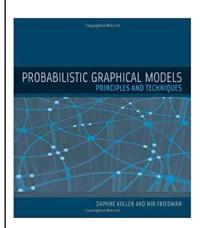
Capturing Dependency of Data using Graphical Models

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Objectives

- •Understand equivalence of conditional independence of R.Vs and factorizations of their probability distribution over a graph.
- •Simple undirected graphical models:
 - •Gaussian Markov Network
 - Logistic Model

References



•Today's class roughly follows Chapter 2.14 and Chapter 4 in Probabilistic Graphical Models by Koller and Friedman.

Dependency in Dataset: A Unit Score Example

Example: Scores of Units

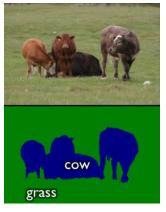
•Imagine a table of unit scores.

Name	SM1	Math	Python	Mach. Learn.
Song	80	70	50	60
Harry	50	40	70	80
Ron	50	50		45
Hermione	90	100		100
				5

Dependency of R.V.s and Probabilistic Models

- •How do you construct a good $p(D|\theta)$ as the likelihood of this dataset?
- •Scores of units are dependent!
 - •Student with **high** Math, Python score is likely to receive **high** SM1 score.
 - •Student with **high** SM1 score is likely to receive **a high** Mach. Learn. score.

Example: Pixel Correlation



•The likelihood of one pixel being "Cow" is dependent with labels of adjacent pixels.

Jamie Shotton et. al. IJCV 2009

How the dependencies between R.V.s would affect likelihood modelling?

Problem Formulation

•Given a dataset
$$\{\boldsymbol{x}_i\}_{i=1}^n$$
,
• $\boldsymbol{x}_i = \left[x_i^{(1)}, x_i^{(2)} \dots x_i^{(d)}\right] \in R^d$

- • x_i is a vector of a student i's scores. •e.g., $x^{(1)}$ is SM1, $x^{(2)}$ is Math...
- •What does $p\!\left(x^{(1)}, x^{(2)} \dots x^{(d)}\right)$ look like?

Note, here we do not distinguish the lower case x, an assignment of a random variable, and upper case X, a random variable.

Dependency and Likelihood

- •If we assume $x_1 \dots x_n$ are IID.
- Likelihood factorizes into product over each x_i

•
$$p(x_1, x_2, ... x_n | \theta) = \prod_{i=1}^n p(x_i | \theta)$$

•Maximum Likelihood Estimation

- - $\operatorname{-max}_{\theta} \prod_{i=1}^{n} p(x_i | \theta)$
 - •First Lecture!

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We can do the factorization of the likelihood function because of the independence of X!!!

Dependency and Likelihood

- •IIDness is an extremely simple assumption.
- What about complicated dependencies?
 How do we factorize our likelihood?
- •To solve this problem, we **first** need to convert our dependences into a graphical representation, **then** use the graph to guide our factorization.
- Study of factorization of prob. distributions and dependencies of R.V.s is called graphical modelling.

Review: Independence and Conditional Independence

Independence of R.V.s

- •Let's look at how independence between R.V.s are **expressed in probability distribution:**
- •R.V. *X* is **independent** of *Y*:
 - $X \perp Y$
 - $\bullet \Leftrightarrow p(X,Y) = p(X)p(Y)$
 - Factorization
 - $\bullet \Leftrightarrow p(X|Y) = p(X) \Leftrightarrow p(Y|X) = p(Y)$
 - •No Information exchange between X and Y.

Notice the independence can be expressed via factorization and information flow.

Conditional Independence of R.V.s

- ullet R.V. X is independent of Y given Z
 - $X \perp Y | Z$
 - • $\Leftrightarrow p(X,Y|Z) = p(X|Z)p(Y|Z)$
 - • \Leftrightarrow $p(X,Y,Z) \propto g_1(X,Z) \cdot g_2(Y,Z)$
 - Factorization
 - $\bullet \Leftrightarrow p(X|Y,Z) = p(X|Z)$
 - Y does not give any additional info which changes the prob. of X given Z.
 - No **direct** information exchange between *X* and *Y*
 - $\bullet \Leftrightarrow p(Y|X,Z) = p(Y|Z)$

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Z is called conditioning random variable.

What are g_1 and g_2? They are just two functions, does not have to be probability, does not have to be in any specific form. **Their existence guarantees** the conditional independence.

g function is called factor

(Conditional) Independence and Information Exchange

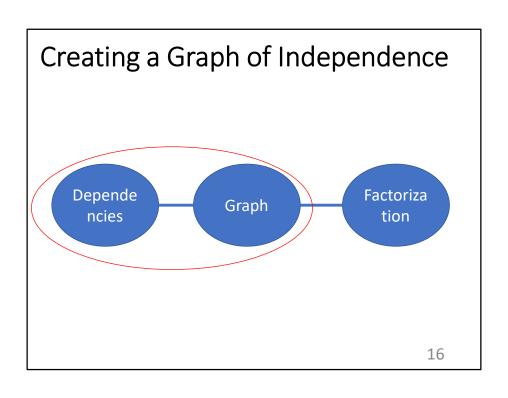
- •(Conditional) Independ. tells how information **exchange** between R.V.s
 - • $X \perp Y \Leftrightarrow$ no information exchanges inbetween X and Y.
 - • $X \perp Y | Z \Leftrightarrow$ no **direct** information exchanges between X and Y

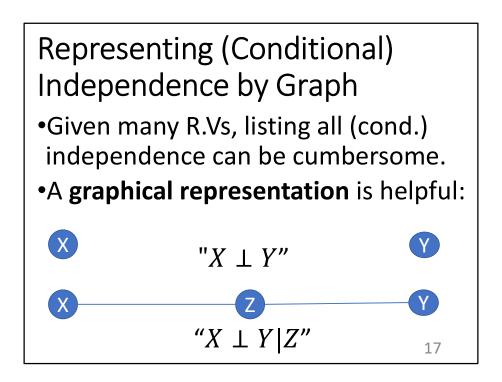
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The analogy is like relationship between people.

X and Y are independent: they do not talk to each other.

X and Y are conditional indepdent, they talk to each other via a middle man.





Because in many machine learning tasks, (conditional) independence are **valuable prior knowledge**, you may want to specify (conditional) independence of R.Vs in your dataset.

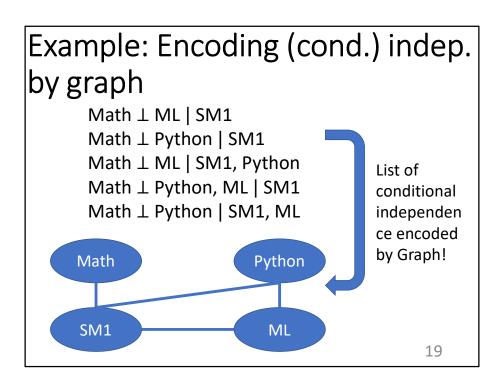
Imagining listing all the (conditional) independence in a very long document...

Representing Conditional Independence by Graph

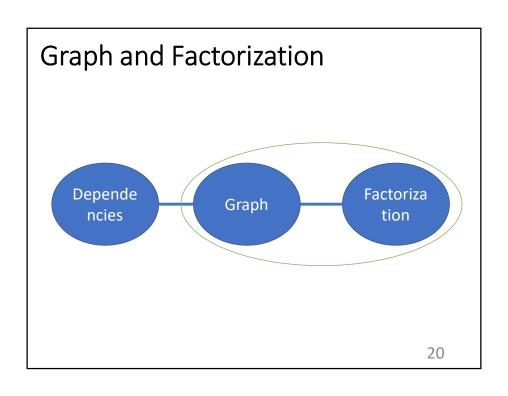
- •Given a graph $G = \langle E, V \rangle$,
 - •V contains all the R.V.
- •Given three subsets of R.V.: $X, Y, Z \subseteq V$
 - •if X and Y are completely "**blocked**" in the graph by Z, we say $X \perp Y | Z$ is represented by G.

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Blocked, means there is no path linking X and Y



Graph is a powerful tool to encode/visualize (conditional) indepedence.



Factorization and Graph

- •Factorizing a probability dist. greatly reduces complexity of modelling and computation of a probability dist.
 - •Think about that Maximum Likelihood under IID assumption!

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The motivation of factorizing a probability dist.

Representing Prob. Distribution Factorization by Graph

- •Writing the factorization of a probability distribution of many factors can be cumbersome.
- •Can we also use graph to help??



"P(X,Y) = P(X)P(Y)"









" $P(X,Y,Z) \propto g_1(X,Z)g_2(Y,Z)_2$ "

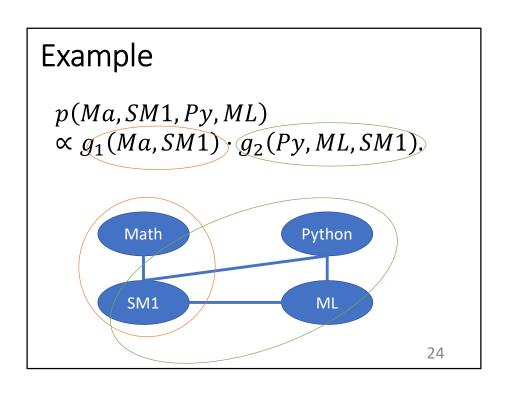
Representing Prob. Distribution Factorization by Graph

- •Given a graph $G = \langle E, V \rangle$,
- •We say p(X) factorizes over G:
- •If $p(X) \propto \prod_{c \in C} g_c(X^{(c)})$
 - •where C is set of all **cliques** in G.
 - •Clique: fully connected subgraph.
 - • g_c is a function defined on $X^{(c)}$, which is the subset of X restricted on c.

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Like what we saw before, g_c is a function that can be in any form.

g is called "factor"



Equivalency between Factorization and Conditional Independence over *G*

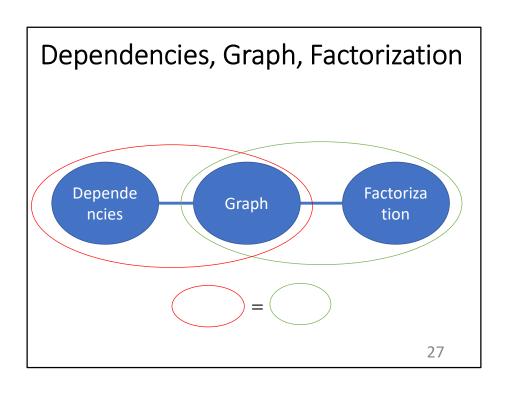
- Using graph represent a factorization of a probability distribution
- Using graph represent a list of conditional independence
- •Remarkably, these two seemingly irrelevant notions are equivalent!

Equivalency between Factorization and Conditional Independence over G

- •If p factorizes over G, p satisfies all conditional independence represented by G.
- •If p satisfies all conditional independence represented by G, then p factorizes over G.

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What does that mean

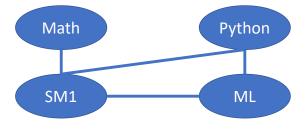


Equivalency between Factorization and Conditional Independence over G

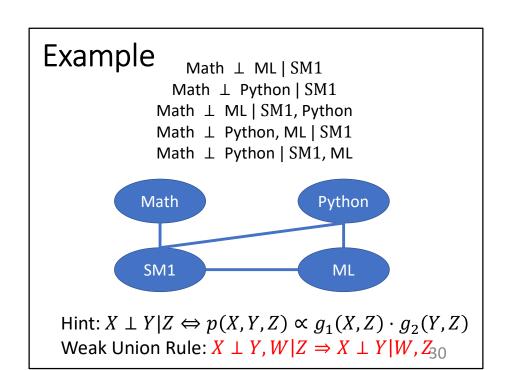
- Verify this on Scores of Units example!
- •Homework:
 - •Create G using factorization on page 25 and check if the graph encodes all conditional Independence of p(Ma, SM1, Py, ML).
 - •Create G using all conditional independence on page 20 and check if it encodes the factorization of p(Ma, SM1, Py, ML).

Example

p(Ma, SPS, Py, ML) $\propto g_1(Ma, SPS) \cdot g_2(Py, ML, SPS).$



Hint: $X \perp Y | Z \Leftrightarrow p(X,Y,Z) \propto g_1(X,Z) \cdot g_2(Y,Z)$ $X \perp Y, W | Z \Rightarrow X \perp Y | Z$



Markov Network

•A probability distribution p(X) which uses undirected graph representing its conditional independence, is called an **undirected graphical model**, or a **Markov network**.

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The definition of Markov network.

Gaussian Markov Network

•Multivariate Gaussian distribution:

•
$$x \in R^d$$
, $x \sim N(\mathbf{0}, \mathbf{\Sigma})$

• $p(x) \propto \exp\left[-\frac{x(\mathbf{\Sigma})^{-1}x^{\mathsf{T}}}{2}\right]$ Let $\mathbf{0} = (\mathbf{\Sigma})^{-1}$.

 $\propto \exp\left[-\frac{\sum_{u,v} \Theta^{(u,v)}x^{(u)} x^{(v)}}{2}\right]$
 $\propto \lim_{u,v;\Theta^{(u,v)}\neq 0} \exp\left(-\Theta^{(u,v)}x^{(u)} x^{(v)}\right)$

aBa^T = \sum_ij B_ij ai aj

You can factorize the joint Gaussian using the pairwise factors

Gaussian Markov Network

•
$$p(\mathbf{x}) \propto \prod_{u,v;\Theta^{(u,v)}\neq 0} g_{u,v}(\mathbf{x}^{(u)},\mathbf{x}^{(v)})$$

•p(x) factorizes over G!•G defined by the adjacency matrix

$$A^{(u,v)} = \begin{cases} 0, \Theta^{(u,v)} = 0 \\ 1, \Theta^{(u,v)} \neq 0 \end{cases}$$

• G must be an undirected graph (why?)

This pairwise factorization implies the distribution factorizes over a G whose edges are defined by the structure of Theta

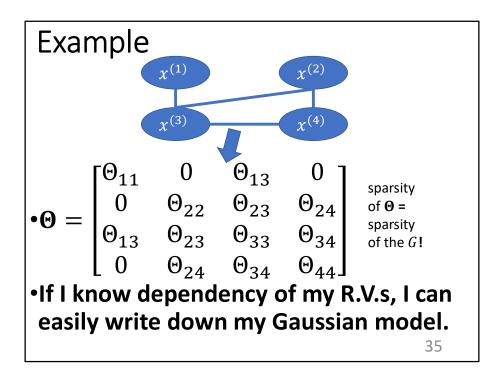
Gaussian Markov Network

•Give me a graph G that encodes all conditional independence of your Gaussian R.V., I can infer the sparsity of your Θ .

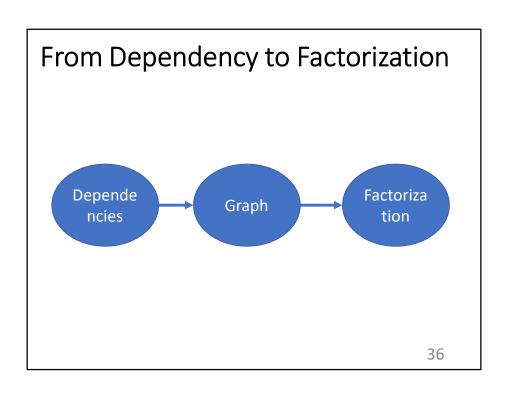
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Theta must be positive definite!!

We are using graph to construct our probabilistic model, hence the name, graphical model!!



Theta must be positive definite!!



Homework question:

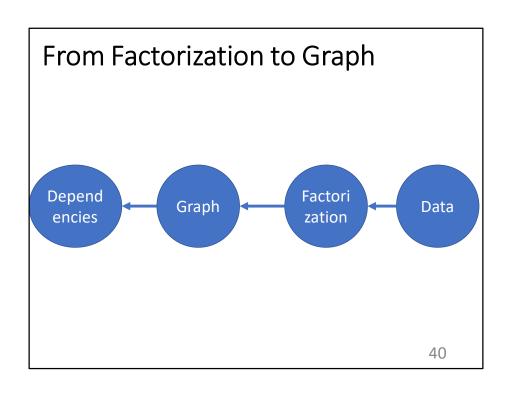
- •Suppose graph G encodes all cond. indep. in your Gaussian distribution p. G contains **three edges**, **five nodes**. How many **non-zero elements** are there **in inverse covariance** matrix of p?
- •A.3
- •B.8
- •C.6
- •D.10
- •E.11

Constructing Likelihood

- •PC: If (x_0, x) are drawn from a joint Gaussian $p(x_0, x)$, show log likelihood $\log p(x_0|x)$ has the form:
 - • $-(x_0 \sum_i \beta_i x_i)^2/b$, where $\beta_i \neq 0$ iff (X_0, X_i) is an edge in the Markov network structure of p.
 - How does it help us select good features in least squares fitting?

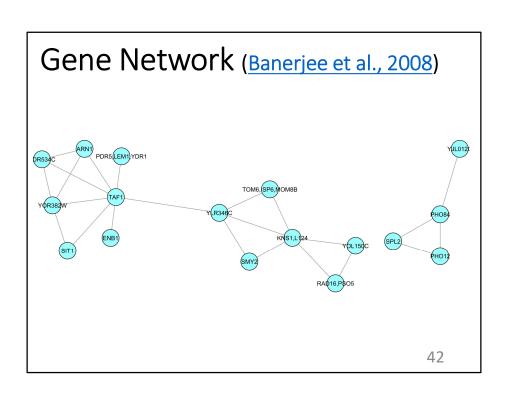
Gaussian Markov Network

- •If we do not know, cond. independence of p(x), we can infer it from data!
- •Given dataset D, we can fit a $\widehat{\mathbf{\Theta}}$.
 - •Using MLE: $\widehat{\mathbf{\Theta}} = \underset{\mathbf{\Theta}}{\operatorname{argmax}} \log p(D; \mathbf{\Theta})$
 - •The sparsity of $\widehat{\mathbf{O}}$ gives a graph corresponds to factorization of $p(\mathbf{x})$!
 - •Such graph also reveals how R.V. are dependent on each other!



Example: Gene Expression Data

Time stamp	Gene1	Gene2	Gene3	Gene4
t1	.1	.2	.5	.2
t2	.5	.4	.7	.8
t3	.5	.5		.45
t4	.9	.2		.01
		•••		



Exponential Family Distribution

- Gaussian Markov network belongs to a wider family of distributions, which are defined using a generic form:
- • $p(x; \theta) := \frac{\exp(\langle \theta, f(x) \rangle)}{Z(\theta)}$
 - •f(x) is a feature transform on x.
 - • $Z(\theta) := \int \exp(\langle \theta, f(x) \rangle) dx$
- •PC: show when f is 2^{nd} degree poly. transform with pairwise terms, $p(x; \theta)$ is a multivariate Gaussian distribution.

Graphical Lasso (Jerome Friedman et al., 2008)

- •Given $D = \left\{ \boldsymbol{x}_i \; \right\}_{i=1}^n$, $\boldsymbol{x} \in R^d$,
- Construct a Gaussian likelihood:

•
$$p(D|\mathbf{\Theta}) = \prod_i N_{x_i}(\mathbf{0}, \mathbf{\Theta}^{-1})$$

- $\begin{aligned} \bullet \widehat{\mathbf{\Theta}} &\coloneqq \operatorname{argmax}_{\mathbf{\Theta}} \log p(D|\mathbf{\Theta}) \lambda ||\mathbf{\Theta}||_{1} \\ \bullet &= \operatorname{argmax}_{\mathbf{\Theta}} \operatorname{tr}(\mathbf{S}\mathbf{\Theta}) + \log \det \mathbf{\Theta} \lambda ||\mathbf{\Theta}||_{1} \\ \bullet & \mathbf{S} : \text{sample cov}; ||\mathbf{\Theta}||_{1} = \sum_{i,j} |\mathbf{\Theta}^{(i,j)}| \end{aligned}$
- •Construct a graph using sparsity of $\widehat{\mathbf{\Theta}}$

Conditional Markov Network

- •In many tasks, the conditional distribution is the key interest.
 - •p(Y|X) measures the randomness on Y given X and help us make a prediction.
 - •Both regression and classification requires a **conditional** model.
- •How to factorize a conditional distribution over *G*?

Conditional Markov Network

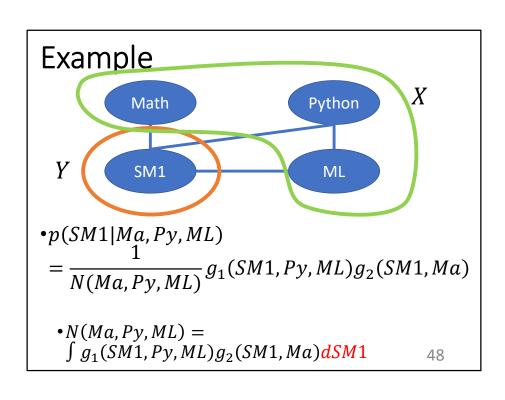
•We say a conditional probability distribution P(Y|X) factorizes over G whose nodes V = $X \cup Y$, if

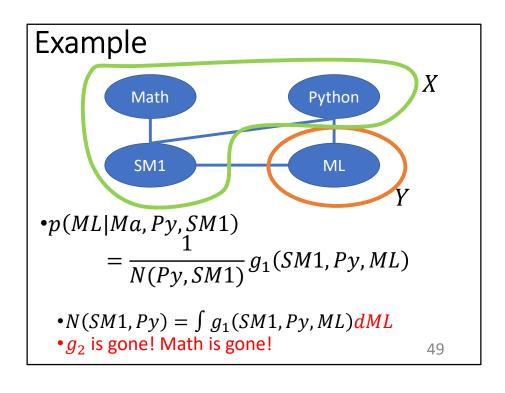
•
$$p(Y|X) = \frac{1}{N(X)} \prod_{c \in C} g_c(V_c)$$
,
• $C := \{c \text{ is a clique in } G|V_c \not\subseteq X\}$

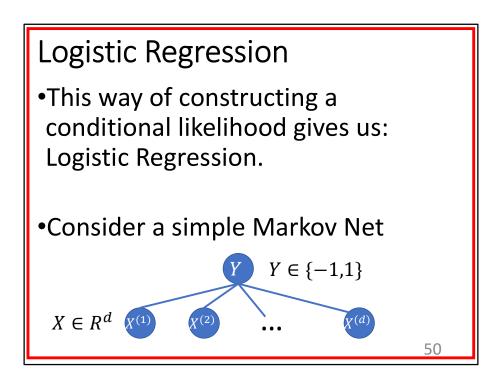
- • $N(X) := \int \prod_{c \in C} g_c(V_c) \frac{dY}{dY}$
- •Normalizing constant:
 - •It normalizes the distribution to 1 over the domain of the random variable (Y).

Conditional Markov Network

•p(Y|X) does not include factors defined on subsets of conditioning variable X!







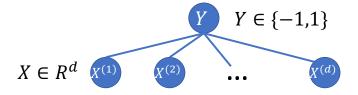
Y is the variable for class labels, that can be either positive +1 or negative -1 as we saw before.

Logistic Model

Using the factorization rule above,

$$\bullet p(Y|X) = \frac{1}{N(X)} \prod_i g_i(Y, X^{(i)})$$

•
$$N(X) = \sum_{Y \in \{-1,1\}} \prod_{i} g_i(Y, X^{(i)})$$



Logistic Model

- •Let us construct a model of cond. likelihood p(Y|X)!
- •By setting $g_i(Y = y, X_i = x^{(i)}; \beta_i, \beta_0) \coloneqq \exp\left(y(\beta^{(i)} \cdot x^{(i)} + \beta_0)\right)$

•
$$N(X; \boldsymbol{\beta}, \beta_0) = \sum_{y \in \{1, -1\}} \exp(y(\langle \boldsymbol{\beta}, \boldsymbol{x} \rangle + d\beta_0))$$

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This is another example, of graphical modelling. We have a graph, which encodes the conditional independence. We then create a probabilistic model based on that graph.

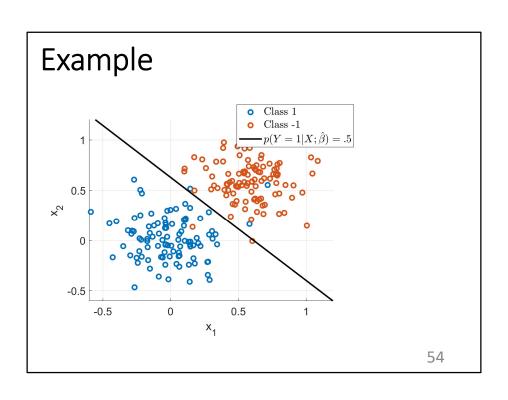
We replaced the integral by sum in the normalizing term, which is required by a discrete variable Y

Logistic Regression

- •Logistic model:
- • $p(y|\mathbf{x}; \boldsymbol{\beta}, \beta_0) = \frac{1}{N(X)} \exp(y(\langle \boldsymbol{\beta}, \mathbf{x} \rangle + d\beta_0))$

•
$$N(x) = \exp(\langle \boldsymbol{\beta}, \boldsymbol{x} \rangle + d\beta_0) + \exp(-\langle \boldsymbol{\beta}, \boldsymbol{x} \rangle - d\beta_0)$$

- • $oldsymbol{eta}$, eta_0 can be fitted using MLE.
 - $\bullet \hat{\beta}, \hat{\beta}_0 = \arg \max_{\beta, \beta_0} \sum_{i=1}^n \log p(y_i | x_i; \beta, \beta_0)$
- •Homework: Show this is the same Logistic Regression we talked about in Lec 10.



Conclusion

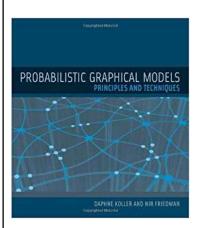
- •Markov network uses an **undirected graph** to represent conditional independencies and factorizations of a probability distribution.
- •Two examples of Markov network
 - •Gaussian Markov network factorizes over the graph defined by its **inverse covariance**.
 - •Logistic model is a conditional prob. dist. factorizes over a classification network.



Judea Pearl

Bayesian Network

References



 Today's class roughly follows Chapter 3 in Probabilistic Graphical Models by Koller and Friedman.

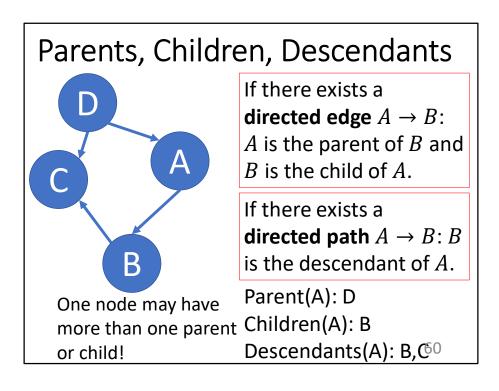
A Directed Graphical Model

- •Markov network is an **undirected graphical model**.
 - •which encodes cond. indep.
 - •and factorization of a probability dist.
- •Can we use a directed graphical model to do the same job?
 - •Some dependencies are better addressed using a directed model.

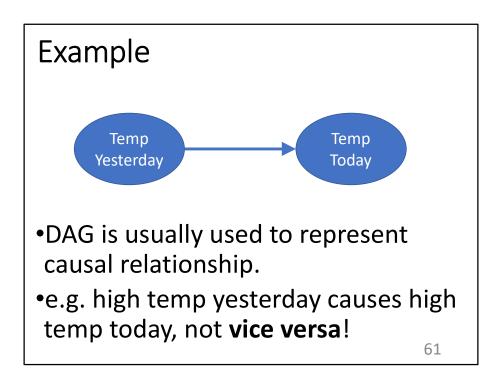
Directed Acyclic Graph

- •The directed graphical model uses Directed Acyclic Graph (DAG) as its graphical representation.
 - • $G := \langle E, V \rangle$, E is directed edge set.
 - •DAG: G without directed cycles.

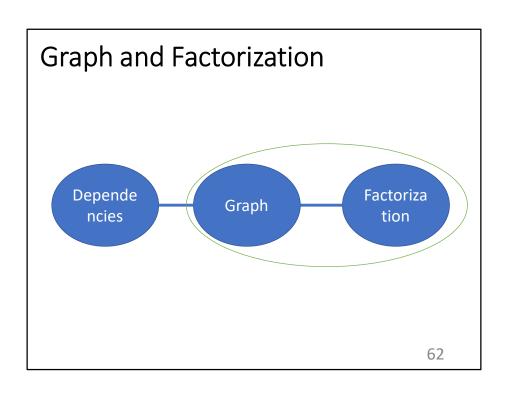




However, a Bayesian network not necessarily comes with causal information. This is important but not in this class



However, a Bayesian network not necessarily comes with causal information. This is important but not in this class



Representing Factorization using DAG

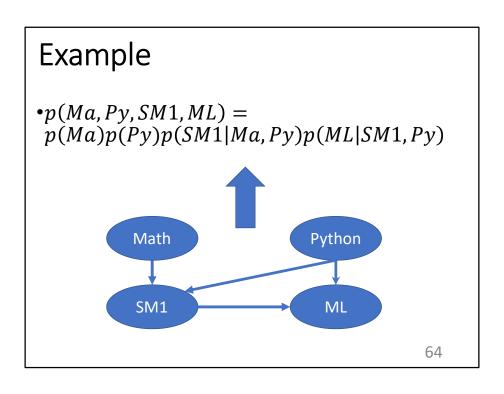
- •DAG can also be used to represent the factorization of a probability dist.
- •We say a probability dist. p(X) factorizes over a DAG G if

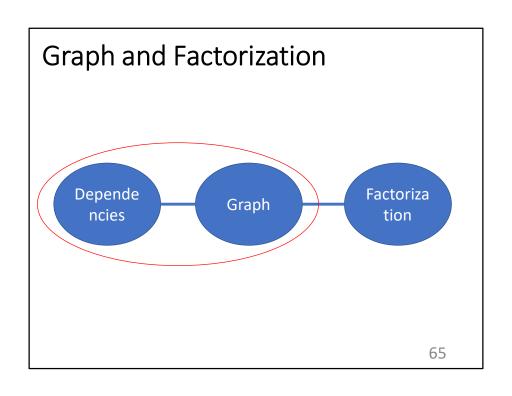
•
$$p(X) = \prod_{v \in V} p(X_v | X_{\text{parent}(X_v)})$$

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Equality

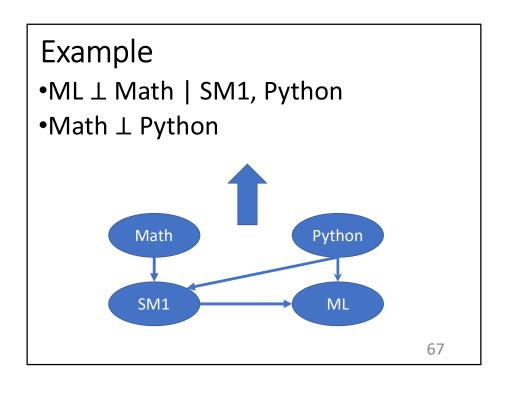
Probability





Represent Cond. Indep. using DAG

- •Given DAG G.
- • X_v is independent of $X_{\text{non-desc}(X_v)}$ given $X_{\text{parent}(X_v)}$, $\forall v$.
 - •This is an analogy to Markov net, as X_v and all non-descendants of X_v are "blocked" by the parents of X_v .
 - •Knowing $X_{\operatorname{parent}(X_v)}$, $X_{\operatorname{non-desc}(X_v)}$ tell us nothing new about X_v .

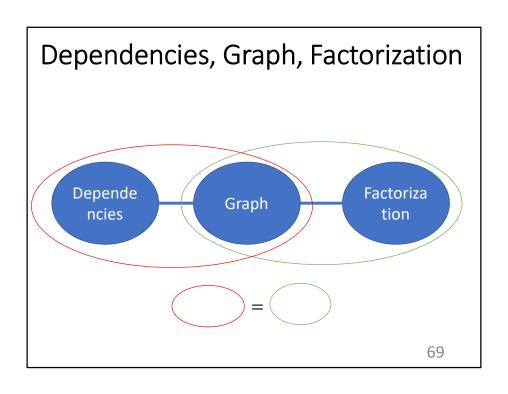


Equivalency between Factorization and Conditional Independence over DAG *G*•If *p* factorizes over *G*, *p* satisfies all

- •If p factor e es over G, p satisfies all conditional independence represented by G.
- •If p satisfies all conditional independence represented by G, then p factorizes over G.

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PC: verify this on unit score example.



Bayesian Network

•A probability dist. p(x) factorizes over a DAG G is called Bayesian network.

Bayesian Network for Classification $Y \in \{-1,1\}$ $X \in \mathbb{R}^d \text{ (1)} \text{ (2)} \dots \text{ (d)}$ •Looks familiar?

Bayesian Network for Classification

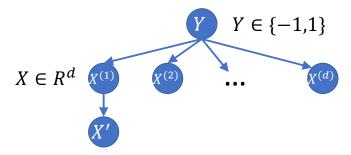
Write down the conditional probability P(Y|X).

•
$$P(Y|X) = \frac{\prod_{i} P(X^{(i)}|Y)P(Y)}{P(X)}$$
•This is how Naïve Bayes is derived!

Bayesian Network for Classification

- Compare NB and Logistic regression from the following perspectives:
 - The graphical structure
 - Same structure
 - Directed vs. Undirected
 - The factorization
 - Pairwise factors between Y and X_i .
 - Factor on cliques vs. Conditional Prob.
 - The probabilistic model
 - Both use p(Y|X) to make prediction
 - NB does not give you p(Y|X), only up to a constant
 - The training/fitting of a classifier
 - Estimation of p(Y|X) vs. P(X|Y)
 - Prediction rule
 - Both $\hat{y} := \operatorname{argmax}_{y} p(Y|X)$

Question



•Homework: Given this Bayesian Net for a classification task, should you include feature X' for classification? Why?

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$$P(Y|X) = \frac{\prod_i P(X_i|Y)P(Y)}{P(X)} p(X'|X)$$

$$\hat{y} \coloneqq \operatorname{argmax}_y p\left(\frac{\prod_i P(X_i|Y)P(Y)}{P(X)} p(X'|X)\right), \text{ for a specific } x!$$

Constant!

Conclusion

- •Bayesian Net uses a **DAG** to represent factorization and conditional independence of a probability distribution .
 - Similar to Makov net
- •Naïve Bayes is derived from a simplified Bayesian net for a conditional probability P(Y|X).