DS 4400

Machine Learning and Data Mining I
Spring 2024

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Outline

- Announcements on homework, final project, and midterm.
- Generative classifiers
  - Difference from discriminative classifiers
- Linear Discriminant Analysis (LDA)
  - Training and inference
  - Why LDA is a linear classifier
  - Comparison with Logistic Regression

Announcements

- Please submit Homework 2. Deadline is tonight at 11:59pm
- Reminder that you have five late days to use over the course of the semester for homework assignments.
- Please tag pages to questions in Gradescope.
- Homework 1 grades will be released this afternoon. Re-grade requests feature is enabled on Gradescope.
  - Questions 1 and 2: Dhanush
  - Question 3: Jai
  - Questions 4 and 5: Caleb

Announcements - Midterm

Midterm is next Friday February 23.

Please come to class a few minutes early so that we can give as much time as possible for the exam.

You are allowed a one-page cheat sheet and a calculator.

Announcements – Final Project

- Final project resources released on Canvas
  - Document with example datasets
  - Examples of past submissions

- Project proposal due on Friday March 1 before Spring Break.

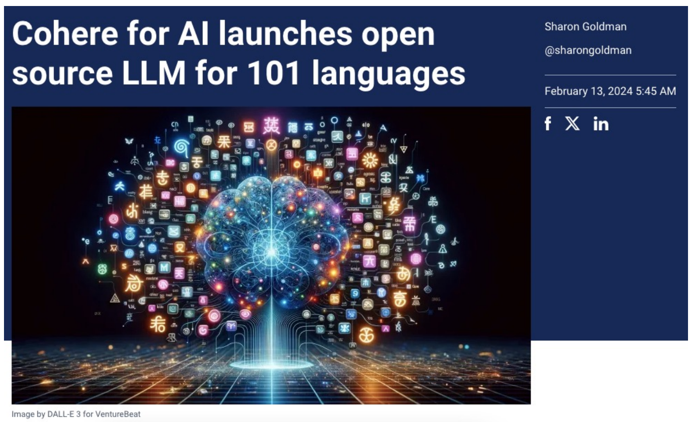
Announcements – Tuesday's Lecture

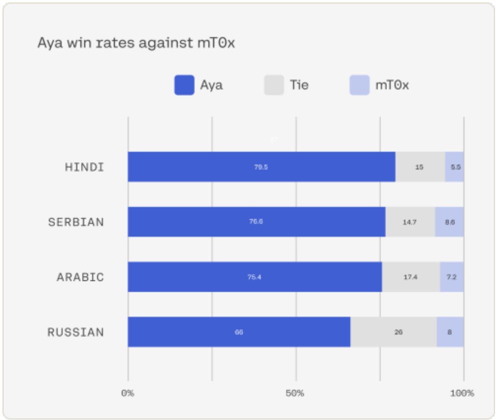
Next Tuesday February 20, we will have a lecture on the Ethics of AI / the societal impacts of AI.

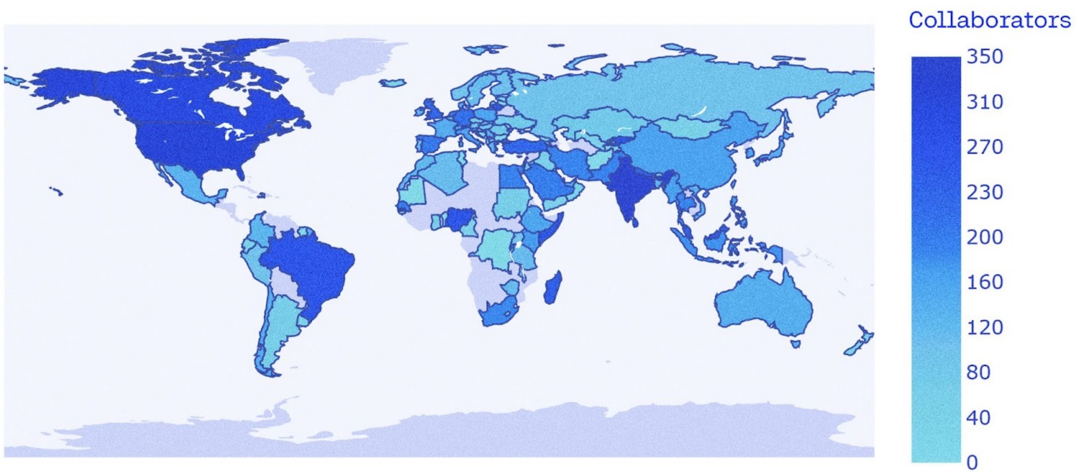
Please bring a laptop to the call as there will be an interactive component led by my labmate Samantha Dies.

News

Cohere for AI launches an open-source LLM, Aya, supporting 101 languages







Generative vs Discriminative

- Generative model
  - Given X and Y, learns the joint probability $P(X, Y)$
  - Can generate more examples from distribution
  - Examples: LDA, Naïve Bayes, language models (GPT-2, GPT-3, BERT)

- Discriminative model
  - Given X and Y, learns a decision function for classification

LDA

- Classify to one of k classes
- Logistic regression computes directly
  - $\mathrm{P}[Y = 1 | X = x]$
- LDA uses Bayes Theorem to estimate it

LDA

- Classify to one of k classes
- Logistic regression computes directly
  - $\mathrm{P}[Y = 1|X = x]$
  - Assume sigmoid function
- LDA uses Bayes Theorem to estimate it
  - $\mathrm{P}[Y = k|X = x] = \frac{\mathrm{P}[X = x|Y = k]\mathrm{P}[Y=k]}{\mathrm{P}[X=x]}$
  - Let $\pi_k = \mathrm{P}[Y = k]$ be the prior probability of class k and $f_k(x) = \mathrm{P}[X = x|Y = k]$

LDA

Assume $f_k(x)$ is Gaussian!
Unidimensional case (d=1)

$$f_k(x) = \frac{1}{\sqrt{2\pi}\sigma_k} \exp\left(-\frac{1}{2\sigma_k^2}(x-\mu_k)^2\right)$$

Continuous Random Variables

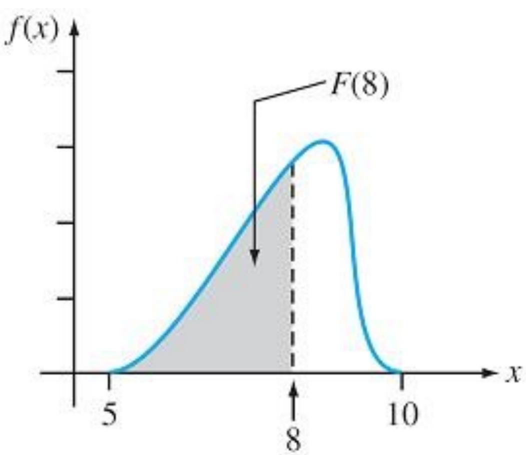
- X:U⟶V is continuous RV if it takes infinite number of values
- The **cumulative distribution function CDF** *F: R* ⟶ {0,1} for *X* is defined for every value *x* by:

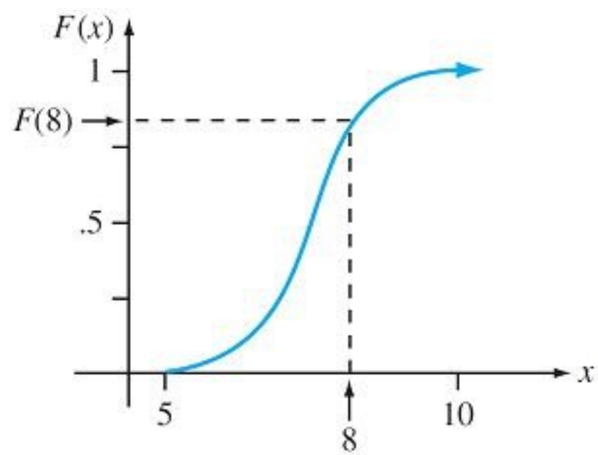
$$F(x) = \Pr(X \leq x)$$

- The **probability distribution function PDF** $f(x)$ for *X is*

$$f(x) = dF(x)/dx$$

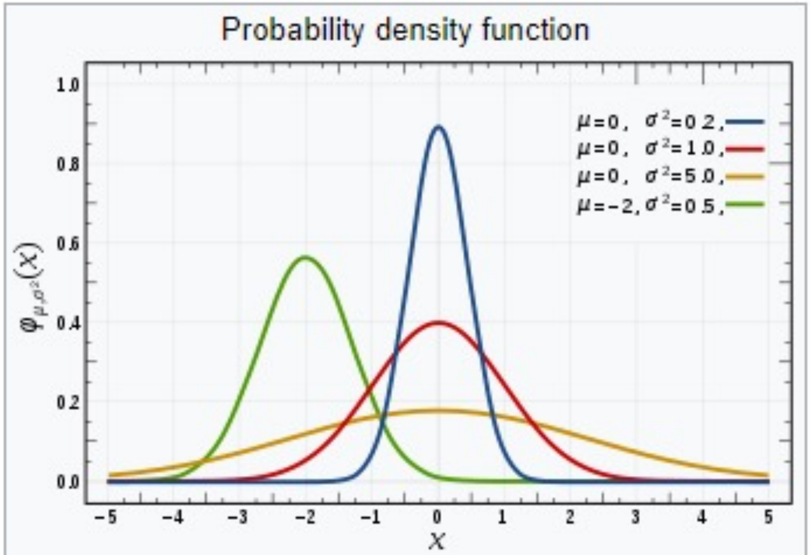
Increasing



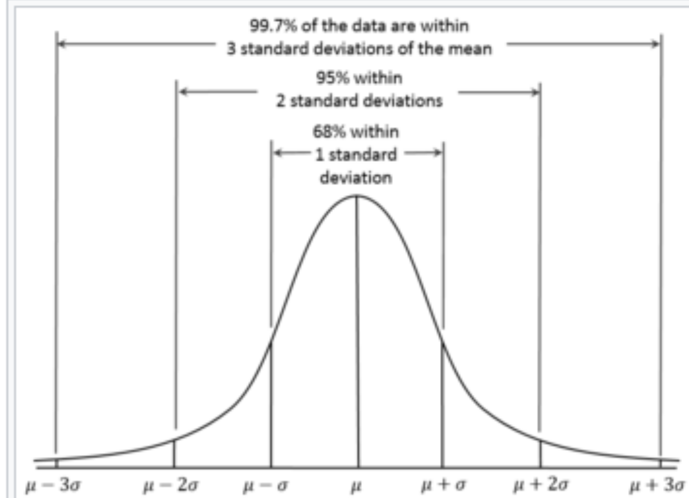


Gaussian Distribution

Normal Distribution



The red curve is the *standard normal distribution*



For the normal distribution, the values less than one standard deviation away from the mean account for 68.27% of the set; while two standard deviations from the mean account for 95.45%; and three standard deviations account for 99.73%.

Notation	$\mathcal{N}(\mu, \sigma^2)$
Parameters	$\mu \in \mathbb{R}$ = mean (location) $\sigma^2 > 0$ = variance (squared scale)
Support	$x \in \mathbb{R}$
PDF	$\frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{(x-\mu)^2}{2\sigma^2}}$

LDA

Assume $f_k(x)$ is Gaussian!
Unidimensional case (d=1)

$$f_k(x) = \frac{1}{\sqrt{2\pi}\sigma_k} \exp\left(-\frac{1}{2\sigma_k^2}(x-\mu_k)^2\right)$$

LDA

$$\Pr(Y = k|X = x) = \frac{\pi_k f_k(x)}{\sum_{l=1}^{K} \pi_l f_l(x)}.$$

Assume $f_k(x)$ is Gaussian!
Unidimensional case (d=1)

$$f_k(x) = \frac{1}{\sqrt{2\pi}\sigma_k} \exp\left(-\frac{1}{2\sigma_k^2}(x - \mu_k)^2\right)$$

$$p_k(x) = \frac{\pi_k \frac{1}{\sqrt{2\pi}\sigma} \exp\left(-\frac{1}{2\sigma^2}(x - \mu_k)^2\right)}{\sum_{l=1}^{K} \pi_l \frac{1}{\sqrt{2\pi}\sigma} \exp\left(-\frac{1}{2\sigma^2}(x - \mu_l)^2\right)}.$$

Assumption: $\sigma_1 = \ldots \sigma_k = \sigma$

LDA Training and Testing

Given training data $(x_i, y_i), i = 1, \dots, n, y_i \in \{1, \dots, K\}$

1. Estimate sample mean and variance

$$\boxed{\begin{aligned} \hat{\mu}_k &= \frac{1}{n_k} \sum_{i:y_i=k} x_i \\ \hat{\sigma}^2 &= \frac{1}{n-K} \sum_{k=1}^{K} \sum_{i:y_i=k} (x_i - \hat{\mu}_k)^2 \end{aligned}}$$

2. Estimate prior

$$\boxed{\hat{\pi}_k = n_k / n.}$$

Given testing point x, predict k that maximizes:

$$\boxed{p_k(x) = \frac{\pi_k \frac{1}{\sqrt{2\pi}\sigma} \exp\left(-\frac{1}{2\sigma^2}(x - \mu_k)^2\right)}{\sum_{l=1}^{K} \pi_l \frac{1}{\sqrt{2\pi}\sigma} \exp\left(-\frac{1}{2\sigma^2}(x - \mu_l)^2\right)}.}$$

LDA decision boundary

LDA decision boundary

Pick class k to maximize

$$\delta_k(x) = x \cdot \frac{\mu_k}{\sigma^2} - \frac{\mu_k^2}{2\sigma^2} + \log(\pi_k)$$

Example: $k = 2, \pi_1 = \pi_2$

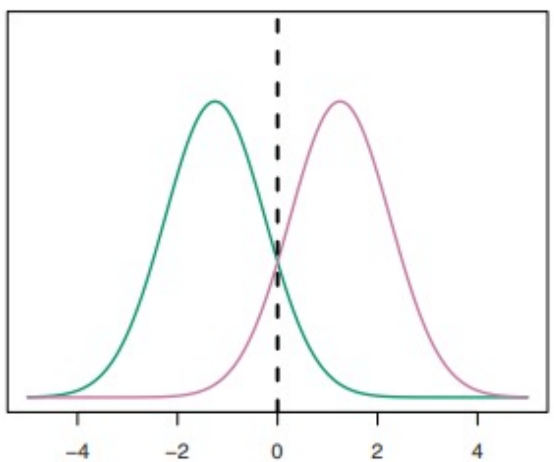
LDA decision boundary

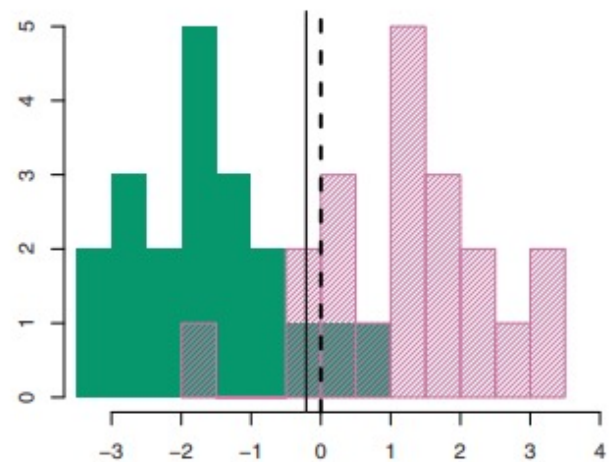
Pick class k to maximize

$$\delta_k(x) = x \cdot \frac{\mu_k}{\sigma^2} - \frac{\mu_k^2}{2\sigma^2} + \log(\pi_k)$$

Example: $k = 2, \pi_1 = \pi_2$

Classify as class 1 if $x > \frac{\mu_1 + \mu_2}{2}$





True decision boundary   Estimated decision boundary

LDA Training and Testing

Given training data $(x_i, y_i), i = 1, \dots, n, y_i \in \{1, \dots, K\}$

1. Estimate mean and variance

$$\hat{\mu}_k = \frac{1}{n_k} \sum_{i: y_i = k} x_i$$

$$\hat{\sigma}^2 = \frac{1}{n-K} \sum_{k=1}^{K} \sum_{i: y_i = k} (x_i - \hat{\mu}_k)^2$$

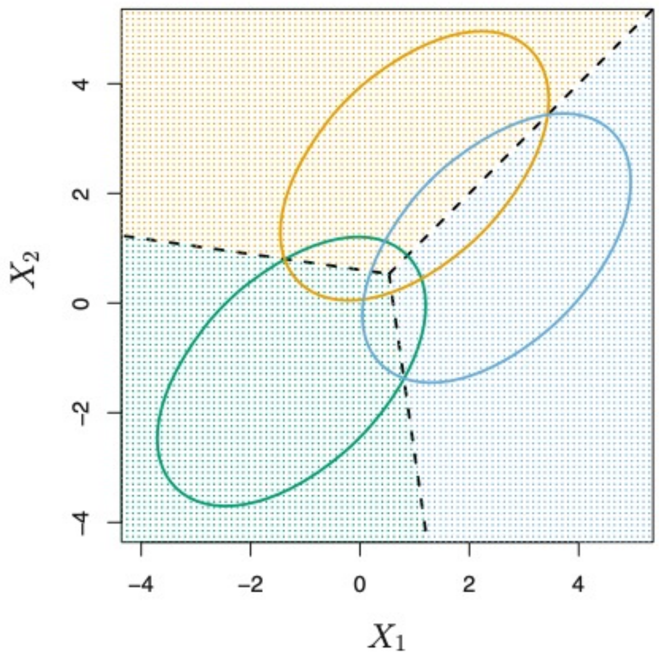
2. Estimate prior

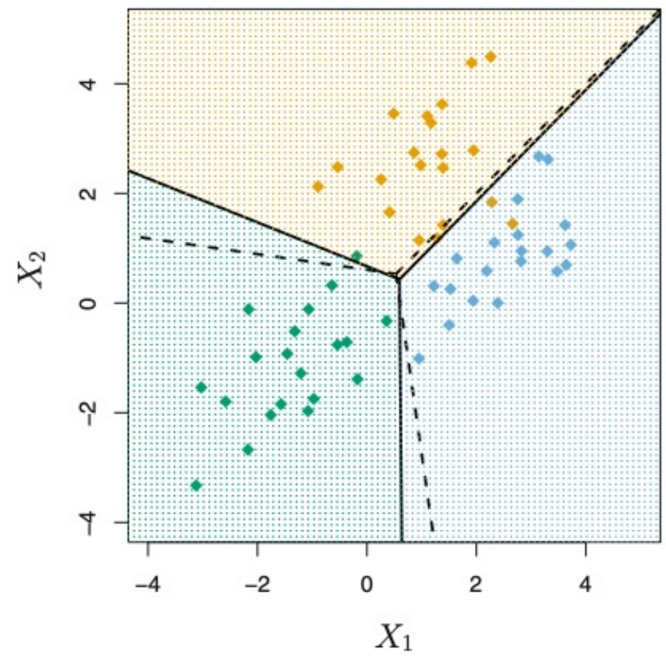
$$\hat{\pi}_k = n_k / n.$$

Given testing point x, predict k that maximizes:

$$\hat{\delta}_k(x) = x \cdot \frac{\hat{\mu}_k}{\hat{\sigma}^2} - \frac{\hat{\mu}_k^2}{2\hat{\sigma}^2} + \log(\hat{\pi}_k)$$

Multi-Dimensional LDA



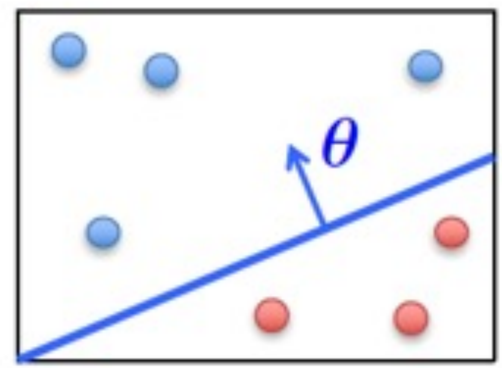


- LDA can be extended to multi-dimensional data
- Assumption that $f_k(x)$ is a multi-variate Gaussian

Linear models

- Logistic regression

$$h_{\boldsymbol{\theta}}(\boldsymbol{x}) = \frac{1}{1 + e^{-\boldsymbol{\theta}^\top \boldsymbol{x}}}$$



- LDA

$$Max_k \;\; \delta_k(x) = x \cdot \frac{\mu_k}{\sigma^2} - \frac{\mu_k^2}{2\sigma^2} + \log(\pi_k)$$

LDA vs Logistic Regression

LDA vs Logistic Regression

- Logistic regression computes directly $\Pr[Y = 1|X = x]$ by assuming sigmoid function
  - Uses Maximum Likelihood Estimation
  - Discriminative Model
- LDA uses Bayes Theorem to estimate it
  - Estimates mean, co-variance, and prior from training data
  - Generative model
  - Assumes Gaussian distribution for $f_k(x) = \Pr[X = x|Y = k]$
- Which one is better?
  - LDA can be sensitive to outliers
  - LDA works well for Gaussian distribution
  - Logistic regression is more complex to solve, but more expressive