CS 583: Probabilistic Graphical Models

Bayesian Networks

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Motivation

- We would like to represent a joint distribution P over $\mathcal{X} = \{X_1, X_2, \ldots, X_n\}$
- Why is such a P useful?
- The naïve representation ⇒ Specify a value for each possible combination
- If all X_i are binary, how many numbers are needed to represent P with 1000 variables?
- How many atoms in the observable universe?

Why is 2^N bad?

- **Computational** challenges
  - Answering queries requires manipulating exponential number of entries
  - Storing exponential number of entries is almost always impossible
- **Cognitive** challenges
  - How can we wrap our minds around about a specific assignment and its corresponding, extremely small, probability?
  - How can an expert provide those numbers or even verify they are correct?
- **Statistical** challenges
  - We often would like to estimate probabilities from data; estimation requires repetition. How can we have a dataset where an exponential number of events are present and repeated multiple times?

We would like to have a representation that is

- Compact
  - Easy to store, manipulate, understand, and estimate
- Intuitive
  - Easy to understand, verify, and construct
- Modular
  - Easy to add and remove variables
- Declarative
  - Separates representation and reasoning

Compactness

- A joint distribution P over $\mathcal{X} = \{X_1, X_2, \ldots, X_n\}$ requires exponential number of numbers
- Reduce the number of parameters through independence
  1. Marginal independence
  2. Conditional independence

Marginal Independence

- Represent a joint distribution P over $\mathcal{X} = \{X_1, X_2, \ldots, X_n\}$, where all X_i are binary
- How many independent parameters?
- Assume for $\forall i \neq j$, $X_i \perp X_j$
- $P(\mathcal{X}) = P(X_1)P(X_2)\ldots P(X_n)$
- Now, how many independent parameters?

Conditional Probabilities

- Two variables, Industrious (I) and SAT score (S)
- Industrious: false (i^0), true (i^1)
- SAT score: low (s^0), high (s^1)

I	S	P(I, S)
i^0	s^0	0.665
i^0	s^1	0.035
i^1	s^0	0.06
i^1	s^1	0.24

What's the number of independent parameters needed?

Conditional Probabilities

- $P(I, S) = P(I)P(S \mid I)$

P(I)

i^0	i^1
0.7	0.3

P(S | I)

I	s^0	s^1
i^0	0.95	0.05
i^1	0.2	0.8

What's the number of independent parameters needed?

A NEW VARIABLE

- Let's add the variable grade (G), with three possible values, A (g^1), B (g^2), and C (g^3).
- Can we assume that G is independent of I or S in real life?
- A more reasonable assumption is to assume that I determines S and G; that is, S and G are conditionally independent
  - This is not totally true either, but then, in the real-world, we cannot really assume anything is independent of anything
    - Butterfly effect?

Conditional independence

- $P(I, S, G) = P(S, G \mid I)P(I) = P(S \mid I)P(G \mid I)P(I)$
- $P(I, S, G) = P(I)P(S \mid I)\,P(G \mid S, I) = P(I)P(S \mid I)\,P(G \mid I)$
- We already have $P(I)$ and $P(S \mid I)$. We need to specify $P(G \mid I)$

$P(G \mid I)$

I	g^1	g^2	g^3
i^0	0.2	0.34	0.46
i^1	0.74	0.17	0.09

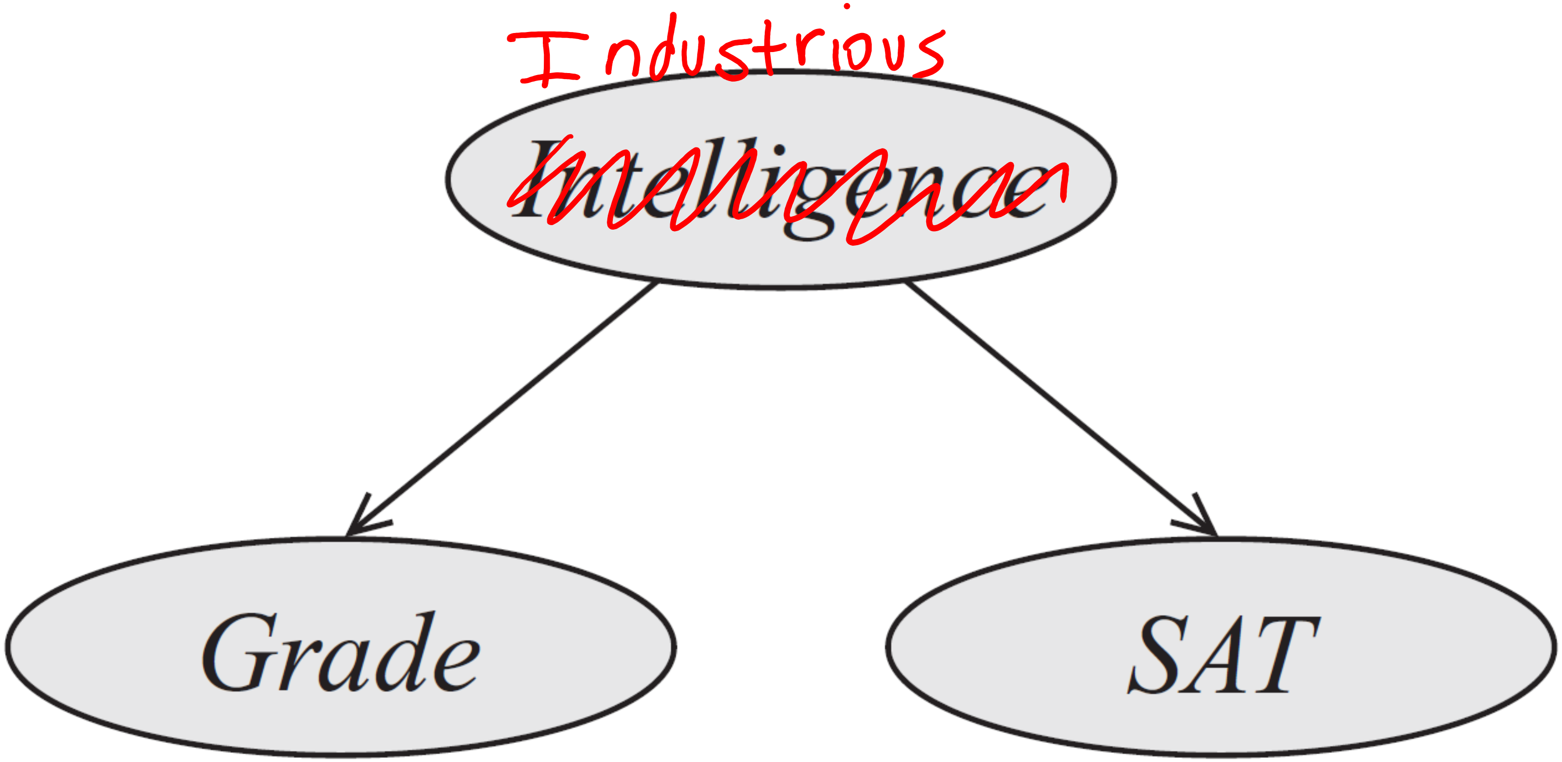
What's the number of independent parameters needed for $P(I, S, G)$ if we use the full joint table?

What if we use the factorization $P(I, S, G) = P(I)P(S|I)\,P(G|I)$?

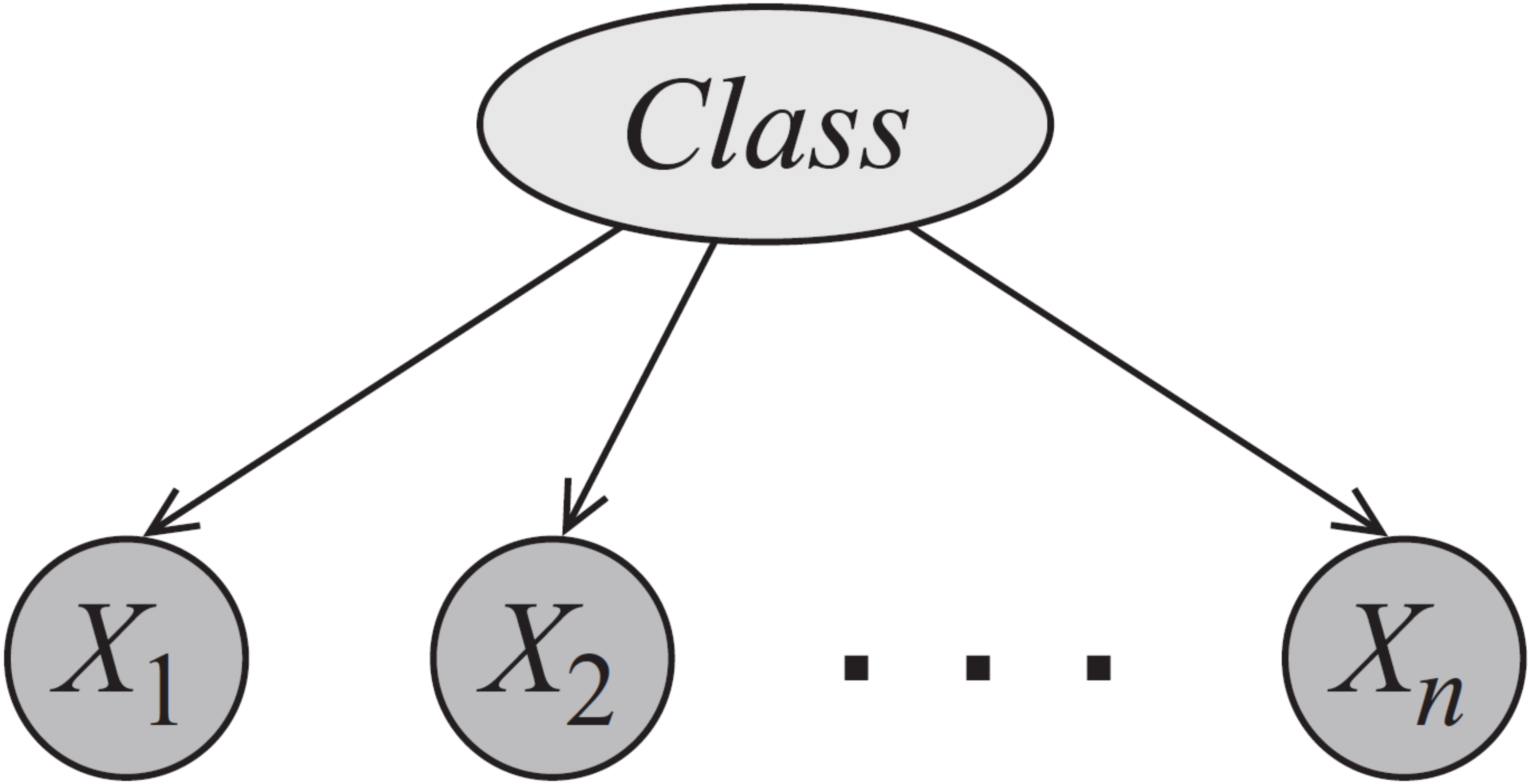
Conditional independencies

- Compactness
  - Fewer parameters to specify
- Intuition
  - Easier to specify
- Modularity
  - Adding a new variable does not cause us to change all the entries in the joint table

Bayesian network representation



NAÏVE BAYES



Naïve Bayes

- How do we write the joint $P(C, X_1, X_2, \ldots, X_n)$?
- How many independent parameters are needed if C and X_i are all binary?
- Naïve Bayes is used for **classification**: given attributes of an object (X_i), classify it into one of pre-given categories (C) (i.e., $P(C \mid X_1, \ldots, X_n)$).
- Read Box 3.A in the textbook for more details

Bayesian Networks

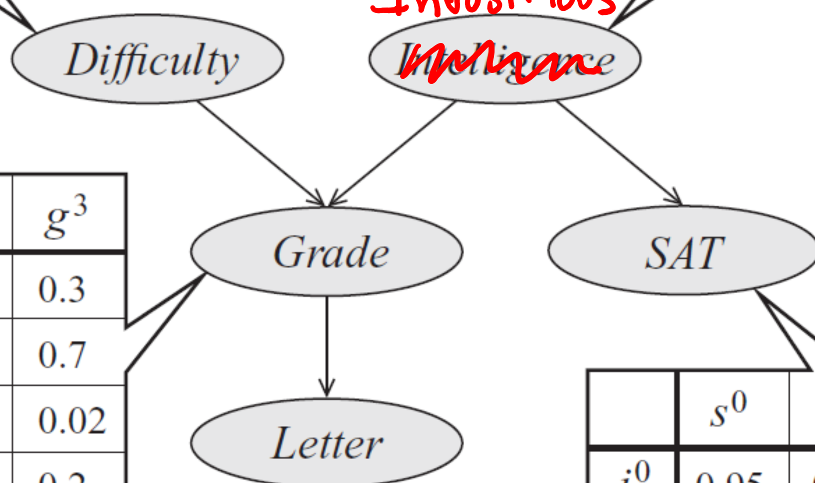
- *A Bayesian Network is a directed acyclic graph whose nodes are random variables and edges represent, intuitively, the direct influence of one node on another*
- Naïve Bayes is a special Bayesian network
- Bayesian networks is
  - A data structure that provides the skeleton for representing a joint distribution compactly in a factorized way
  - A compact representation for a set of conditional independence assumptions about a distribution

THE STUDENT EXAMPLE

- So far we have I, S, G
- We add two more random variables
  - Student's grade also depends on the difficulty (D) of the class: Val(D) = {easy(d^0), hard(d^1)}
  - Student's professor writes a recommendation letter (L), where Val(L)={weak (l^0), strong(l^1)}
    - Professor writes the letter based only the grade and it is a stochastic function of the grade

The student network

1. The structure



d^0	d^1
0.6	0.4

i^0	i^1
0.7	0.3

	g^1	g^2	g^3
i^0, d^0	0.3	0.4	0.3
i^0, d^1	0.05	0.25	0.7
i^1, d^0	0.9	0.08	0.02
i^1, d^1	0.5	0.3	0.2

	s^0	s^1
i^0	0.95	0.05
i^1	0.2	0.8

	l^0	l^1
g^1	0.1	0.9
g^2	0.4	0.6
g^3	0.99	0.01

2. Parameters:
Local probability model
Conditional probability distribution

How many parameters?

The joint?

- What is the meaning of $P(i^1, d^0, g^2, s^1, l^0)$?
- Probability that
  - The student is industrious
  - The class is easy
  - The smart student gets a B in an easy class
  - The smart students get a high score in SAT
  - The student who got a B in the class gets a weak letter
  - $= P(i^1)\, P(d^0)\, P(g^2 \mid i^1, d^0)\, P(s^1 \mid i^1) P(l^0 \mid g^2)$

Reasoning Patterns

- Causal reasoning
  - Causes to effects
- Evidential reasoning
  - Effects to causes
- Intercausal reasoning
  - Explaining away

Causal Reasoning

- Causes to effects
- Don't know anything. Probability of a strong letter
  - $P(l^1) = 0.502$
- Learn that the student is not industrious
  - $P(l^1 \mid i^0) = 0.389$
- Additionally, learn the class is easy
  - $P(l^1 \mid i^0, d^0) = 0.513$

EVIDENTIAL REASONING

- Effects to causes
- Don't know anything. Probability of a student being industrious
  - $P(i^1) = 0.3$
- Learn that the student got a C in a class
  - $P(i^1 \mid g^3) = 0.079$
- Or, learn that the student received a weak letter
  - $P(i^1 \mid l^0) = 0.14$
- Learn both
  - $P(i^1 \mid g^3, l^0) = 0.079$

Intercausal reasoning

- Different causes of the same effect interact
- Don't know anything. Probability of a student being industrious
  - $P(i^1) = 0.3$
- Learn that the student got a B in a class
  - $P(i^1 \mid g^2) = 0.175$
- Learn that the class was difficult
  - $P(i^1 \mid g^2, d^1) = 0.34$
- Student's B is *explained away* with the other cause

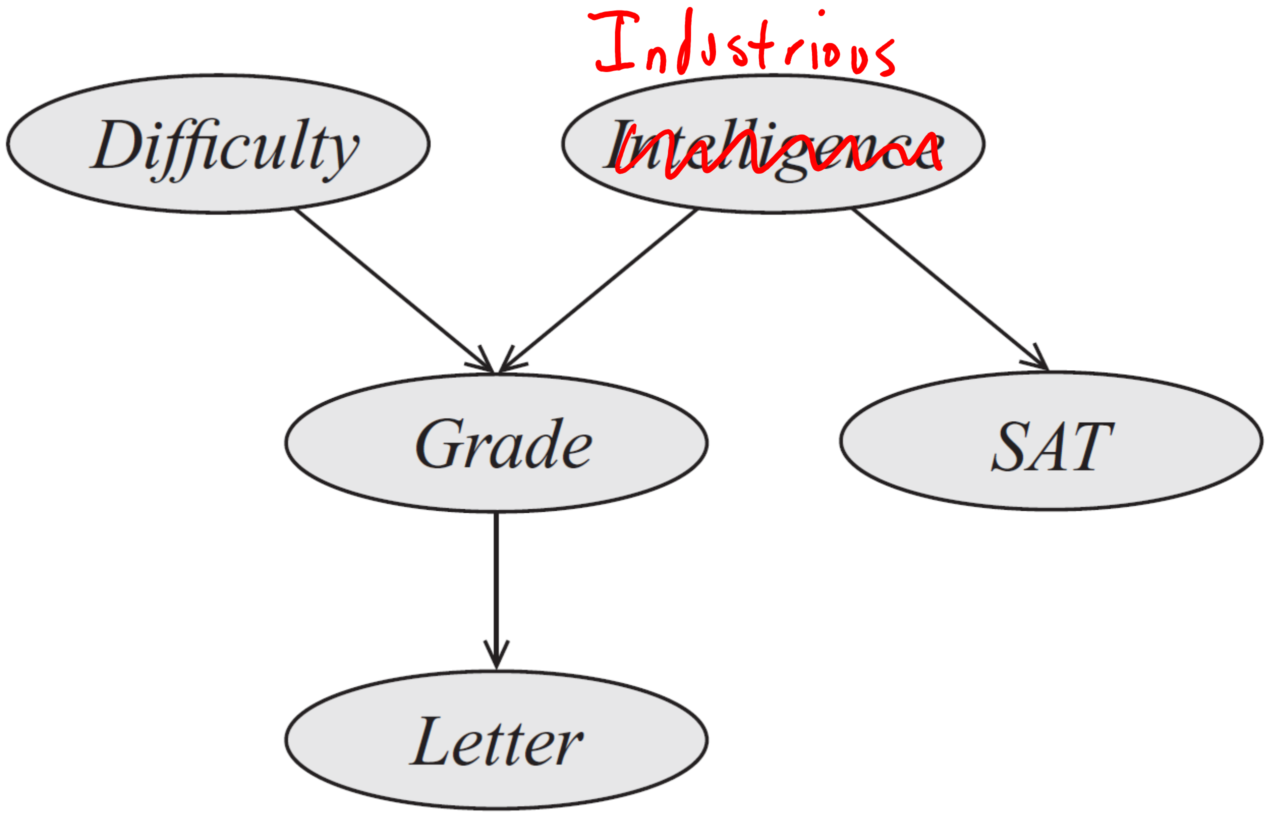
HUGIN LITE

- Download Hugin Lite
  - https://www.hugin.com/index.php/hugin-lite/
- Get the student example from GitHub
- Try a few causal, evidential, and intercausal queries
- Extra fun
  - Get more .net files from https://www.bnlearn.com/bnrepository/ and load them to Hugin and play with them
- Double-extra fun
  - Install pgmpy Python package https://github.com/pgmpy/pgmpy
  - Check out the examples at http://pgmpy.org/

Bayesian Network Structure

- A *Bayesian network structure* $\mathcal{G}$ is a directed acyclic graph whose nodes represent random variables $X_1, \ldots, X_n$. Let $\mathrm{Pa}(X_\mathrm{i})$ denote the parents of X_i, and $\mathrm{ND}(X_i)$ denote the variables that are not descendants of X_i. Then $\mathcal{G}$ encodes the following set of conditional independence assumptions:
  - $\boldsymbol{X_i \perp \mathrm{ND}(X_i) \mid \mathrm{Pa}(X_i)}$
- These independencies are called the *local independencies*
- Clarification. A node itself and its parents are part of non-descendants according the definition of ND. A clearer statement would be, in my opinion:
  - $X_i \perp \mathrm{ND}(X_i) \setminus \{X_i \cup \mathrm{Pa}(X_i)\} \mid \mathrm{Pa}(X_i)$

Local independencies example



1. $D \perp I, S$
2. $I \perp D$
3. $S \perp D, G, L \mid I$
4. $G \perp S \mid D, I$
5. $L \perp D, I, S \mid G$

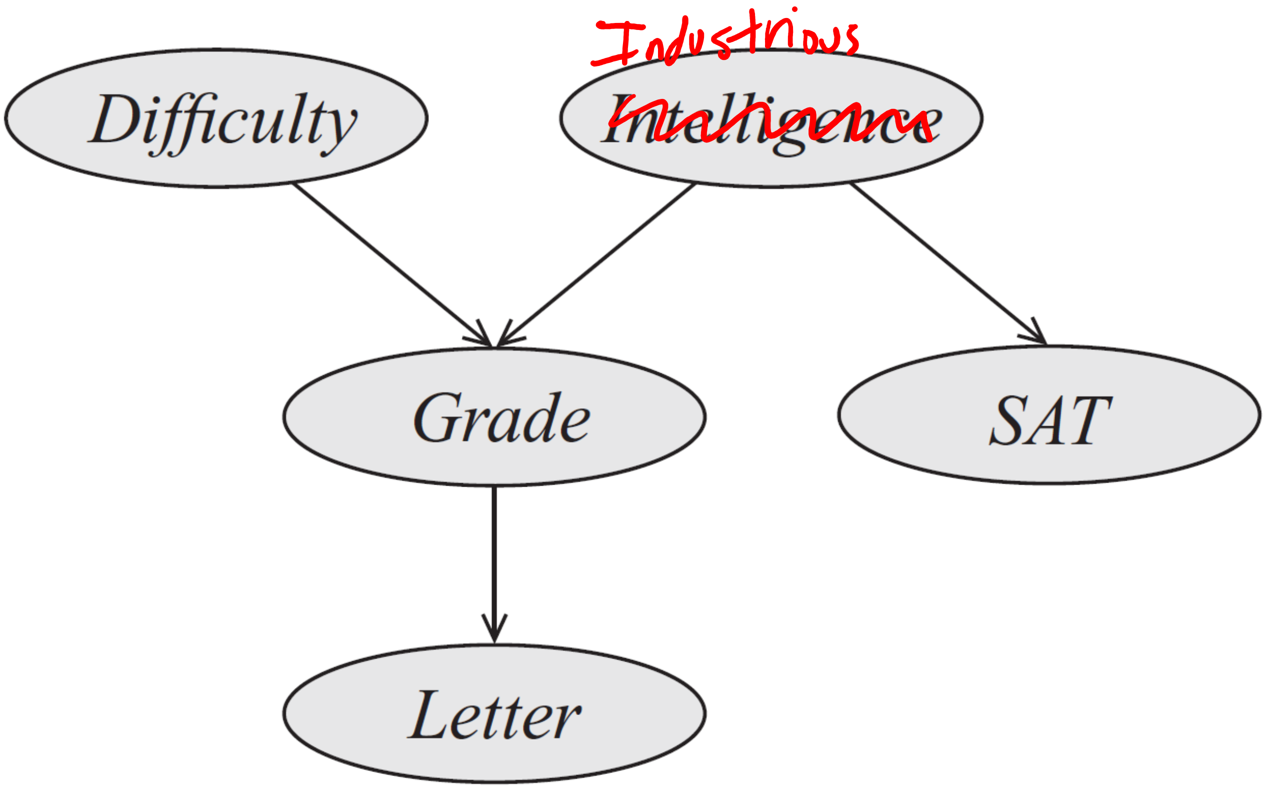
Bayesian Network Factorization

$$P(X_1, \ldots, X_n) = \prod_i P(X_i \mid Pa(X_i))$$

Why is this factorization useful?

How can you prove this factorization holds?

FACTORIZATION EXAMPLE



P(I, D, S, G, L) =
P(I)*
P(D)*
P(S | I)*
P(G | I, D)*
P(L | G)

WE'LL PROVE

1. Local conditional independence assertions $\Rightarrow$ Bayesian network factorization
2. Bayesian network factorization $\Rightarrow$ Local conditional independence assertions

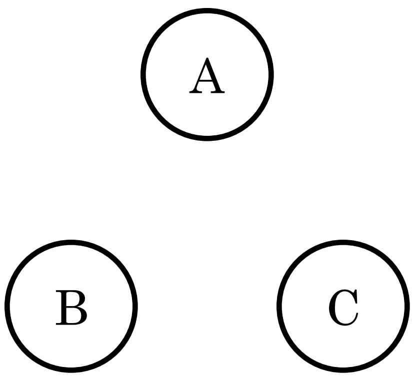
I-Map

- Let P be a distribution over $\mathcal{X}$. We define I(P) to be the set of independencies of the form $\mathbf{X} \perp \mathbf{Y} \mid \mathbf{Z}$ that hold in P.
- "P satisfies independencies of the structure $\mathcal{K}$" $\equiv \mathrm{I}(\mathcal{K}) \subseteq \mathrm{I}(\mathrm{P})$
- If $\mathrm{I}(\mathcal{K}) \subseteq \mathrm{I}(\mathrm{P}) \Rightarrow \mathcal{K}$ is an I-Map for P
- For $\mathcal{K}$ to be an I-Map of P, any independence assertion made by $\mathcal{K}$ has to be true in P. However, it is possible that P can contain additional independencies
  - That is, whatever $\mathcal{K}$ says independent is independent in P, but $\mathcal{K}$ may not know all the independencies in P

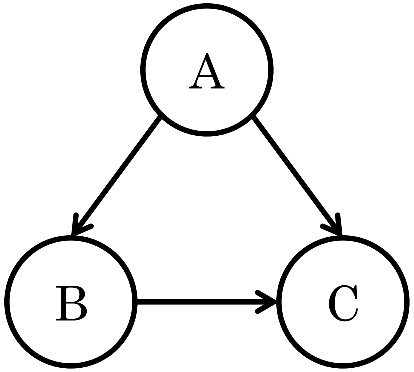
P-Map

- **Definition:** *Perfect Map*: A graph structure $\mathcal{G}$ is a perfect map (P-Map) for a distribution P, if I($\mathcal{G}$) = I(P)

Two Graphs



$\mathcal{G}_1$



$\mathcal{G}_2$

What are the local independence assertions made by $\mathcal{G}_1$? $\mathcal{G}_2$?

WE'LL PROVE

1. Local conditional independence assertions $\Rightarrow$ Bayesian network factorization
   - I-Map to Factorization
2. Bayesian network factorization $\Rightarrow$ Local conditional independence assertions
   - Factorization to I-Map

I-Map to Factorization

- **<u>Theorem</u>**: Let $\mathcal{G}$ be a BN structure over $\mathcal{X}$, and let P be joint distribution over the same space. If $\mathcal{G}$ is an I-Map for P, then P factorizes according to $\mathcal{G}$.
- Proof?

Factorization to I-Map

- Theorem: Let $\mathcal{G}$ be a BN structure over X and let P be a joint distribution over the same space. If P factorizes over $\mathcal{G}$, then $\mathcal{G}$ is an I-Map for P.
- Proof?

Independencies in graphs

- We have already seen the local independence assertions
- Are there additional independence statements we can make simply based on the graph structure?
  - Yes.
- Will these additional independencies help us reduce the number parameters further?
  - No.
- Why are they useful then?

Dependence ≡ Information flow

- X and Y <u>are</u> independent if the information <u>cannot</u> flow from one to the other

1. No trail between X and Y
   - Information <u>cannot</u> flow; X and Y <u>are</u> independent
2. X and Y are connected by an edge
   - Information <u>can</u> flow; X and Y <u>are not</u> independent
3. X and Y are not connected by an edge, but there is a trail between them
   - Depends…

Trails 1-2

- Causal trail
  - $X \to Z \to Y$
  - Information can flow between X and Y if Z is not observed; if Z is observed, it blocks the information flow. $X \perp Y \mid Z$
  - E.g, $I \to G \to L$
    - If we don't know the student's grade, then knowing her intelligence tells us something about the strength of the letter. But, once we know her grade, I and L are independent
- Evidential trail
  - $X \leftarrow Z \leftarrow Y$
  - Information can flow between X and Y if Z is not observed; if Z is observed, it blocks the information flow. $X \perp Y \mid Z$

Trails 3

- Common cause
  - $X \leftarrow Z \rightarrow Y$
  - Information can flow between X and Y if Z is not observed; if Z is observed, it blocks the information flow. $X \perp Y \mid Z$
  - E.g, $G \leftarrow I \rightarrow S$
    - If we don't know the student's intelligence, then knowing his SAT score tells us something about his grade. If we know his intelligence, then his grade and SAT score are independent

TRAILS 4

- Common effect
  - $X \rightarrow Z \leftarrow Y$ (v-structure)
  - Information can flow between X and Y only if Z or at least one of Z's descendants is observed
  - E.g. $D \rightarrow G \leftarrow I$
    - If we do not know the grade or the letter quality, then D and I are independent. If we know, however, the grade or the letter quality, then D and I interact

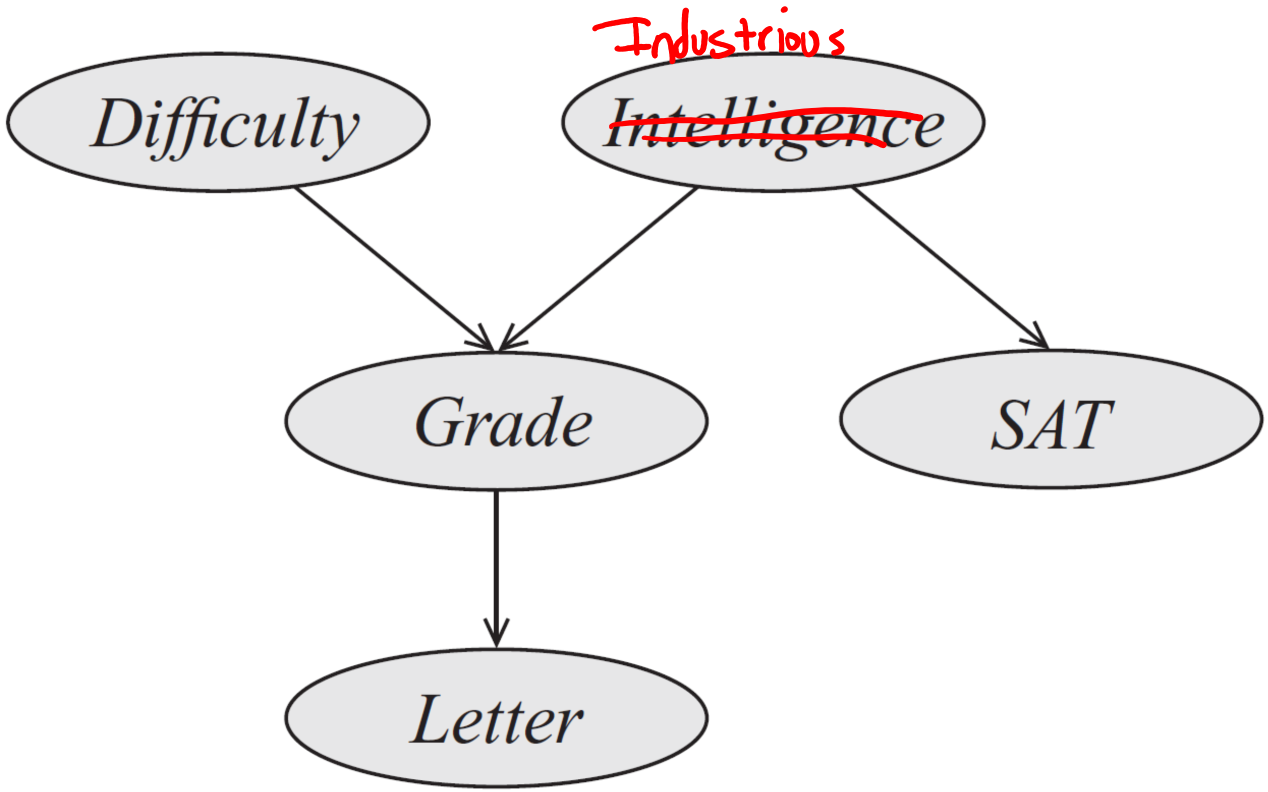
D-Separation

- To answer whether X_i and X_j are independent given $\mathbf{E}$
  - Find all trails between X_i and X_j
  - If information can flow through at least one trail, then X_i and X_j are dependent given $\mathbf{E}$; otherwise they are independent given $\mathbf{E}$

More Formally

- Let $\mathcal{G}$ be a BN structure and $X_1 \leftrightarrow \ldots \leftrightarrow X_n$ a trail in $\mathcal{G}$. Let **E** be the observed set of variables. The information <u>can</u> flow along the trail $X_1 \leftrightarrow \ldots \leftrightarrow X_n$ if
  - Whenever we have a v-structure $X_{i\text{-}1} \rightarrow X_i \leftarrow X_{i+1}$, then X_i or one of its descendants is in **E**; and
  - No other node along the trail is in **E**

D-separation example



Are the following statements true?

1. $D \perp G$?
2. $D \perp L$?
3. $D \perp I$?
4. $D \perp I \mid G$?
5. $D \perp I \mid L$?
6. $D \perp S \mid L$?

I-Equivalence

- If two BN structures $\mathcal{G}_i$ and $\mathcal{G}_j$ encode exactly the same independencies, i.e., if $I(\mathcal{G}_i) = I(\mathcal{G}_j)$, then $\mathcal{G}_i$ and $\mathcal{G}_j$ are I-equivalent
- Why is this an important concept?
- A given distribution can be represented with one of I-equivalent structures and it might be impossible to identify a unique structure
  - E.g., $X \rightarrow Y$ and $X \leftarrow Y$ are I-equivalent. Then, we cannot readily argue whether X causes Y or Y causes X.

I-Equivalence

- *Definitions*:
  - *Skeleton* of Bayesian network G is the undirected version of G
    - That is, G and its skeleton have the same node and edge set, except edges in G are directed, whereas in its skeleton, the edges are undirected
  - A v-structure $X \rightarrow Z \leftarrow Y$ is an *immorality* if there is no direct edge between X and Y (informally, it is an immorality if the parents are not married)
- *Theorem*: Two Bayesian networks are I-Equivalent if and only if they have the same skeleton and the same set of immoralities

From Distributions to Graphs

- For a given P, we would like to find a structure that represents P
- One approach is to take any graph that is an I-Map for P
  - This is not a good idea. Why?
- **Definition:** *Minimal I-Map*: A graph $\mathcal{G}$ is a minimal I-Map for a P, if it is an I-Map for P, and removal of a single edge from $\mathcal{G}$ renders it to be not an I-Map

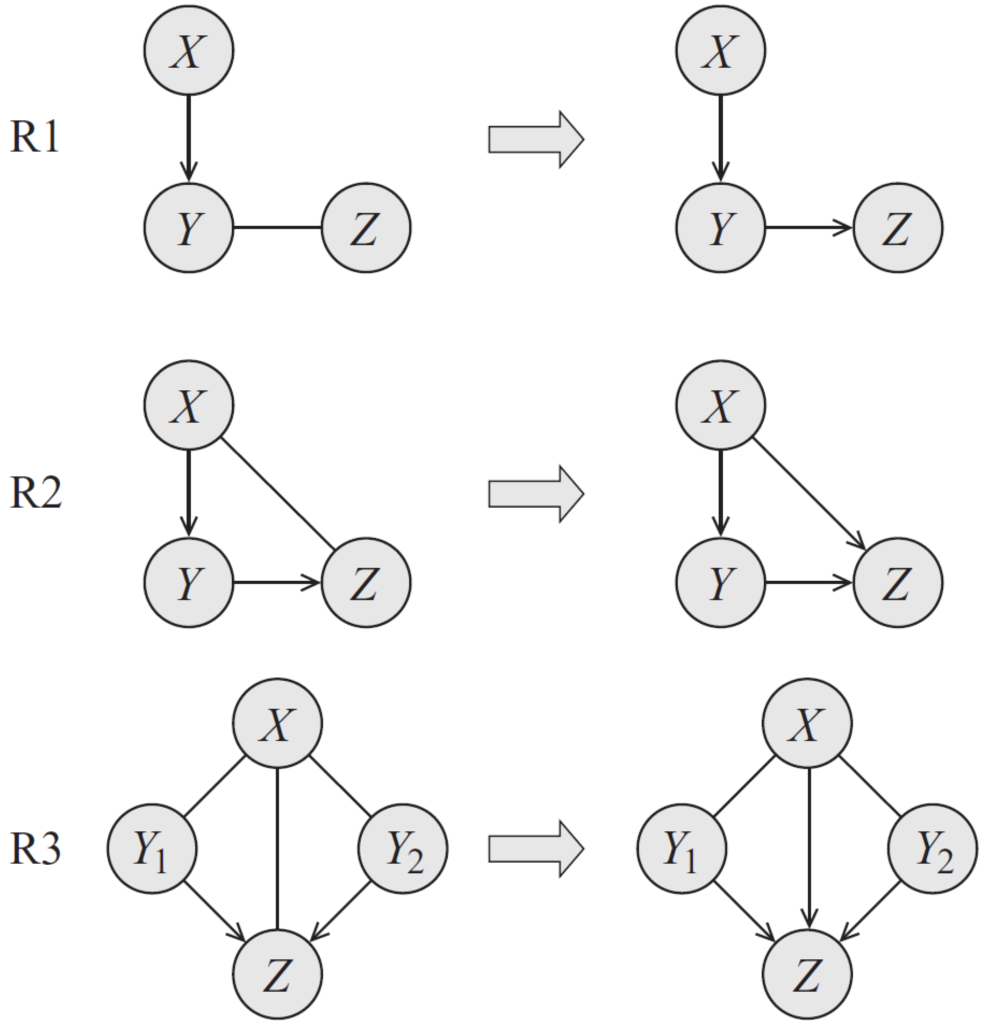
Finding Minimal I-Maps

- Given a distribution P over $\mathcal{X}$, how can we find a structure $\mathcal{G}$ that is a minimal I-Map for P?
- The procedure is given on page 79
  - Pick an ordering of the variables, $X_1, X_2, \ldots, X_n$
  - For each X_i, find minimal subset $\mathbf{U}$ of $\{X_1, X_2, \ldots, X_{i-1}\}$ such that $X_i \perp \{X_1, X_2, \ldots, X_{i-1}\} \setminus \mathbf{U} \mid \mathbf{U}$
  - Set $\mathbf{U}$ to be the parents of X_i
- Assume $I(P^{student}) = I(G^{student})$. Construct a minimal network using the order
  - D, I, S, G, L
  - L, S, G, I, D
  - L, D, S, I, G

Finding I-equivalent structures

- Start with a fully connected undirected graph
- Assume a max indegree of d
- For all pairs X-Y
  - Search for a set $\boldsymbol{U}$ where $X \perp Y \mid \boldsymbol{U}$ and $|\boldsymbol{U}| \leq d$ ($\boldsymbol{U}$ has to be a subset of neighbors of X or neighbors of Y)
  - If such a $\boldsymbol{U}$ cannot be found, then X and Y are connected, otherwise,
  - Remove the edge X-Y and record $\boldsymbol{U}$ as the witness set for X and Y
- Find all immoralities; For all X-Z-Y where X and Y are not directly connected
  - If $Z \in \boldsymbol{U}$, then X-Z-Y is not an immorality, otherwise
  - It is an immorality, orient the edges as $X \rightarrow Z \leftarrow Y$
- Orient any other edges if necessary by applying three rules

Rules for orienting the edges



NEXT

- Markov networks