Capturing Dependency of Data using Graphical Models

Song Liu
(song.liu@bristol.ac.uk)

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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

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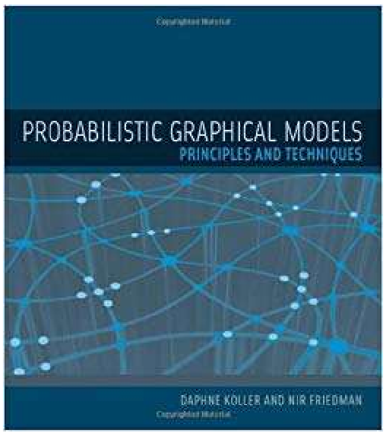
References



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

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Dependency in Dataset:
A Unit Score Example

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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
…	…	…	…	…

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.

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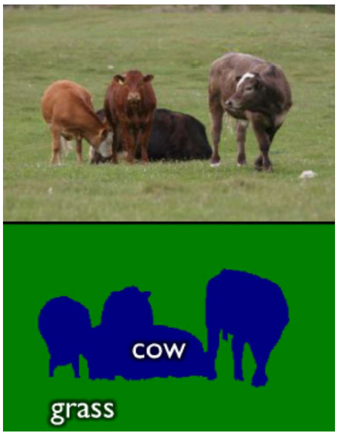
Example: Pixel Correlation



- 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 $\{\boldsymbol{x}_i\}_{i=1}^{n}$,
  - $\boldsymbol{x}_i = \left[x_i^{(1)}, x_i^{(2)} \ldots x_i^{(d)}\right] \in R^d$
  - $\boldsymbol{x}_i$ is a vector of a student i's scores.
  - e.g., $x^{(1)}$ is SM1, $x^{(2)}$ is Math…

- **What does $p\left(x^{(1)}, x^{(2)} \ldots\ x^{(d)}\right)$ look like?**

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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
  - $p(x_1, x_2, \dots x_n|\theta) = \prod_{i=1}^{n} p(x_i|\theta)$
- Maximum Likelihood Estimation
  - $\max_\theta \prod_{i=1}^{n} p(x_i|\theta)$
  - **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

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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:
  - $X \perp Y$
  - $\Leftrightarrow p(X, Y) = p(X)p(Y)$
    - Factorization
  - $\Leftrightarrow p(X|Y) = p(X) \Leftrightarrow p(Y|X) = p(Y)$
    - No Information exchange between X and Y.

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

Conditional Independence of R.V.s

- 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
  - $\Leftrightarrow p(X|Y,Z) = p(X|Z)$
    - Y does not give any additional info which changes the prob. of X given Z.
    - No **direct** information exchange between X and Y
  - $\Leftrightarrow p(Y|X,Z) = p(Y|Z)$

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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 in-between X and Y.
  - $X \perp Y|Z \Leftrightarrow$ no **direct** information exchanges between X and Y

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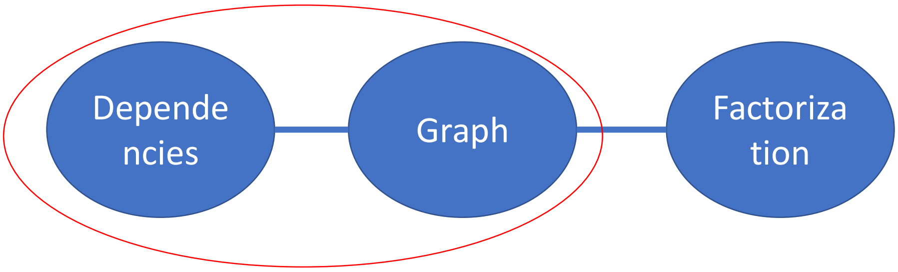
The analogy is like relationship between people.

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.

Creating a Graph of Independence



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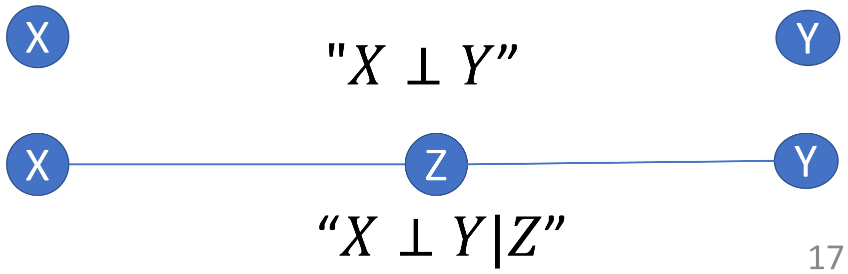
Representing (Conditional) Independence by Graph

- Given many R.Vs, listing all (cond.) independence can be cumbersome.
- A **graphical representation** is helpful:



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 $G =< E, V >$,
  - 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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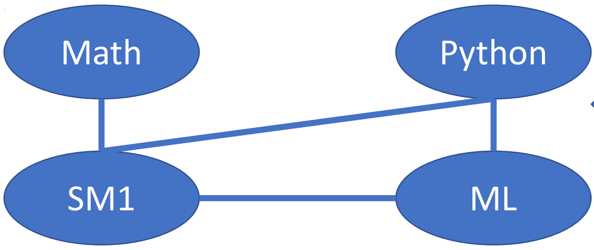
Blocked, means there is no path linking X and Y

Example: Encoding (cond.) indep. by graph

Math $\perp$ ML | SM1
Math $\perp$ Python | SM1
Math $\perp$ ML | SM1, Python
Math $\perp$ Python, ML | SM1
Math $\perp$ Python | SM1, ML



List of conditional independence encoded by Graph!

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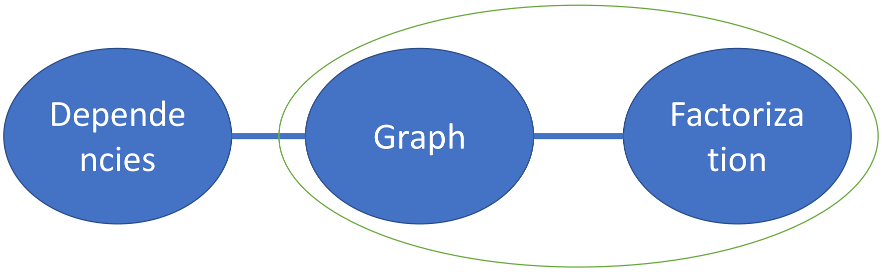
Graph is a powerful tool to encode/visualize (conditional) indepedence.

Graph and Factorization



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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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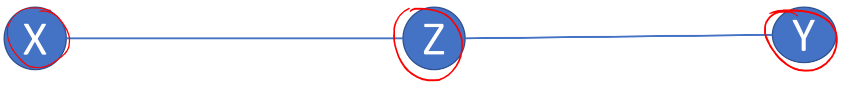
The motivation of factorizing a probability dist.

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??

$$"\underline{P(X,Y)} = \underline{P(X)}\,\underline{P(Y)}"$$



$$\text{“}P(X,Y,Z) \propto \underline{g_1(X,Z)}\,\underline{g_2(Y,Z)}\text{”}$$

Representing Prob. Distribution Factorization by Graph

- Given a graph $G =< E, V >$,
- We say $p(X)$ factorizes over G:
- If $p(X) \propto \prod_{c \in C} g_c\left(X^{(c)}\right)$
  - 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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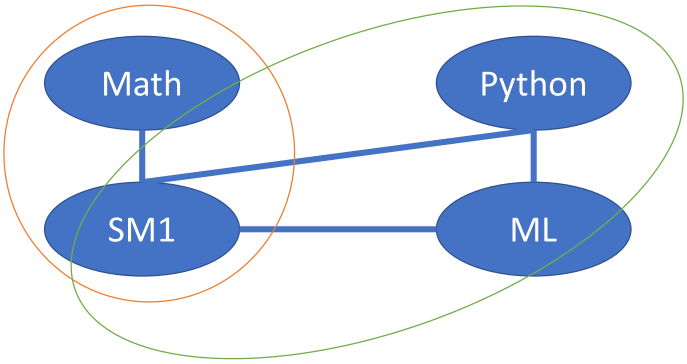
Like what we saw before, g_c is a function that can be in any form.

g is called "factor"

Example

$$p(Ma, SM1, Py, ML) \propto g_1(Ma, SM1) \cdot g_2(Py, ML, SM1).$$



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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!**

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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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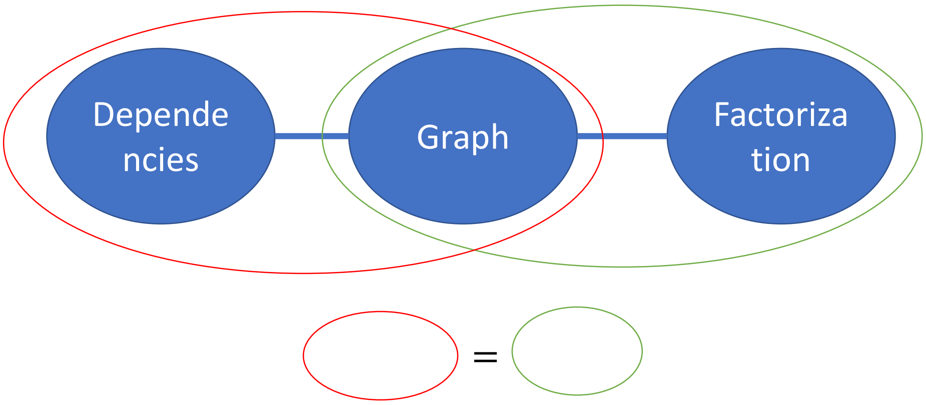
What does that mean

Dependencies, Graph, Factorization



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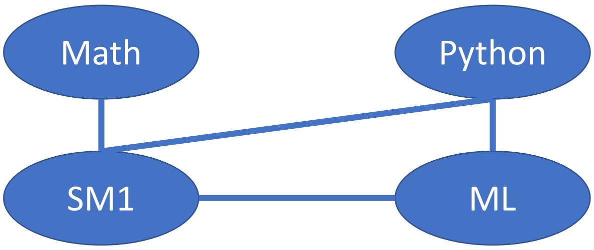
Equivalency between Factorization and Conditional Independence over G

- Verify this on Scores of Units example!
- **Homework:**
  - Create G using factorization on page 24 and check if the graph encodes all conditional Independence of $p(Ma, SM1, Py, ML)$.
  - Create G using all conditional independence on page 19 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: $X \perp Y | Z \Leftrightarrow p(X, Y, Z) \propto g_1(X, Z) \cdot g_2(Y, Z)$

$$X \perp Y, W | Z \Rightarrow X \perp Y | Z$$

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Example

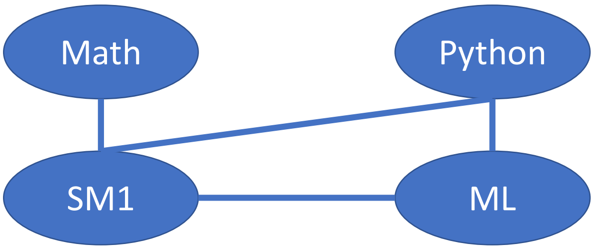
Math $\perp$ ML | SM1

Math $\perp$ Python | SM1

Math $\perp$ ML | SM1, Python

Math $\perp$ Python, ML | SM1

Math $\perp$ Python | SM1, ML



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

Weak Union Rule: $X \perp Y,W|Z \Rightarrow X \perp Y|W,Z$

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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:
- $\boldsymbol{x} \in R^d, \boldsymbol{x} \sim N(\mathbf{0}, \boldsymbol{\Sigma})$
- $p(\boldsymbol{x}) \propto \exp\left[-\frac{\boldsymbol{x}(\boldsymbol{\Sigma})^{-1}\boldsymbol{x}^{\top}}{2}\right]$ $\boxed{\text{Let } \boldsymbol{\Theta} = (\boldsymbol{\Sigma})^{-1}}$.

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

$$\propto \prod_{u,v;\Theta^{(u,v)}\neq 0} \exp\left(-\Theta^{(u,v)} x^{(u)}\, x^{(v)}\right)$$

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aBa^T = \sum_ij B_ij ai aj

You can factorize the joint Gaussian using the pairwise factors

Gaussian Markov Network

- $p(\boldsymbol{x}) \propto \prod_{u,v;\Theta^{(u,v)}\neq 0} g_{u,v}\left(x^{(u)}, x^{(v)}\right)$
- $p(\boldsymbol{x})$ **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?)

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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 $\boldsymbol{\Theta}$.

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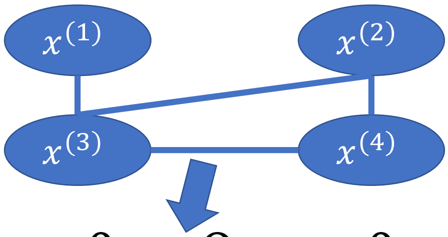
Theta must be positive definite!!

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

Example



- $\mathbf{\Theta} = \begin{bmatrix} \Theta_{11} & 0 & \Theta_{13} & 0 \\ 0 & \Theta_{22} & \Theta_{23} & \Theta_{24} \\ \Theta_{13} & \Theta_{23} & \Theta_{33} & \Theta_{34} \\ 0 & \Theta_{24} & \Theta_{34} & \Theta_{44} \end{bmatrix}$

sparsity of $\mathbf{\Theta}$ = sparsity of the G!

- **If I know dependency of my R.V.s, I can easily write down my Gaussian model.**

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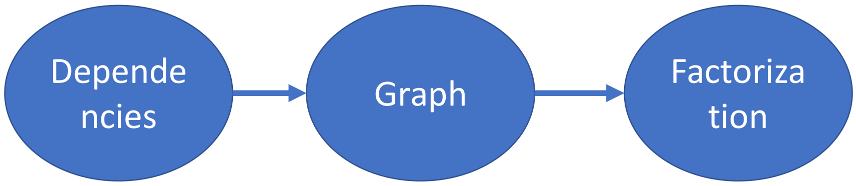
Theta must be positive definite!!

From Dependency to Factorization



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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 $(x_0, \boldsymbol{x})$ are drawn from a joint Gaussian $p(x_0, \boldsymbol{x})$, show log likelihood $\log p(x_0|\boldsymbol{x})$ 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?

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Gaussian Markov Network

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

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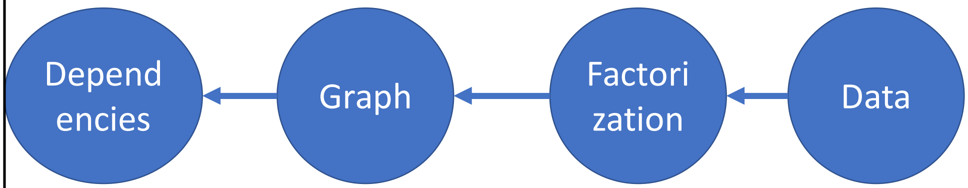
From Factorization to Graph



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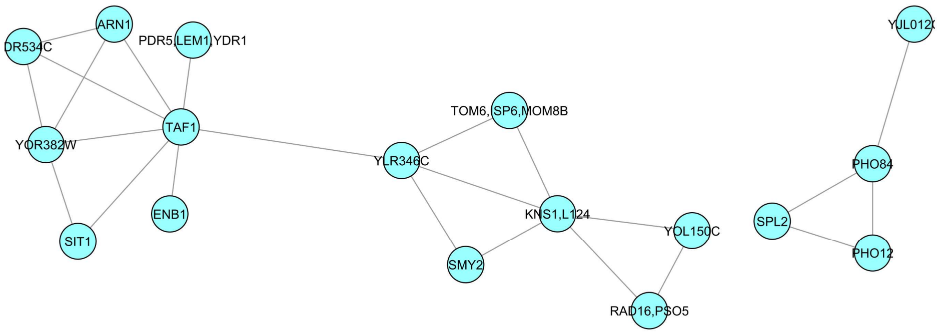
Example: Gene Expression Data

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

Gene Network (Banerjee et al., 2008)



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Exponential Family Distribution

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

Graphical Lasso (Jerome Friedman et al., 2008)

- Given $D = \{\boldsymbol{x}_i\}_{i=1}^{n}, \boldsymbol{x} \in R^d$,
- Construct a Gaussian likelihood:
  - $p(D|\boldsymbol{\Theta}) = \prod_i N_{\boldsymbol{x}_i}(\boldsymbol{0}, \boldsymbol{\Theta}^{-1})$
- $\widehat{\boldsymbol{\Theta}} := \mathrm{argmax}_{\boldsymbol{\Theta}} \log p(D|\boldsymbol{\Theta}) - \lambda||\boldsymbol{\Theta}||_1$
  - $= \mathrm{argmax}_{\boldsymbol{\Theta}} - \mathrm{tr}(\boldsymbol{S}\boldsymbol{\Theta}) + \log\det\boldsymbol{\Theta} - \lambda||\boldsymbol{\Theta}||_1$
  - $\boldsymbol{S}$:sample cov; $||\boldsymbol{\Theta}||_1 = \sum_{i,j}|\Theta^{(i,j)}|$
- Construct a graph using sparsity of $\widehat{\boldsymbol{\Theta}}$

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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?

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Conditional Markov Network

- We say a conditional probability distribution $P(Y|X)$ factorizes over G whose nodes $V = X \cup Y$, if
- $p(Y|X) = \frac{1}{N(X)} \prod_{c \in C} g_c(V_c)$,
  - $C := \{c \text{ is a clique in } G | V_c \nsubseteq X\}$
- $N(X) \coloneqq \int \prod_{c \in C} g_c(V_c)\, dY$
- Normalizing constant:
  - It normalizes the distribution to 1 over the domain of the random variable (Y).

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Conditional Markov Network

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

  - $p(Y|X) = \frac{1}{N(X)} g_1(Y,X) g_2\,(X)$
  - $N(X) =$
    $\int g_1(Y,X) g_2(X) dY = g_2(X) \int g_1(Y,X) dY$
  - $p(Y|X) = \frac{g_1(Y,X) g_2\,(X)}{g_2\,(X) \int g_1(Y,X) d} = \frac{g_1(Y,X)}{\int g_1(Y,X) dy}$

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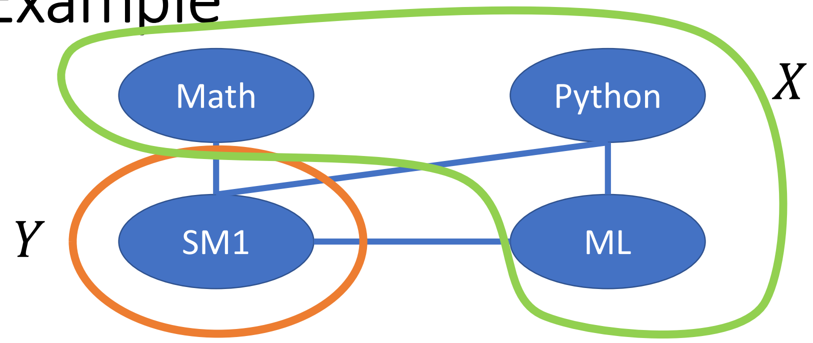
Example

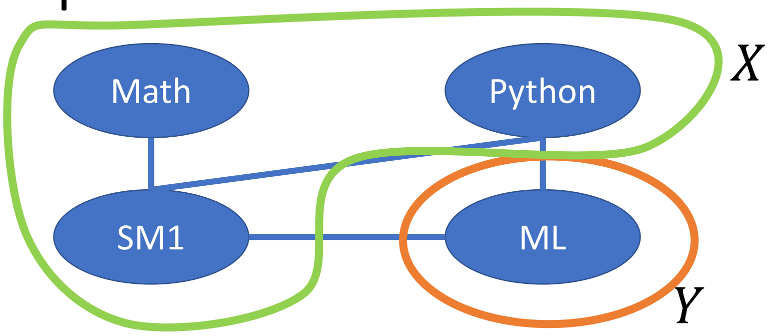


- $p(SM1|Ma, Py, ML)$

$$= \frac{1}{N(Ma, Py, ML)} g_1(SM1, Py, ML) g_2(SM1, Ma)$$

  - $N(Ma, Py, ML) = \int g_1(SM1, Py, ML) g_2(SM1, Ma) dSM1$

Example



- $p(ML|Ma, Py, SM1) = \frac{1}{N(Py, SM1)} g_1(SM1, Py, ML)$
  - $N(SM1, Py) = \int g_1(SM1, Py, ML) dML$
  - g_2 is gone! Math is gone!

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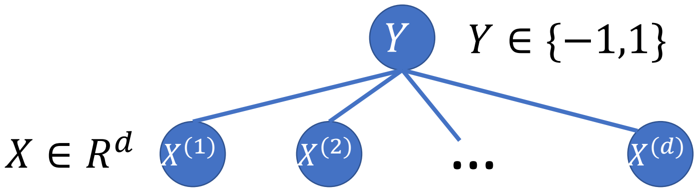
Logistic Regression

- This way of constructing a conditional likelihood gives us: Logistic Regression.

- Consider a simple Markov Net



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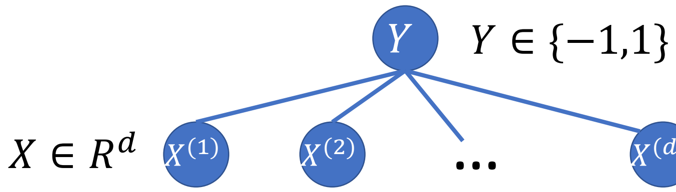
Y is the variable for class labels, that can be either positive +1 or negative -1 as we saw before.

Logistic Model

- Using the factorization rule above,
  - $p(Y|X) = \frac{1}{N(X)} \prod_i g_i(Y, X^{(i)})$
  - $N(X) = \sum_{Y \in \{-1,1\}} \prod_i g_i(Y, X^{(i)})$



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Logistic Model

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

- $p(y|\boldsymbol{x}; \boldsymbol{\beta}, \beta_0) = \frac{1}{N(X)} \prod_i \exp\Big(y\big(\beta^{(i)} \cdot x^{(i)} + \beta_0\big)\Big)$
  $= \frac{1}{N(X)} \exp\big(y(\langle \boldsymbol{\beta}, \boldsymbol{x} \rangle + d\beta_0)\big).$

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

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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

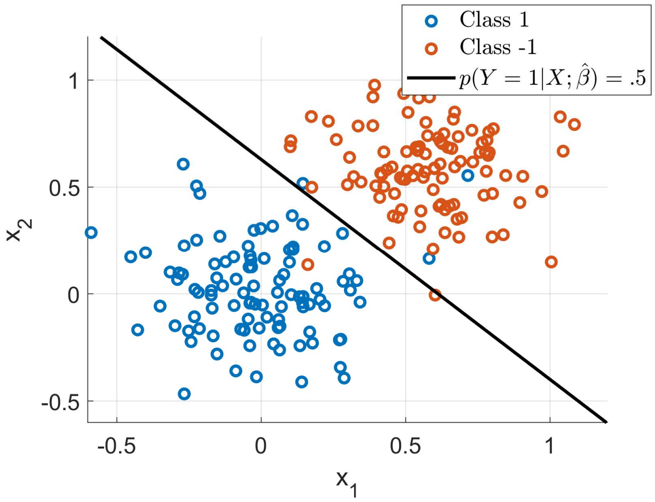
Logistic Regression

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

- $\boldsymbol{\beta}, \beta_0$ can be fitted using MLE.
  - $\widehat{\boldsymbol{\beta}}, \hat{\beta}_0 = \arg\max_{\boldsymbol{\beta}, \beta_0} \sum_{i=1}^{n} \log p(y_i | \boldsymbol{x}_i; \boldsymbol{\beta}, \beta_0)$

- Homework: Show this is the same Logistic Regression we talked about in Lec 10.

Example



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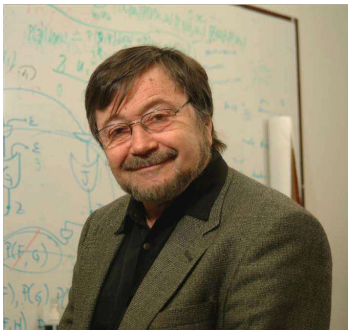
Conclusion

- 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

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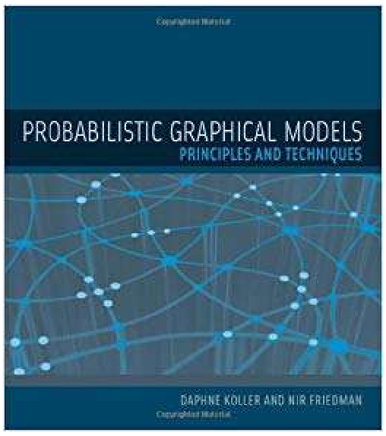
References



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

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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.

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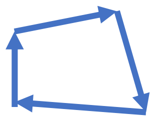
Directed Acyclic Graph

- The directed graphical model uses Directed Acyclic Graph (DAG) as its graphical representation.
  - $G \coloneqq < E, V >, E$ is directed edge set.
  - DAG: G **without directed cycles.**



A directed cycle

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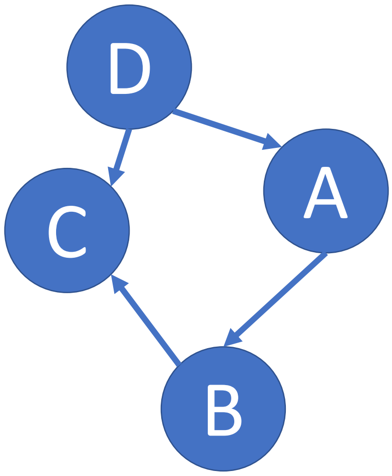
Parents, Children, Descendants



One node may have more than one parent or child!

If there exists a **directed edge** $A \rightarrow B$: A is the parent of B and B is the child of A.

If there exists a **directed path** $A \rightarrow B$: B is the descendant of A.

Parent(A): D

Children(A): B

Descendants(A): B,C

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

Example

- DAG is usually used to represent causal relationship.
- e.g. high temp yesterday causes high temp today, not **vice versa**!

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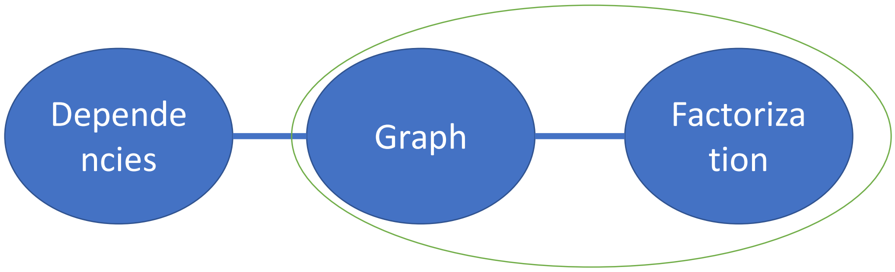
However, a Bayesian network not necessarily comes with causal information. This is important but not in this class

Graph and Factorization



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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
- $p(X) \boxed{=} \prod_{v \in V} \boxed{p}\left(X_v | X_{\mathrm{parent}(X_v)}\right)$

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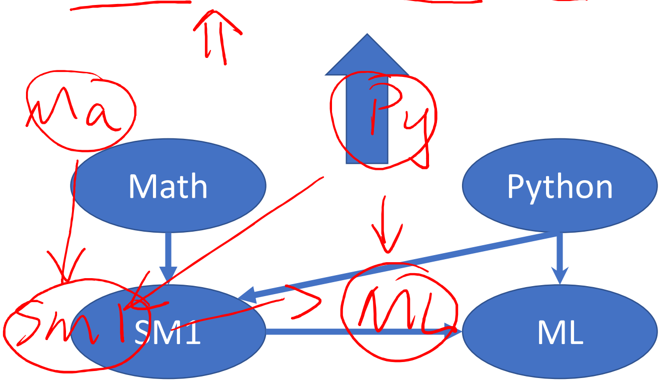
Equality

Probability

Example

- $p(Ma, Py, SM1, ML) =$
  $p(Ma)p(Py)p(SM1|Ma, Py)p(ML|SM1, Py)$



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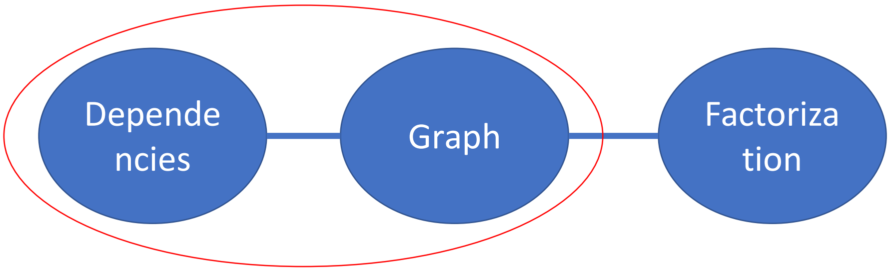
Graph and Dependency



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Represent Cond. Indep. using DAG

- Given DAG G.
- X_v is independent of $X_{\mathrm{non-desc}(X_v)}$ given $X_{\mathrm{parent}(X_v)}$, $\forall v$.
  - 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 $X_{\mathrm{parent}(X_v)}$, $X_{\mathrm{non-desc}(X_v)}$ tell us nothing new about X_v.

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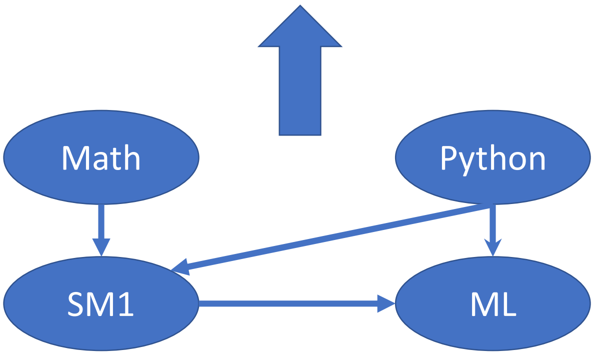
Example

- ML ⊥ Math | SM1, Python
- Math ⊥ Python



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Equivalency between Factorization and Conditional Independence over DAG 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.

Same as Markov Net!!

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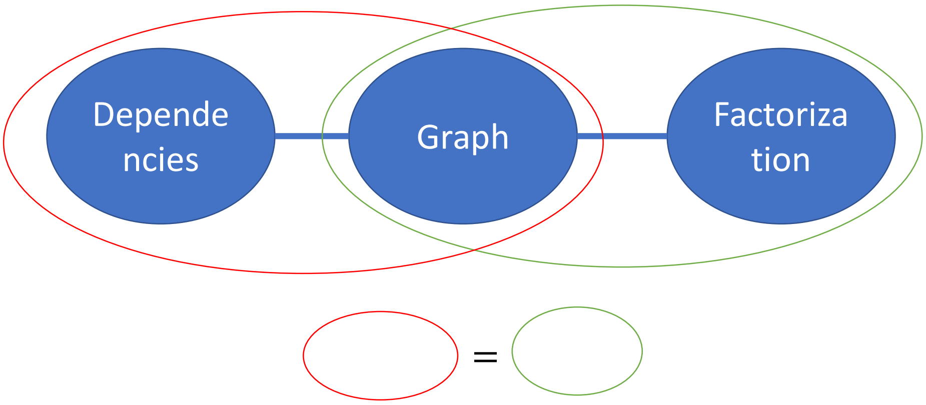
PC: verify this on unit score example.

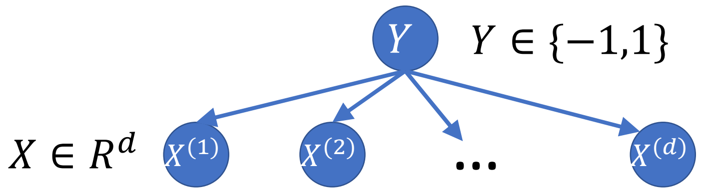
Dependencies, Graph, Factorization



Bayesian Network

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

Bayesian Network for Classification



- Looks familiar?

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Bayesian Network for Classification

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

- $P(Y|X) = \frac{\prod_i P\left(X^{(i)}\middle|Y\right)P(Y)}{P(X)}$
- This is how Naïve Bayes is derived!

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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 $\hat{y} \coloneqq \mathrm{argmax}_y p(Y|X)$

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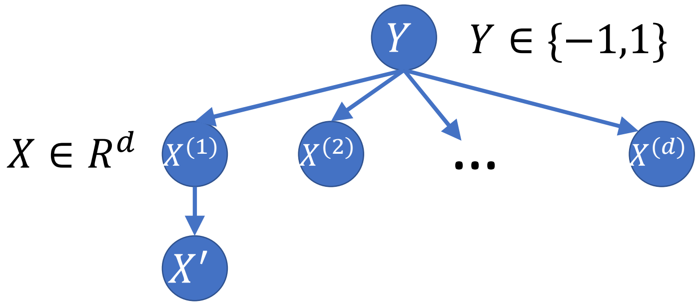
Question



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

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

$\hat{y} \coloneqq \text{argmax}_y p\left(\frac{\prod_i P(X_i|Y)P(Y)}{P(X)} p(X'|X)\right)$, 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 $P(Y|X)$.

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