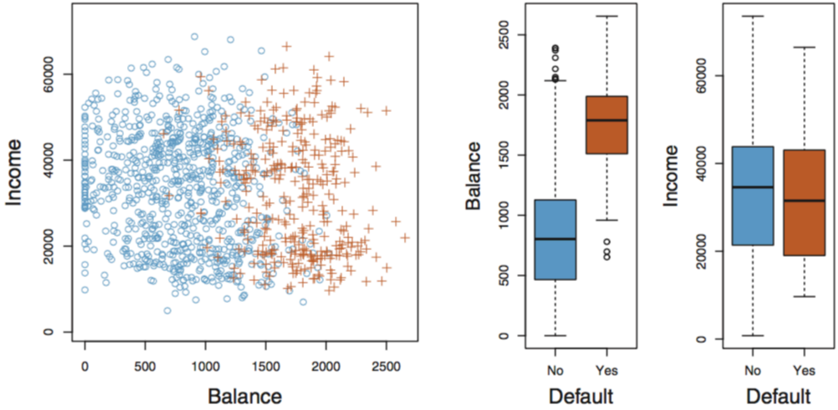
Lecture 8: Classification (Textbook 4.4)

Default Data



It shows the annual incomes and monthly credit card balances of a number of individuals. The individuals who defaulted on their credit card payments are shown in orange, and those who did not are shown in blue.

Linear Discriminant Analysis

- Logistic regression involves directly modeling $P(Y = k|X = x)$.
- Here, **linear discriminant analysis** is to model the distribution of X in each of the classes separately, and then use Bayes' theorem to flip things around and obtain $P(Y = k|X = x)$. The Bayes' theorem is

$$P(Y = k|X = x) = P(X = x|Y = k)P(Y = k)/P(X = x).$$

- We usually assume the distribution of X in each of the classes to be normal distributions.

Why not Logistic Regression

- When the classes are well-separated, the parameter estimates for the logistic regression model are surprisingly unstable. Linear discriminant analysis does not suffer from this problem.
- If n is small and the distribution of the predictors X is approximately normal in each of the classes, the linear discriminant model is again more stable than the logistic regression model.
- Linear discriminant analysis is more convenient when we have more than two response classes. (Multinomial logistic regression and proportional odds model)

Linear Discriminant Analysis

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Using Bayes' Theorem for Classification

- Recall that the Bayes' theorem is

$$P(Y = k|X = x) = P(X = x|Y = k)P(Y = k)/P(X = x).$$

- We can slightly rewrite it as

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

  π_k is the **prior** probability that a randomly chosen observation comes from the kth class, i.e. $P(Y = k)$.

  $f_k(X) = P(X = x|Y = k)$ denotes the **density function** of X for an observation that comes from the kth class.

  $p_k(x) = P(Y = k|X = x)$ is called **posterior** probability. It is the probability that the observation belongs to the kth class, given the predictor value for that observation.

- In the ideal case, we classify a new point according to which posterior probability is highest.

Linear Discriminant Analysis for $p = 1$

- We assume that $f_k(x)$ is normal, which takes the form

$$f_k(x) = \frac{1}{\sqrt{2\pi}\sigma_k} e^{-\frac{1}{2\sigma_k^2}(x-\mu_k)^2},$$

  where μ_k and σ_k^2 are the mean and variance parameters for the kth class. We assume all $\sigma_k = \sigma$ are the same.

- Plugging this into Bayes' formula, we get $p_k(x) = P(Y = k|X = x)$ as

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

Linear Discriminant Analysis for $p = 1$

- To classify at the value $X = x$, we need to see which k has the largest $p_k(x)$.

- Taking logs, and discarding terms that do not depend on k, the Bayes classifier is to assign x to the class with the largest

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

  Note that $\delta_k(x)$ is a linear function of x. That is why it is called linear discriminant analysis (LDA).

- If $K = 2$ and $\pi_1 = \pi_2$, then the Bayes decision boundary corresponds to

$$x = \frac{\mu_1 + \mu_2}{2}.$$

Discriminant functions

- Given training data, we estimate μ_k, and σ by

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

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

  where n_k is the number of training observations in the kth class. We also estimate π_k by

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

- Plugging the estimates into $\delta_k(x)$, we get

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

  which is called **discriminant function**.

- LDA just assigns x to the class with the largest $\hat{\delta}_k(x)$.

Linear Discriminant Analysis for $p > 1$

- We now extend the LDA classifier to the case of multiple predictors $X = (X_1, ..., X_p)$.
- Recall that the posterior probability has the form

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

- Now, we assume $X|Y = k$ follows a multivariate normal distribution $N(\mu_k, \Sigma)$,

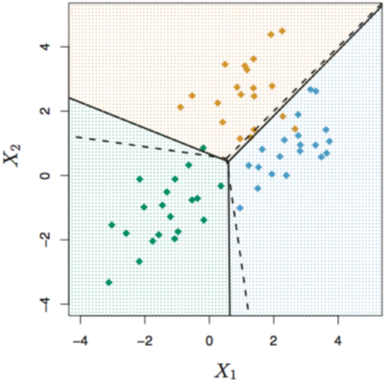
$$f_k(x) = \frac{1}{(2\pi)^{p/2}|\Sigma|^{1/2}} e^{-\frac{1}{2}(x-\mu_k)^T\Sigma^{-1}(x-\mu_k)}.$$

- Similarly, we assign x to the class with the largest

$$\delta_k(x) = x^T\Sigma^{-1}\mu_k - \frac{1}{2}\mu_k^T\Sigma^{-1}\mu_k + \log \pi_k.$$

- The Bayes decision boundaries are the set of x for which $\delta_k(x) = \delta_l(x)$ for $k \neq l$. Again, the boundaries are collection of straight lines, since $\delta_k(x)$ is linear in x.

Example



There are three classes (orange, green and blue) with two predictors X_1 and X_2. Dashed lines are the Bayes decision boundaries. Solid lines are their estimates based on the LDA.

LDA on the Default Data

Our goal is predict whether or not an individual will default on the basis of credit card balance.

		True default status		
		No	Yes	Total
Predicted	No	9,644	252	9,896
default status	Yes	23	81	104
	Total	9,667	333	10,000

The training error rate is $(23 + 252)/10000 = 2.75\%$. For a credit card

company that is trying to identify high-risk individuals, an error rate of $252/333 = 75.7\%$ among individuals who default is unacceptable.

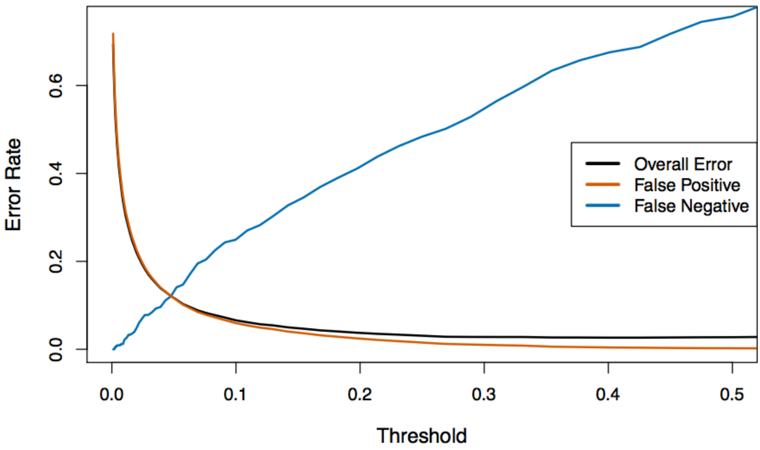
Types of Errors

- **False positive rate (FPR)**: The fraction of negative examples that are classified as positive – $23/9667 = 0.2\%$ in default data.
- **False negative rate (FNR)**: The fraction of positive examples that are classified as negative – 75.7% in default data.
- The false negative rate is too high.
- We can achieve better balance of FPR and FNR by varying the threshold

  $$\mathrm{P(default{=}yes} \mid \mathrm{X{=}x}) > \mathrm{threshold},$$

  for some threshold different from 0.5.

Trade-off between FPR and FNR



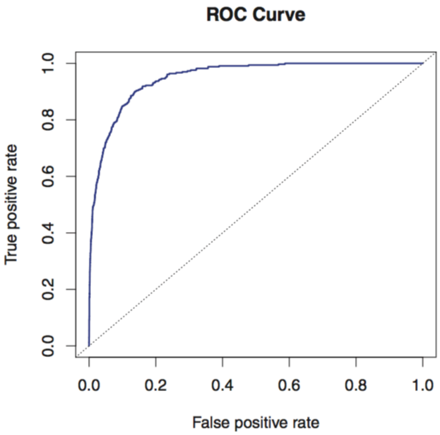
More Terminology

		Predicted class		
		− or Null	+ or Non-null	Total
True	− or Null	True Neg. (TN)	False Pos. (FP)	N
class	+ or Non-null	False Neg. (FN)	True Pos. (TP)	P
	Total	N*	P*	

Name	Definition	Synonyms
False Pos. rate	FP/N	Type I error, 1−Specificity
True Pos. rate	TP/P	1−Type II error, power, sensitivity, recall
Pos. Pred. value	TP/P*	Precision, 1−false discovery proportion
Neg. Pred. value	TN/N*	

This defines **sensitivity** and **specificity**.

ROC Curve



The ROC plot displays both FPR and TPR. We use **AUC** or area under the curve to summarize the overall performance. Higher AUC is good.

Other forms of Discriminant Analysis

Recall that

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

When $f_k(x)$ are Gaussian densities, with the same covariance matrix Σ in each class, this leads to linear discriminant analysis. By altering the forms for $f_k(x)$, we get different classifiers.

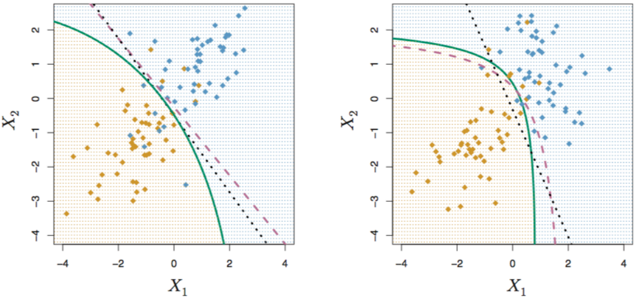
- With Gaussians but different Σ_k in each class, we get **quadratic discriminant analysis** (QDA).
- With $f_k(x) = \prod_{j=1}^{p} f_{jk}(x_j)$ (conditional independence model) in each class we get **naive Bayes**. For Gaussian density, this means the Σ_k are diagonal.
- Many other forms, by proposing specific density models for $f_k(x)$, including nonparametric approaches.

Quadratic Discriminant Analysis

In QDA, the Bayes classifier assigns an observation $X = x$ to the class for which

$$\delta_k(x) = -\frac{1}{2}x^T\Sigma_k^{-1}x + x^T\Sigma_k^{-1}\mu_k - \frac{1}{2}\mu_k^T\Sigma_k^{-1}\mu_k + \log\pi_k - \frac{1}{2}\log|\Sigma_k|.$$

is largest. So, the decision boundary is nonlinear (quadratic).



The Bayes (purple dashed), LDA (black dotted), and QDA (green solid) decision boundaries under two scenarios.

Naive Bayes

Assumes features are independent in each class.

Useful when p is large, and so multivariate methods like QDA and even LDA break down.

- Under Gaussian distributions, naive Bayes assumes each Σ_k is diagonal. The decision boundary is determined by

$$\delta_k(x) = -\frac{1}{2}\sum_{j=1}^{p}\frac{(x_j-\mu_{kj})^2}{\sigma_{kj}^2} + \log \pi_k.$$

- It is easy to extend it to mixed features (quantitative and categorical).

- Despite strong assumptions, naive Bayes often produces good classification results.

Logistic Regression versus LDA

For a two-class problem, one can show that for LDA

$$\log\left(\frac{p_1(x)}{1-p_1(x)}\right) = \log\left(\frac{p_1(x)}{p_2(x)}\right) = c_0 + c1x_1 + ... + c_p x_p,$$

which has the same form as logistic regression.

The difference is in how the parameters are estimated.

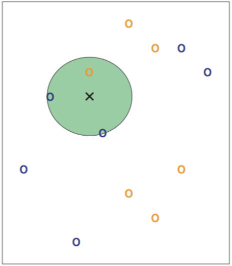
- Logistic regression uses the conditional likelihood based on $P(Y|X)$ (known as discriminative learning).
- LDA uses the full likelihood based on $P(X, Y)$ (known as generative learning).
- Despite these differences, in practice the results are often very similar.

K-Nearest Neighbors (KNN)

K-nearest neighbors (KNN) classifier directly estimates $P(Y = j|X = x_0)$ by

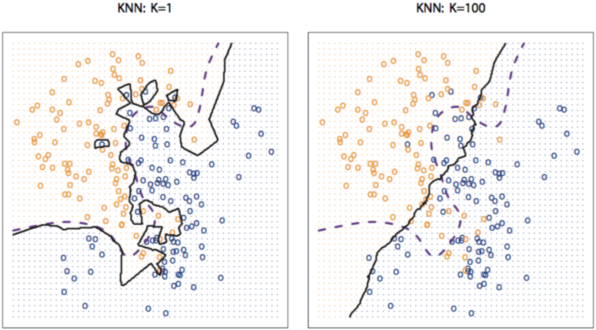
$$\frac{1}{K} \sum_{i \in N_0} I(y_i = j),$$

where N_0 is the set of K points in the training data that are closest to x_0. KNN estimate $P(Y = j|X = x_0)$ as the fraction of points with label j in N_0.



(KNN with $K = 3$).

Effect of K



With $K = 1$, the decision boundary is overly flexible, while with $K = 100$ it is not sufficiently flexible. Again, this represents the bias variance trade-off. The Bayes decision boundary is shown as a purple dashed line.