Revision Class

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General Stuff

What might be given?

- 2 by 2 Matrix Inversion Formula.
- Formulas of
  - Radial Basis Function;
  - Polynomial Kernel function;
  - Radial Basis Kernel function.
- Comp. complexity of matrix inversion.

- You should assume no other information will be given (at least for this part of SPS).

Facts of Exam

- Multiple choices:
  - **Concepts**: e.g. which of … is true/false
  - **Calculation**: e.g. given info, calculate sth.
  - **Practical**: e.g. given a problem setting, which one of the following XXX should be used…

- Part III is new this year!
  - No previous exam available!
- Test yourself using all the mock questions (marked as "**M**" in this presentation).

- Live demonstrations happened off the slides will **not** be tested

Overview

- Feature Transform
  - Different Types of Feature Transforms
  - Variance and Bias Decomposition
  - Kernel Methods
- Feature Redundancy Removal
  - PCA and FDA
- Feature Dependency Modelling
  - Markov Net
  - Bayesian Net

Focus

Prerequisites

- What is Least squares?
  - How to solve it?
- What is Training data/Testing data?
  - What is training error/testing error?
- What is overfitting?

Feature Transforms

Lecture 1.

Key Messages

- Polynomial Transform
  - What is “Polynomial feature transform, with degree b=X”?
  - How choices of b affect classification boundary?

- RBF Transform
  - What is “RBF feature transform, with number of basis, b=X”?
  - How do you select centroids?
  - What does the hyper para. σ do?

Polynomial Transform

- Let $\boldsymbol{f}(\boldsymbol{x})$ be polynomial functions:
- When $x \in R$, $\boldsymbol{f}(x) := [x^0, x^1, x^2, \ldots, x^b]$.
  - b is called the degree of $\boldsymbol{f}$.
  - $\boldsymbol{f}(x) = [0, x, x^2]$ is called a degree 2 polynomial trans. on x.

Polynomial Transform

- When $\boldsymbol{x} \in R^d$,
  - $\boldsymbol{f}(\boldsymbol{x}) := \left[\boldsymbol{h}\left(x^{(1)}\right), \boldsymbol{h}\left(x^{(2)}\right), \dots, \boldsymbol{h}\left(x^{(d)}\right)\right]$.
  - $\boldsymbol{h}(t) := [t^0, t^1, t^2, \dots, t^b] \in R^{b+1}$.
  - $\boldsymbol{f}(\boldsymbol{x}) \in R^{d(b+1)}$, which means $\boldsymbol{\beta} \in R^{d(b+1)}$.

Polynomial Transform on Data Matrix

- $\boldsymbol{X} \in R^{n \times d}$ is data matrix with n observations and d dimensions.
- $\boldsymbol{f}(\boldsymbol{X}) := \begin{bmatrix} \boldsymbol{f}(\boldsymbol{x}_1) \\ \boldsymbol{f}(\boldsymbol{x}_2) \\ \dots \\ \boldsymbol{f}(\boldsymbol{x}_n) \end{bmatrix} \in R^{n \times d(b+1)}$.
- We expanded our data matrix.
    - from d to $d(b+1)$

LS Solution

- $\widehat{\boldsymbol{\beta}} := \arg\min \sum_{i=1}^{n} (y_i - < \boldsymbol{\beta}, \boldsymbol{f}(\boldsymbol{x}_i) >)^2$
- $\widehat{\boldsymbol{\beta}} := \left(\boldsymbol{f}(\boldsymbol{X})^\top \boldsymbol{f}(\boldsymbol{X})\right)^{-\mathbf{1}} \boldsymbol{f}(\boldsymbol{X})^\top \boldsymbol{y}$

- **M:** what is the computational complexity of calculating $\widehat{\boldsymbol{\beta}}$?

Radial Basis Function (RBF)

- RBF is another widely used basis function for function approximation.
- $f^{(i)}(x) := \exp\left(-\frac{||x-x_i||^2}{\sigma^2}\right)$
  - $\sigma > 0$ is called **width** and **is a hyper parameter**.
  - σ is determined before fitting
  - A practice is setting σ as the median of all pairwise distances of $\boldsymbol{x}$ in your data.

Radial Basis Function (RBF)

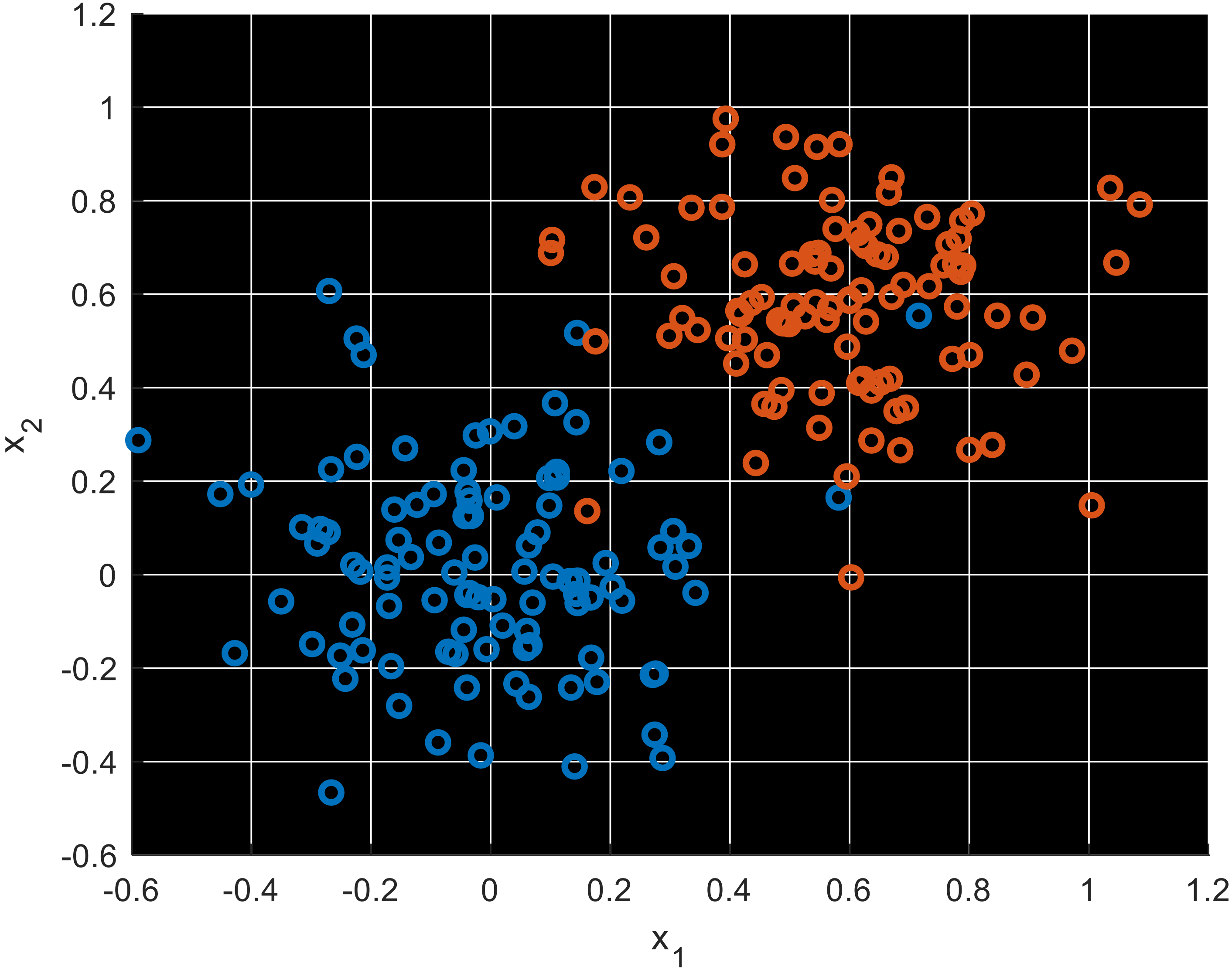
- $\boldsymbol{x}_i$ are called **RBF centroids**.
- $\boldsymbol{x}_i$ can be **randomly chosen** from the $\boldsymbol{x}$ in your dataset
- $\boldsymbol{f}(\boldsymbol{x}) \coloneqq [1, f^{(1)}(x), f^{(2)}(x), \dots, f^{(b)}(x)]$
  - Do not forget 1!

M: How to choose f given data

- Given a dataset D (see next slide), what f should you use for classification? **Hint**: consider computational cost and overfitting
  - Polynomial, $b = 1$
  - Polynomial, $b = 2$
  - Polynomial, $b = 3$
  - RBF, $b = 100$

Use an f that is **just enough** for doing your job without causing heavy computation/overfitting!

M: How to choose f given data



Feature Transforms

Lecture 2. Bias and variance decomposition

Key Messages

- How the choices of b in feature transform affects training and testing error?
  - Training error -> goes down as b increases.
  - Testing error -> goes down and then raise up as b increases.
- What is the expected error at a data point x_i in regression problem?
  - How does it decompose?
  - $\boxed{\text{Remember the decomposition formulas.}}$

Expected Square Error Decomposition

- Given dataset, $D = \{(x_i, y_i)\}$,
- $y_i = g(x_i) + \epsilon$, $\epsilon \sim N(0, \sigma^2)$
- Bias and Variance Decomposition:

$$\mathbb{E}_\epsilon[(y - \hat{y}_i)^2 | \boldsymbol{x}_i]$$

$$= \underline{\mathrm{var}[\epsilon]} + \left[\underline{g(x) - \mathbb{E}_\epsilon[\hat{y}_i | \boldsymbol{x}_i]}\right]^2 + \underline{\mathrm{var}[\hat{y}_i | \boldsymbol{x}_i]}$$

Irreducible error bias variance

- "Variance and Bias decomposition"

M: Calculate Variance.

- Given a data generation scheme, $y_i = x_i + \epsilon$, $\epsilon \sim N(0, \sigma^2), \sum_{i=1} x_i^2 = C$ and a regression model $\hat{y} = \hat{\beta} \cdot x$, where $\hat{\beta}$ is calculated using least squares.
- 1. Write down bias and irreducible error.
  - irr. error = σ^2, bias = 0
- 2. Calculate variance term at a data point $x = 1$. (see next slide for a cheat)

A Closer Look at In Sample $\mathrm{var}[\hat{y}]$

- $\mathrm{var}[\hat{y}|\boldsymbol{x}_i] =< h(\boldsymbol{x}_i), h(\boldsymbol{x}_i) > \cdot\, \sigma^2$
  - Where $h(\boldsymbol{x}_i) := \boldsymbol{f}(\boldsymbol{x}_i)\left(\boldsymbol{f}(\boldsymbol{X})^\top \boldsymbol{f}(\boldsymbol{X})\right)^{-1} \boldsymbol{f}(\boldsymbol{X})^\top$
- Figure out what is $\boldsymbol{f}(\boldsymbol{x})$,$\boldsymbol{f}(\boldsymbol{X})$ and $g(\boldsymbol{x})$ in this example, then you can use this formula to calculate the result.
- $\mathrm{var}[\hat{y}|\boldsymbol{x}_i] = \frac{\sigma^2}{c}$

Feature Transforms

Lecture 3. Kernel methods

Key Messages

- How do we perform kernel least squares?
- Prediction rule: $\hat{\boldsymbol{y}} := \boldsymbol{k}(\boldsymbol{K} + \lambda \boldsymbol{I})^{-1}\boldsymbol{y}$
    - What are $\boldsymbol{k}, \boldsymbol{K}, \boldsymbol{I}, \boldsymbol{y}, \lambda$**?**
    - How do you use this rule to make a prediction?
    - **Remember this prediction rule.**

- What is
    - Linear kernel function
    - Polynomial kernel function
    - RBF kernel function?

M: Example

- Given a dataset $\{(y_1 = 1, x_1 = 1), (y_2 = -1, x_2 = -1)\}$, calculate $\boldsymbol{K}$ in the kernel least square prediction rule using
  - Linear kernel
    - $\boldsymbol{K} = \begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix}$
  - Polynomial kernel $k(x, x') := (< x, x' > +1)^2$.
    - $\boldsymbol{K} = \begin{bmatrix} 4 & 0 \\ 0 & 4 \end{bmatrix}$

- Calculate $\boldsymbol{k}$ for a prediction $\hat{y}$ at data point $x = 2$ using
  - Linear kernel: $\boldsymbol{k} = [2, -2]$
  - Polynomial kernel: $\boldsymbol{k} = [9,1]$

Feature Redundancy

Lecture 4. PCA

Key Messages

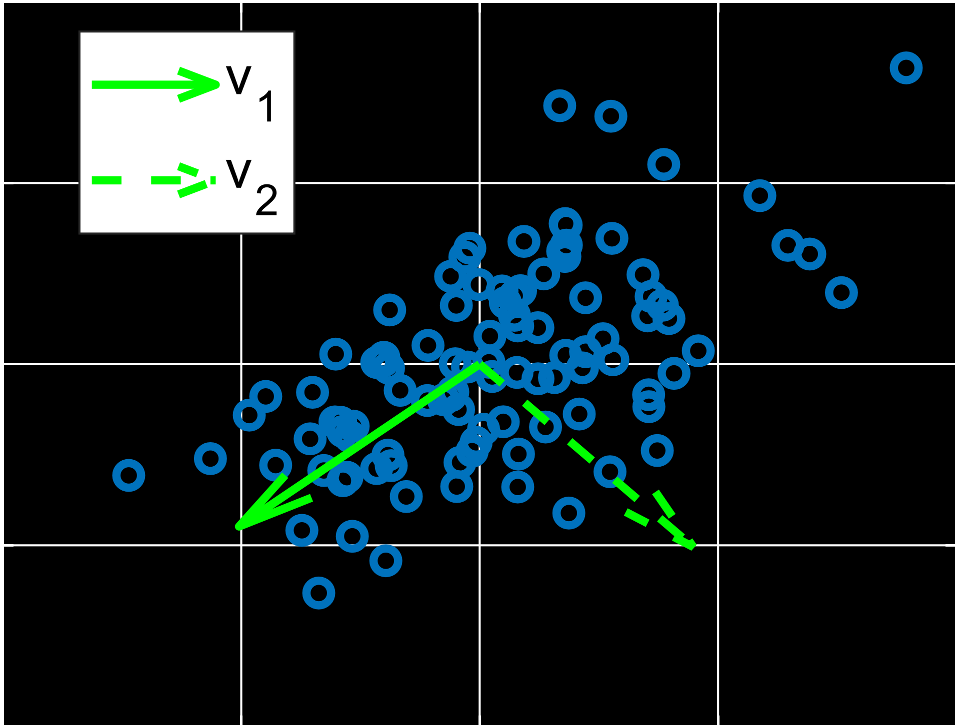
- What is curse of dimensionality?
  - The performance of machine learning algorithm degrades when the dimensionality of dataset increases.

- What kind of information is most likely preserved in a PCA projection?

Minimizing Projection Error

- $\min_{\boldsymbol{B}, \boldsymbol{B}\boldsymbol{B}^\top = \boldsymbol{I}} \sum_{i=1}^{n} \left\| \boldsymbol{x}_i^\top - \boldsymbol{B}^\top \boldsymbol{B} \boldsymbol{x}_i^\top \right\|^2$
  - We minimize square error between original data points and its projection.

Example



v_1 always points at the direction where your dataset has the largest variance!

Intuitively explain why.

Feature Redundancy

Lecture 5. FDA

Key Messages

- Why PCA does **NOT** preserve cluster/class information?
  - It does not take class information into account

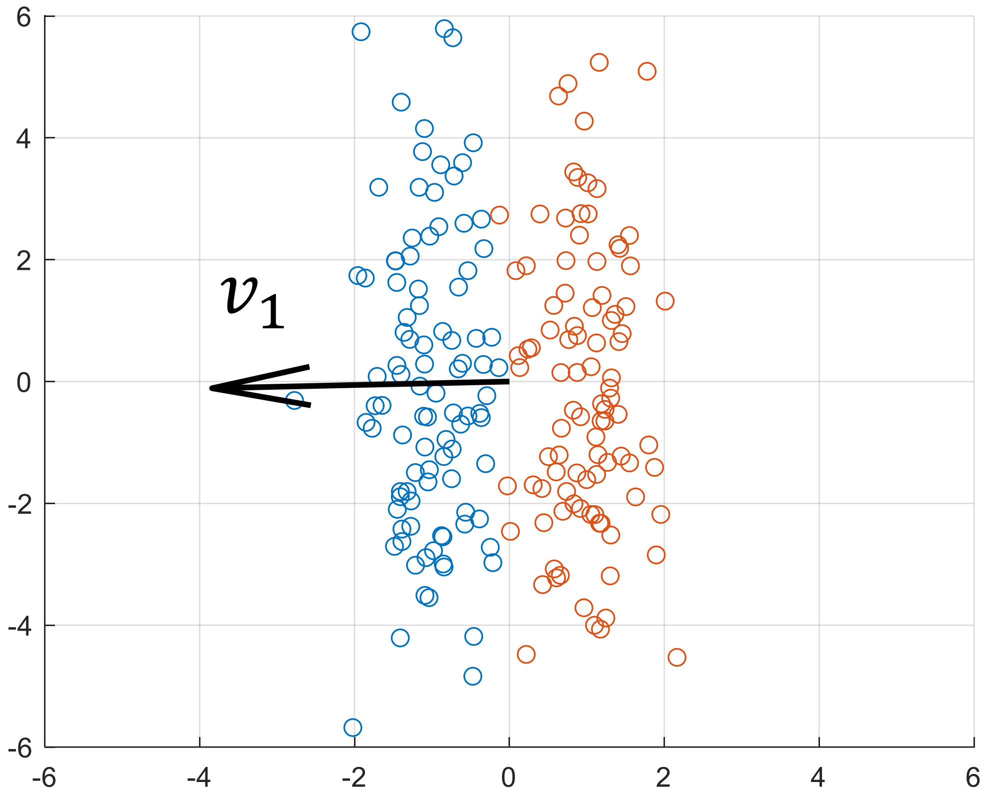
- What is within class scatterness?
- What is between class scatterness?

- What **kind of information** is most likely preserved in a FDA projection?

Objective of FDA

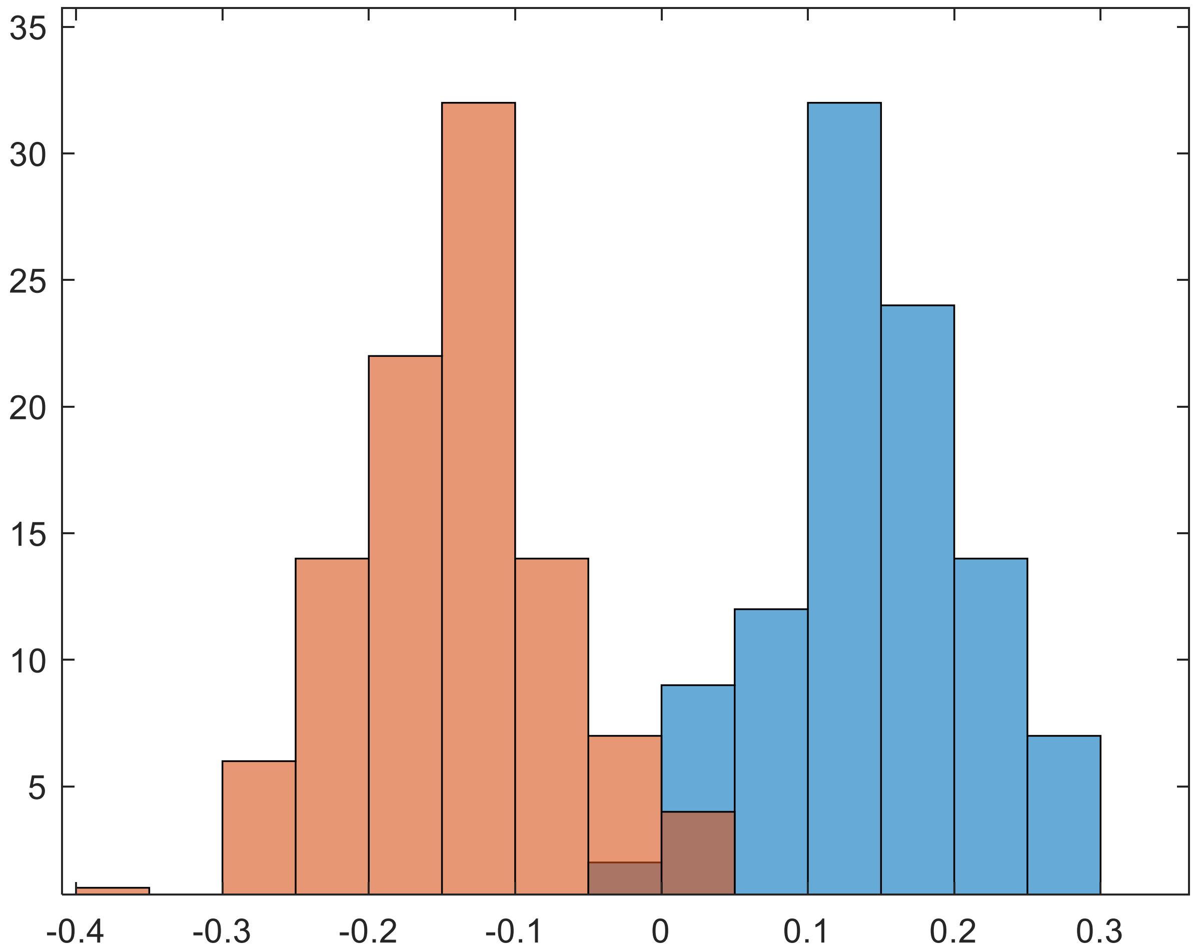
- **Maximizing** between class scatterness $\forall_k$.
  - **Minimize** within class scatterness $\forall_k$.

Example: Binary Classification Dataset



FDA embeds samples to a subspace that is the most **linearly** separable.

Example: embedding, $\boldsymbol{v}_1^\top \boldsymbol{x}^\top$



Class separation is preserved after embedding.

Feature Dependency

Lecture 6. Markov Net

Key Messages

- Cond. independence in a distribution can be encoded by a graph.
- The density of such a distribution factorizes over the same graph.

- What is **Gaussian Markov net**?

Gaussian Markov Network

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

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

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

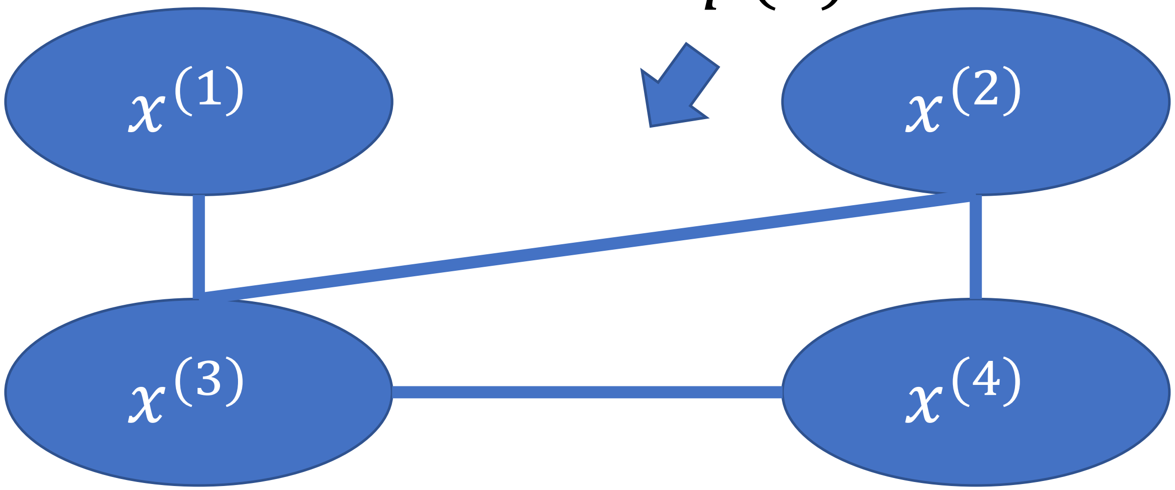
Gaussian Markov Network

- $p(\boldsymbol{x}) \propto \prod_{u,v;\Theta^{(u,v)}\neq 0} g_{u,v}\left(x^{(u)}, x^{(v)}\right)$
- $p(\boldsymbol{x})$ **factorizes over** G**!**
  - G defined by the adjacency matrix $\boldsymbol{A}$

    $$A^{(u,v)} = \begin{cases} 0, \Theta^{(u,v)} == 0 \\ 1, \Theta^{(u,v)} \neq 0 \end{cases}$$
  - G must be an undirected graph (why?)
- $\Leftrightarrow p(\boldsymbol{x})$ satisfies the conditional independence encoded in G.

Example

This G encodes cond. independence in a Gaussian MN $p(\boldsymbol{x})$



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

Notice how the sparsity of G translates into the sparsity of Θ!

Diagonal must be filled!

M

- Suppose graph G encodes all cond. indep. in your Gaussian MN 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

#Edges *2 + #Vertices
Understand why #Edges times 2
Understand why vertices must be non-zero

Feature Dependency

Lecture 7. Bayesian Net

Important Concepts

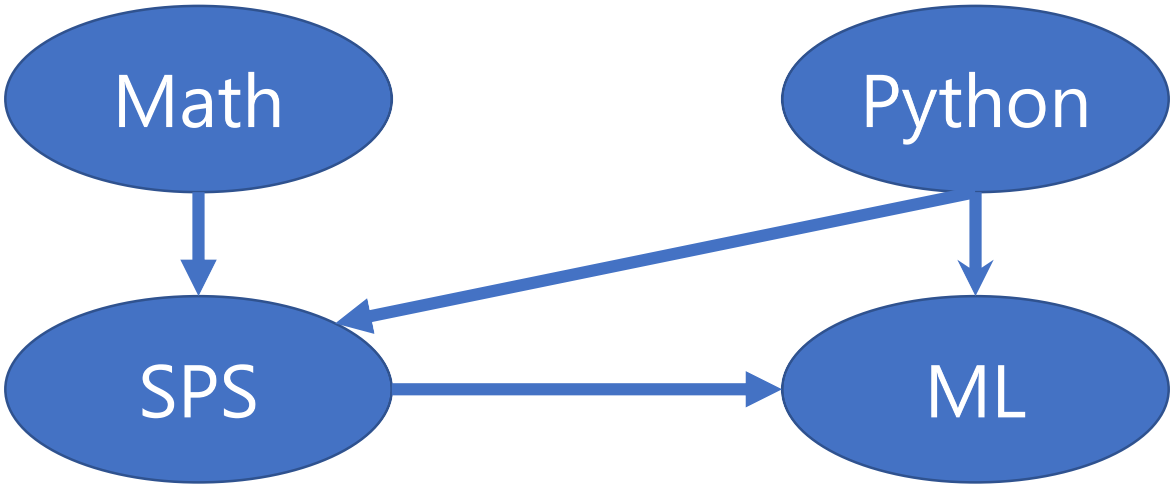
- What is a DAG?
- How a density is represented by a DAG? (Chain rule)
- How do you read conditional independence from a DAG?
- How Naïve Bayes Classifier is derived from a Bayesian net?

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

M: Expressing Density using DAG

- Write down the Bayesian net represented by this graph:



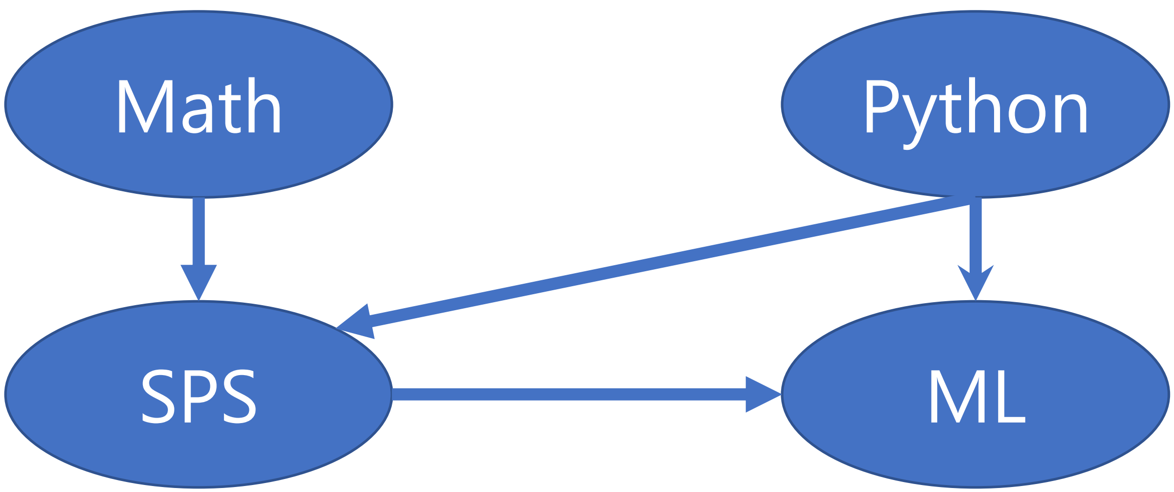
$$p(Ma, Py, SPS, ML)$$
$$= p(Ma)p(Py)p(SPS|Ma, Py)p(ML|SPS, Py)$$

Represent Cond. Indep. using DAG

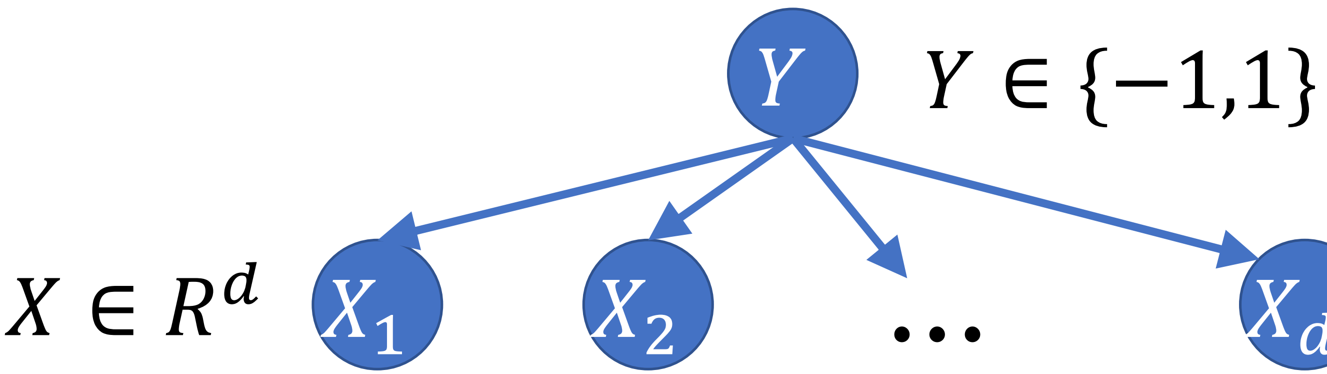
- Given DAG G.
- $\boxed{X_v \text{ is independent of } X_{\mathrm{non-desc}(X_v)} \text{ given } X_{\mathrm{parent}(X_v)},\ \forall v.}$
  - This is an analogy to Markov net, as X_v and all non-descendants of X_v are "blocked" by the parents of X_v.
  - Knowing $X_{\mathrm{parent}(X_v)}, X_{\mathrm{non-desc}(X_v)}$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

M: Expressing Cond. Indep. Using DAG

- Which of the following Cond. Indep. is **not** encoded by the graph?
  - ML ⊥ Math | SPS, Python
  - Math ⊥ Python
  - SPS ⊥ ML | Math



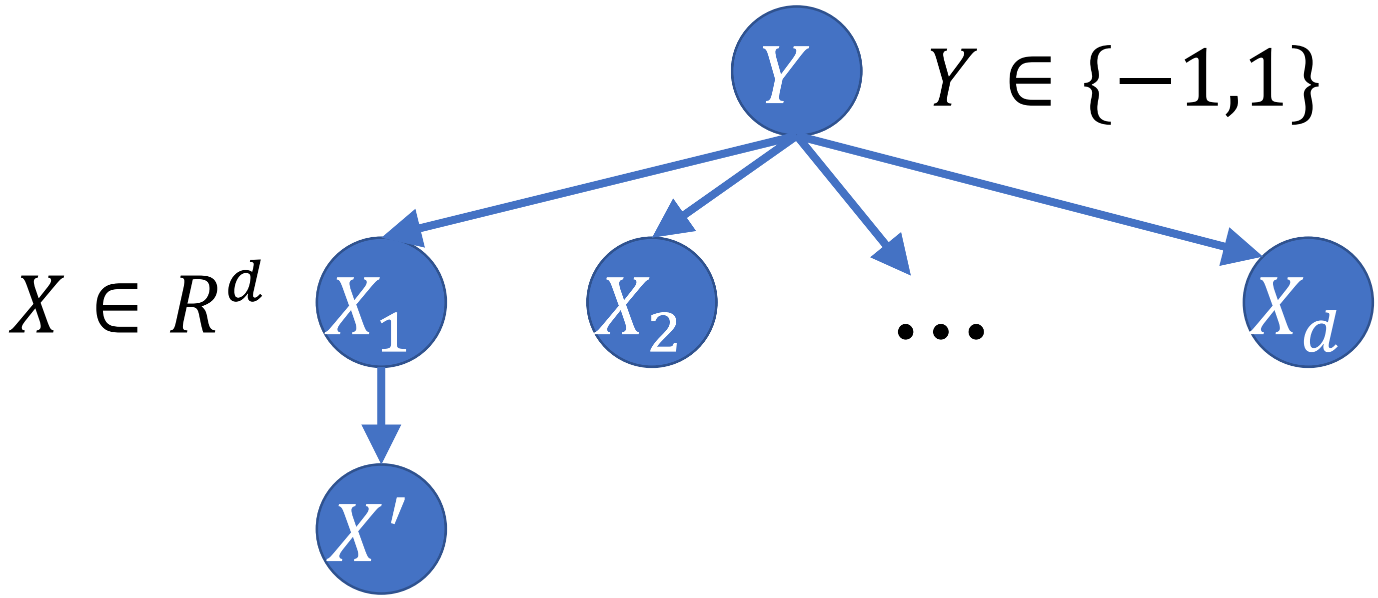
Bayesian Network for Classification



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!

M: “useless feature”



- Given this Bayesian Net for a classification task, should you include feature X' for training? Why?
- $P(Y|X) = \frac{\prod_i P(X_i|Y)P(Y)}{P(X)} p(X'|X)$
- $\hat{y} := \mathrm{argmax}_y p\left(\frac{\prod_i P(X_i|Y)P(Y)}{P(X)} \underbrace{p(X'|X)}_{}\right)$, for a specific x!

  Does not depends on y
- You should not include X' for training.

In Conclusion…

- Take your time to do all questions.
- Bring a Calculator!

- Office Hour:
  - next week Tuesday 3-5pm;
  - next week Thursday 3-5pm.