INTRODUCTION

To Statistical Learning

Introduction to Statistical Learning

Generative Models - Class 12

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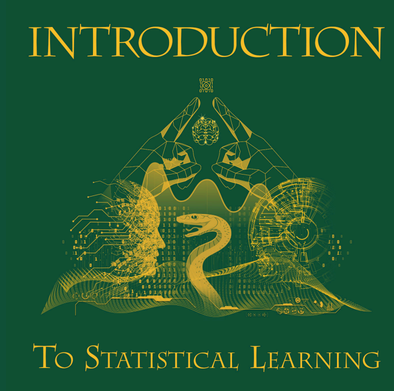
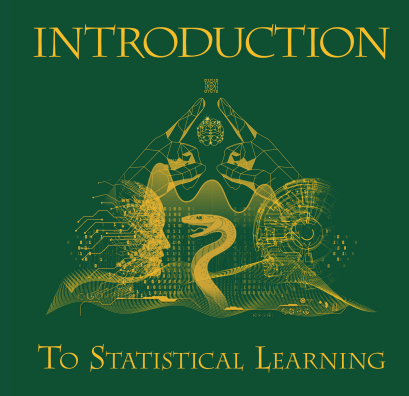


Intro. to Generative Models



Generated images

Face recognition using eigenfaces by Turk & Pentland (1991)

Image generated using DALL·E by OpenAI with: “a realistic image of a dog and a cat hugging in front of the eiffel tower”

How did we get here?

Discriminative models

- We are constanly trying to *model* $E(Y|X=x)$ (regression) or $P(Y|X=x)$ (Bayes classifier):

- Linear:
  - linear regression, ridge, lasso
  - logistic regression
- Non-linear:
  - KNN
  - Trees, RF, Boosting

> ⓘ Even our Bias-variance tradeoff analysis assumed a Fixed-X scenario!

Generative models

But for classification:

$$P(Y|X) = \frac{P(X,Y)}{P(X)}$$

- Generative models focus on modeling the joint distribution $P(X, Y)$, or more specifically:

$$P(Y|X) = \frac{P(X,Y)}{P(X)} = \frac{P(Y)P(X|Y)}{P(X)} \propto P(Y)P(X|Y)$$

- Focus on the mechanism which **generated** the data, not just the data
- Especially useful when n is small

Classification using generative models

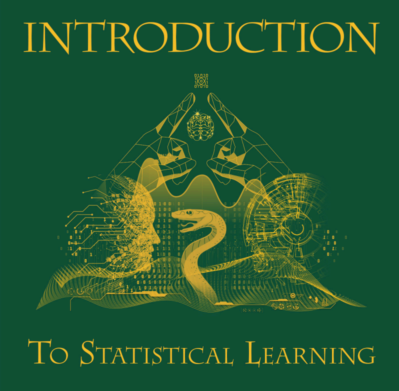
- Even more specifically, if $Y \in \{1, \ldots, K\}$:

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

- We focus on estimating π_k, $f_k(x)$

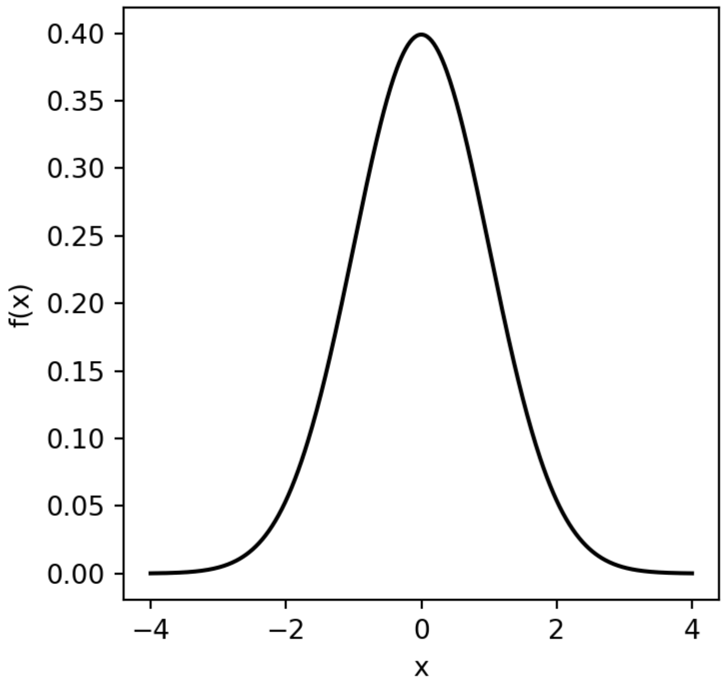
> And if we are so good at estimaing $f_k(x) = P(X = x|Y = k)$ why not generate more!

Detour: multivariate normal



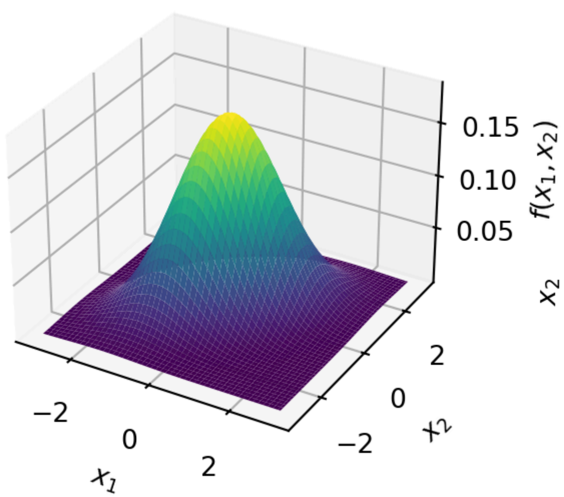
Univariate normal

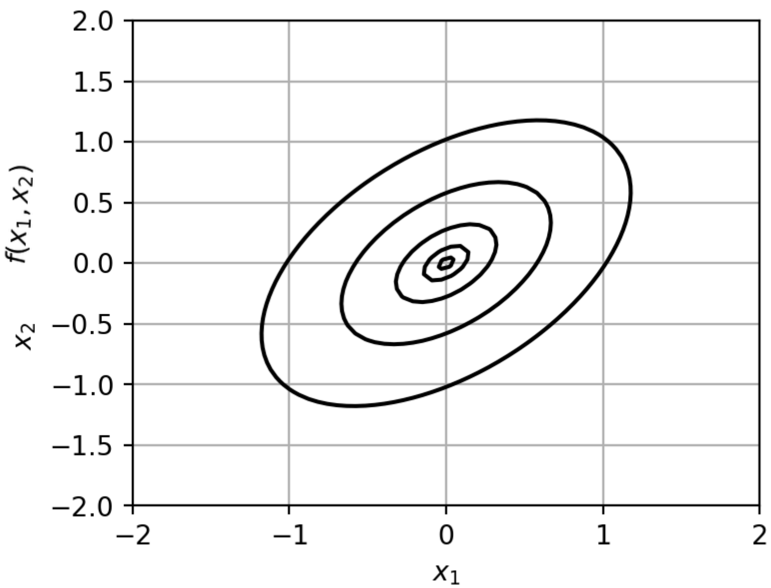
- $X \in \mathbb{R} \sim \mathcal{N}(\mu, \sigma^2) \Rightarrow E(X) = \mu; \quad V(X) = \sigma^2 > 0$
- $f(x) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{1}{2\sigma^2}(x-\mu)^2\right)$
- $F(x) = P(X \leq x) = \int_{-\infty}^{x} f(x)dx = \Phi\left(\frac{x-\mu}{\sigma}\right)$



Bivariate normal

- $X \in \mathbb{R}^2 \sim \mathcal{BVN}(\mu, \mathbf{\Sigma}) \Rightarrow E(X) = \mu = \begin{pmatrix} \mu_1 \\ \mu_2 \end{pmatrix}; \quad V(X) = \mathbf{\Sigma} = \begin{pmatrix} \sigma_1^2 & \rho\sigma_1\sigma_2 \\ \rho\sigma_1\sigma_2 & \sigma_2^2 \end{pmatrix}$
- $\Leftrightarrow X_1 \sim \mathcal{N}(\mu_1, \sigma_1^2), X_2 \sim \mathcal{N}(\mu_2, \sigma_2^2); \quad \rho = \mathrm{Cor}(X_1, X_2) = \frac{\mathrm{Cov}(X_1, X_2)}{\sigma_1\sigma_2}$
- $f(\mathbf{x}) = \frac{1}{2\pi\sigma_1\sigma_2\sqrt{1-\rho^2}} \exp\left(-\frac{1}{2(1-\rho^2)}\left[\frac{(x_1-\mu_1)^2}{\sigma_1^2} + \frac{(x_2-\mu_2)^2}{\sigma_2^2} - \frac{2\rho(x_1-\mu_1)(x_2-\mu_2)}{\sigma_1\sigma_2}\right]\right)$
- $F(\mathbf{x}) = P(X_1 \le x_1, X_2 \le x_2) = \int_{-\infty}^{x_2}\int_{-\infty}^{x_1} f(x_1, x_2)dx_1dx_2$





Multivariate normal

- $X \in \mathbb{R}^p \sim \mathcal{MVN}(\mu, \mathbf{\Sigma})$
- $E(X) = \mu = \begin{pmatrix} \mu_1 \\ \vdots \\ \mu_p \end{pmatrix}; \quad V(X) = \mathbf{\Sigma} = \begin{pmatrix} \sigma_1^2 & \cdots & \rho_{1,p}\sigma_1\sigma_p \\ \vdots & \ddots & \vdots \\ \rho_{1,p}\sigma_1\sigma_p & \cdots & \sigma_p^2 \end{pmatrix}$
- $\Leftrightarrow X_1 \sim \mathcal{N}(\mu_1, \sigma_1^2), \ldots, X_p \sim \mathcal{N}(\mu_p, \sigma_p^2); \quad \rho_{j,k} = \mathrm{Cor}(X_j, X_k) = \frac{\mathrm{Cov}(X_j, X_k)}{\sigma_j \sigma_k}$
- $f(\mathbf{x}) = f(x_1, \ldots, x_p) = \frac{1}{(2\pi)^{p/2}|\Sigma|^{1/2}} \exp\left(-\frac{1}{2}(\mathbf{x} - \mu)^T \mathbf{\Sigma}^{-1}(\mathbf{x} - \mu)\right)$

> ⓘ How many unique params in $\mathbf{\Sigma}$?

Linear Discriminant Analysis

INTRODUCTION

To Statistical Learning

Linear discriminant analysis (LDA)

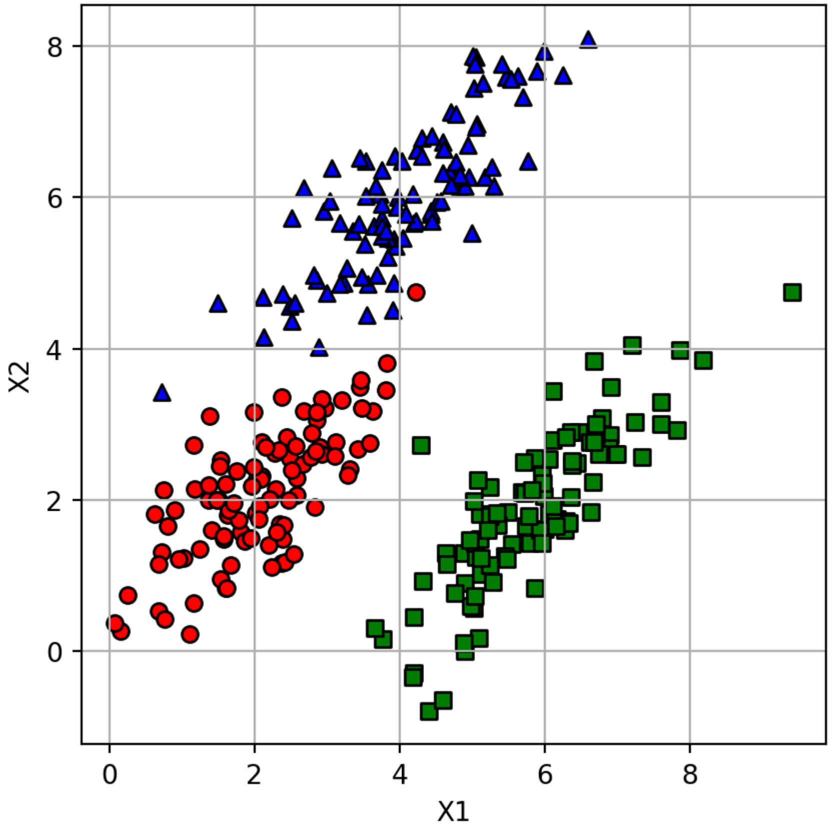
- Recall:

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

- $\hat{f}(x_0) = \arg\max_k \pi_k f_k(x_0)$

- In LDA:
  - π_k are priors, or (spoiler): $\hat{\pi}_k = \frac{\sum_{i=1}^{n} \mathbb{I}[Y_i = k]}{n}$
  - $f_k(x)$ are multivariate Gaussian, or: $X|Y=k \sim \mathcal{N}(\mu_k, \Sigma)$
  - Notice the covariance matrix Σ is the same $\forall k$

LDA: What to expect



What do you expect the decision rule(s) to look like?

LDA: $k - j$ classes decision rule

- Why choose class k over j?

$$P(Y = k|X = x) > P(Y = j|X = x)$$
$$\Leftrightarrow \pi_k f_k(x) > \pi_j f_j(x)$$
$$\Leftrightarrow \log\left[\pi_k f_k(x)\right] > \log\left[\pi_j f_j(x)\right]$$

- Assume $\pi_k, \pi_j, \mu_k, \mu_j, \Sigma$ known
- $X|Y = k \sim \mathcal{N}(\mu_k, \Sigma) \Rightarrow f_k(x) = \frac{1}{(2\pi)^{p/2}|\Sigma|^{1/2}} \exp\left(-\frac{1}{2}(x - \mu_k)^T \Sigma^{-1}(x - \mu_k)\right)$
- $\log\left[\pi_k f_k(x)\right] = \log(\pi_k) + \log(f_k(x)) = \log(\pi_k) + C - \frac{1}{2}(x - \mu_k)^T \Sigma^{-1}(x - \mu_k)$

LDA: $k - j$ classes decision rule

So, select class k over class j if $\log\left[\pi_k f_k(x)\right] > \log\left[\pi_j f_j(x)\right]$ means:

$$\log(\pi_k) - \frac{1}{2}(x-\mu_k)^T\Sigma^{-1}(x-\mu_k) > \log(\pi_j) - \frac{1}{2}(x-\mu_j)^T\Sigma^{-1}(x-\mu_j)$$

$$\delta_{k>j}(x) : x^T\Sigma^{-1}(\mu_k-\mu_j) + \left[-\frac{1}{2}\mu_k^T\Sigma^{-1}\mu_k + \frac{1}{2}\mu_j^T\Sigma^{-1}\mu_j + \log(\pi_k) - \log(\pi_j)\right] > 0$$

What shape is $\delta_{k>j}(x)$?

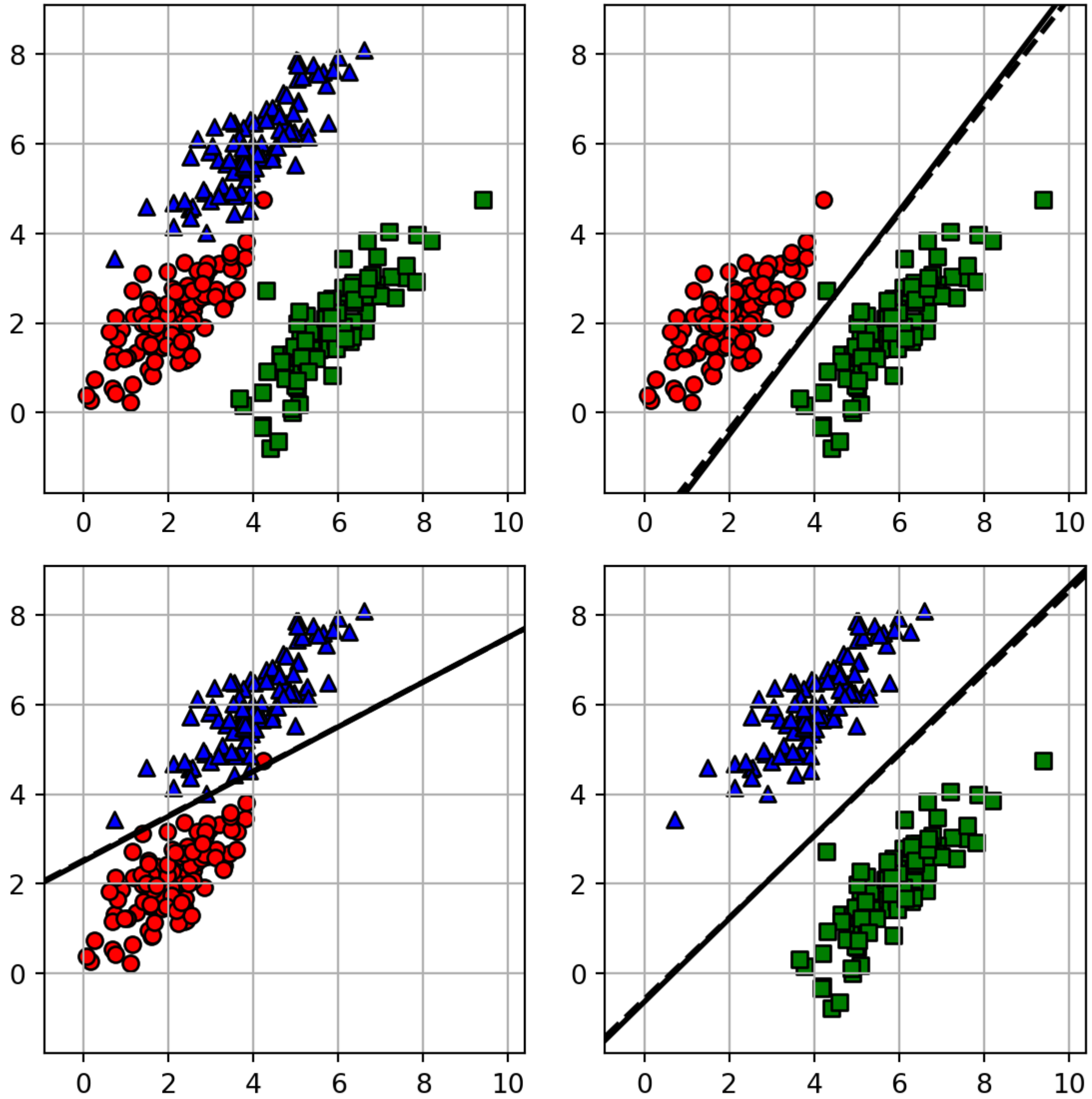
LDA: Estimation

- If we want to fit LDA to data, we need to estimate the parameters: $\mu_1, \ldots, \mu_K,\ \Sigma,\ \pi_1, \ldots, \pi_K$.
- This is naturally done from the data (e.g. by maximum likelihood):

$$\hat{\pi}_k = \frac{\sum_{i=1}^{n} \mathbb{I}\left[Y_i = k\right]}{n}, \ \hat{\mu}_k = \frac{\sum_{\mathbb{I}[Y_i=k]} x_i}{\sum_{i=1}^{n} \mathbb{I}\left[Y_i = k\right]}$$

$$\hat{\Sigma} = \frac{1}{n-K} \sum_{k=1}^{K} \sum_{\mathbb{I}[Y_i=k]} (x_i - \hat{\mu}_k)(x_i - \hat{\mu}_k)^T$$

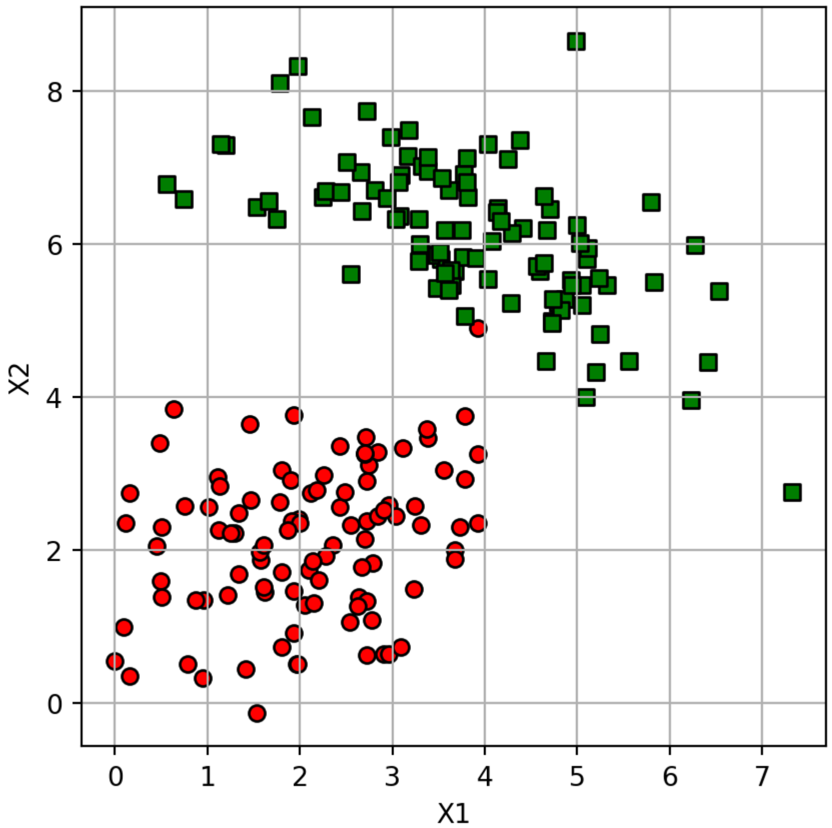
LDA: Example



Quadratic Discriminant Analysis

INTRODUCTION TO STATISTICAL LEARNING

A common covariance?



Quadratic linear analysis (QDA)

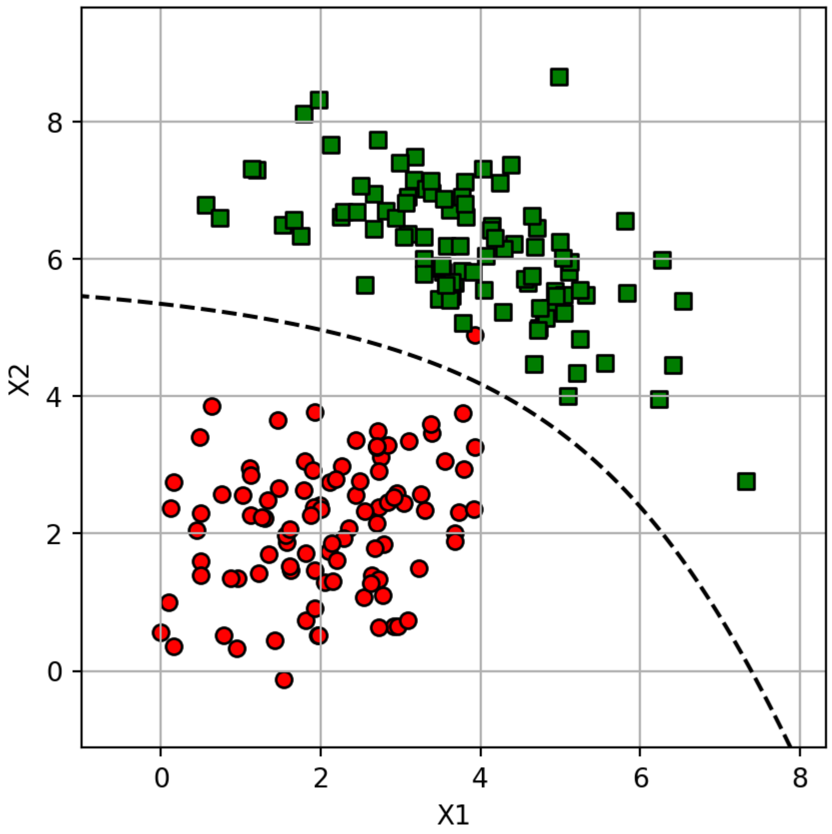
- Now assume: $X|Y=k \sim \mathcal{N}(\mu_k, \Sigma_k)$
- Decision rule stays the same:
  - select class k over class j if $\log\left[\pi_k f_k(x)\right] > \log\left[\pi_j f_j(x)\right]$
- $\log\left[\pi_k f_k(x)\right] = \log(\pi_k) + C - \frac{1}{2}(x-\mu_k)^T \Sigma_k^{-1}(x-\mu_k) - \frac{1}{2}\log(|\Sigma_k|)$

$$
\begin{aligned}
\delta_{k>j}(x) :& \\
& -\frac{1}{2} x^T \left(\Sigma_k^{-1} - \Sigma_j^{-1}\right) x + x^T \left(\Sigma_k^{-1}\mu_k - \Sigma_j^{-1}\mu_j\right) \\
& + \left[-\frac{1}{2}\mu_k^T \Sigma^{-1}\mu_k + \frac{1}{2}\mu_j^T \Sigma^{-1}\mu_j + \log(\pi_k) - \log(\pi_j) \right. \\
& \qquad \left. + \frac{1}{2}(\log(|\Sigma_j| - \log(|\Sigma_k|))\right] > 0
\end{aligned}
$$

> What shape is $\delta_{k>j}(x)$?

QDA: Estimation

- Estimate μ_k, π_k as in LDA and:
  - $\hat{\Sigma}_k = \frac{1}{n_k - 1} \sum_{\mathbb{I}[Y_i=k]} (X_i - \hat{\mu}_k)(X_i - \hat{\mu}_k)^T$



How many params are estimated in QDA? LDA?

Naive Bayes

INTRODUCTION

To Statistical Learning

Naive Bayes

- Recall: $P(Y=k|X=x)=\frac{P(Y=k)P(X=x|Y=k)}{P(X=x)}=\frac{\pi_k f_k(x)}{\sum_{l=1}^{K}\pi_l f_l(x)}$

- In Naive Bayes:
  - π_k are priors, or: $\hat{\pi}_k=\frac{\sum_{i=1}^{n}\mathbb{I}[Y_i=k]}{n}$
  - Within the k-th class, the p predictors are **independent**
  - $f_k(x)=f_{k1}(x_1)\times f_{k2}(x_2)\times\cdots\times f_{kp}(x_p)$
    - $f_{kj}(x_j)$ for a continuous feature: $\mathcal{N}(\mu_{jk},\sigma_{jk}^2)$, $Exp(\lambda_{jk})$, KDE, …
    - $f_{kj}(x_j)$ for a discrete feature: $\hat{f}_{kj}(x_j)=\begin{cases}0.2 & \text{if } x_j=1\\ 0.8 & \text{if } x_j=2\end{cases}$

> ⓘ We don't really believe this independence… when is this naive assumption particularly useful?

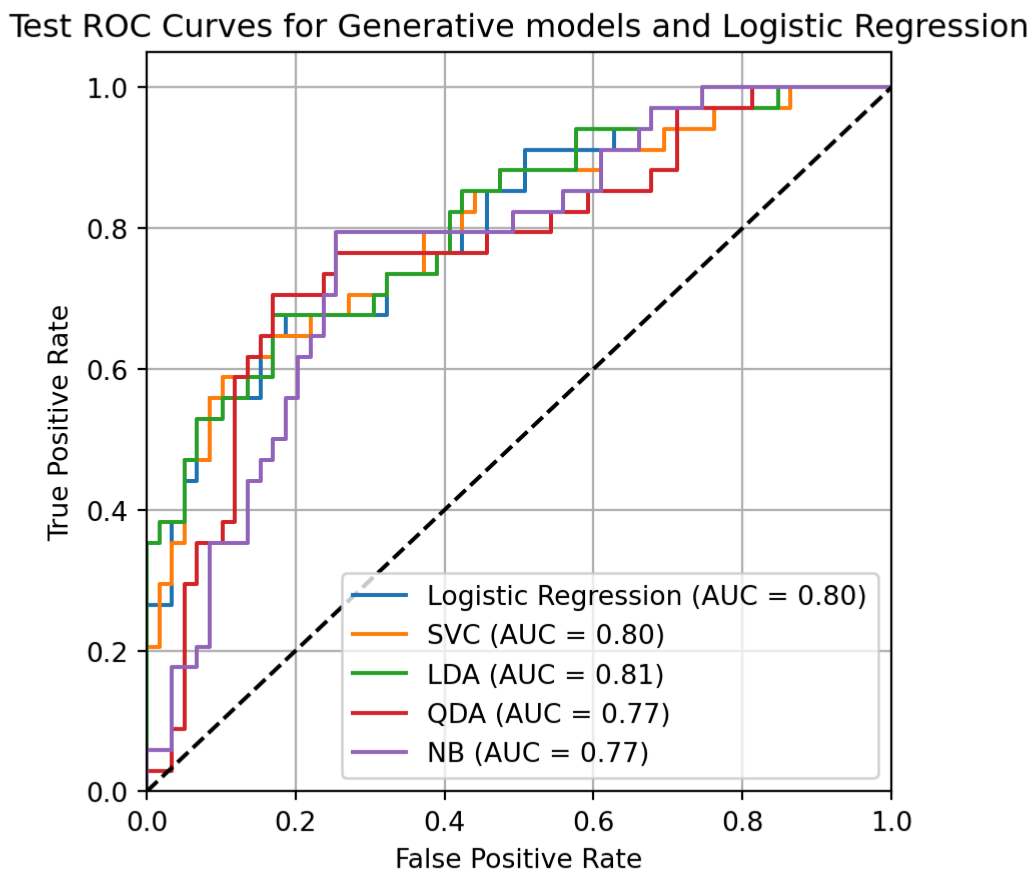
> ⓘ How is Naive Bayes = LDA/QDA?

Comparing classifiers

INTRODUCTION

To Statistical Learning

Example: SAHeart data



LDA vs. logistic regression

- For $K = 2$ (though we can show this for any K), logistic regression:

$$\begin{aligned}\text{logit}(P(Y=1|X)) &= \log\left(\frac{P(Y=1|X)}{1-P(Y=1|X)}\right) \\ &= \log\left(\frac{P(Y=1|X)}{P(Y=0|X)}\right) = \beta_0 + x^T\beta\end{aligned}$$

- For $K = 2$ (though we can show this for any K), LDA:

$$\begin{aligned}\log\left(\frac{P(Y=1|X)}{P(Y=0|X)}\right) &= \log\left(\frac{\pi_1 f_1(x)}{\pi_0 f_0(x)}\right) = \log(\pi_1 f_1(x)) - \log(\pi_0 f_0(x)) \\ &= x^T\Sigma^{-1}(\mu_1 - \mu_0) \\ &+ \left[-\frac{1}{2}\mu_1^T\Sigma^{-1}\mu_1 + \frac{1}{2}\mu_0^T\Sigma^{-1}\mu_0 + \log(\pi_1) - \log(\pi_0)\right] \\ &= \alpha_0 + x^T\alpha\end{aligned}$$

Similarly for all methods

$$\delta_{1>0}(x) = \log\left(\frac{P(Y=1|X=x)}{P(Y=0|X=x)}\right) =$$

method	type	$\delta_{1>0}(x)$
LR	discriminative, linear	$\beta_0 + x^T\beta$
LDA	generative, linear	$\alpha_0 + x^T\alpha$
QDA	generative, non-linear	$\gamma_0 + x^T\gamma + x^T\Gamma x$
NB	generative, non-linear	$\tau_0 + \sum_{j=1}^{p} \tau_j(x_j)$