begin by moralizing the Bayesian network
 - Get parent nodes married if they have a common child
 - Ignore directedness of the graph







Hopefully by now you can decipher



And maybe even ...

