Lecture 9: Classification, LDA

Reading: Chapter 4

STATS 202: Data mining and analysis

October 11, 2019

Review: Main strategy in Chapter 4

Find an estimate $\hat{P}(Y \mid X)$. Then, given an input x_0, we predict the response as in a Bayes classifier:

$$\hat{y}_0 = \text{argmax}_{\,y} \; \hat{P}(Y = y \mid X = x_0).$$

Linear Discriminant Analysis (LDA)

Instead of estimating $P(Y \mid X)$ directly, we will estimate:

1. $\hat{P}(X \mid Y)$: Given the response, what is the distribution of the inputs?
2. $\hat{P}(Y)$: How probable is each category?

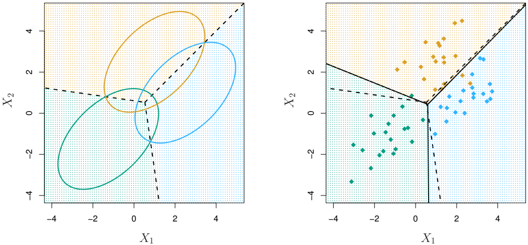
Then, we use *Bayes rule* to obtain the estimate:

$$\begin{aligned}\hat{P}(Y = k \mid X = x) &= \frac{\hat{P}(X = x \mid Y = k)\hat{P}(Y = k)}{\hat{P}(X = x)} \\ &= \frac{\hat{P}(X = x \mid Y = k)\hat{P}(Y = k)}{\sum_j \hat{P}(X = x \mid Y = j)\hat{P}(Y = j)}\end{aligned}$$

Linear Discriminant Analysis (LDA)

Instead of estimating $P(Y \mid X)$, we compute estimates:

1. $\hat{P}(X = x \mid Y = k) = \hat{f}_k(x)$, where each $\hat{f}_k(x)$ is a *Multivariate Normal Distribution* density:



2. $\hat{P}(Y = k) = \hat{\pi}_k$ is estimated by the fraction of training samples of class k.

LDA has linear decision boundaries

Suppose that:

- We know $P(Y = k) = \pi_k$ exactly.
- $P(X = x | Y = k)$ is Mutivariate Normal with density:

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

μ_k : Mean of the inputs for category k.
$\mathbf{\Sigma}$: Covariance matrix (common to all categories).

Then, what is the Bayes classifier?

LDA has linear decision boundaries

By Bayes rule, the probability of category k, given the input x is:

$$P(Y = k \mid X = x) = \frac{\text{likelihood} \cdot \text{prior}}{\text{marginal}} = \frac{f_k(x)\pi_k}{P(X = x)}$$

The denominator does not depend on the response k, so we can write it as a constant:

$$P(Y = k \mid X = x) = C \times f_k(x)\pi_k$$

Plugging in the formula for $f_k(x)$:

$$P(Y = k \mid X = x) = \frac{C\pi_k}{(2\pi)^{p/2}|\mathbf{\Sigma}|^{1/2}} e^{-\frac{1}{2}(x-\mu_k)^T \mathbf{\Sigma}^{-1}(x-\mu_k)}$$

LDA has linear decision boundaries

$$P(Y = k \mid X = x) = \frac{C\pi_k}{(2\pi)^{p/2}|\mathbf{\Sigma}|^{1/2}} e^{-\frac{1}{2}(x-\mu_k)^T \mathbf{\Sigma}^{-1}(x-\mu_k)}$$

Now, let us absorb everything that does not depend on k into a constant C':

$$P(Y = k \mid X = x) = C'\pi_k e^{-\frac{1}{2}(x-\mu_k)^T \mathbf{\Sigma}^{-1}(x-\mu_k)}$$

and take the logarithm of both sides:

$$\log P(Y = k \mid X = x) = \log C' + \log \pi_k - \frac{1}{2}(x - \mu_k)^T \mathbf{\Sigma}^{-1}(x - \mu_k).$$

This constant is the same for every category, k.
So we want to find the maximum of this over k.

LDA has linear decision boundaries

Goal, maximize the following over k:

$$
\begin{aligned}
&\log \pi_k - \frac{1}{2}(x - \mu_k)^T \boldsymbol{\Sigma}^{-1}(x - \mu_k). \\
=&\log \pi_k - \frac{1}{2}\left[x^T \boldsymbol{\Sigma}^{-1} x + \mu_k^T \boldsymbol{\Sigma}^{-1} \mu_k\right] + x^T \boldsymbol{\Sigma}^{-1} \mu_k \\
=&C'' + \log \pi_k - \frac{1}{2}\mu_k^T \boldsymbol{\Sigma}^{-1} \mu_k + x^T \boldsymbol{\Sigma}^{-1} \mu_k
\end{aligned}
$$

We define the objective:

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

At an input x, we predict the response with the highest $\delta_k(x)$.

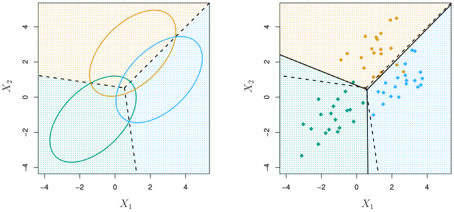
LDA has linear decision boundaries

What is the decision boundary? It is the set of points in which 2 classes are equally probable:

$$\delta_k(x) = \delta_\ell(x)$$

$$\log \pi_k - \frac{1}{2}\mu_k^T \boldsymbol{\Sigma}^{-1}\mu_k + x^T \boldsymbol{\Sigma}^{-1}\mu_k = \log \pi_\ell - \frac{1}{2}\mu_\ell^T \boldsymbol{\Sigma}^{-1}\mu_\ell + x^T \boldsymbol{\Sigma}^{-1}\mu_\ell$$

This is a linear equation in x.



Estimating π_k

$$\hat{\pi}_k = \frac{\#\{i\ ;\ y_i = k\}}{n}$$

In words, the fraction of training samples of class k.

Estimating the parameters of $f_k(x)$

Estimate the the mean vector μ_k for each class:

$$\hat{\mu}_k = \frac{1}{\#\{i \; ; \; y_i = k\}} \sum_{i \; ; \; y_i = k} x_i$$

Estimate the common covariance matrix $\mathbf{\Sigma}$:

- One predictor ($p = 1$):

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

- Many predictors ($p > 1$): Compute the vectors of deviations $(x_1 - \hat{\mu}_{y_1}), (x_2 - \hat{\mu}_{y_2}), \ldots, (x_n - \hat{\mu}_{y_n})$ and use an unbiased estimate of its covariance matrix, $\mathbf{\Sigma}$.

LDA prediction

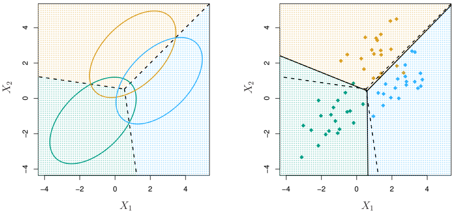
For an input x, predict the class with the largest:

$$\hat{\delta}_k(x) = \log \hat{\pi}_k - \frac{1}{2}\hat{\mu}_k^T \hat{\mathbf{\Sigma}}^{-1}\hat{\mu}_k + x^T \hat{\mathbf{\Sigma}}^{-1}\hat{\mu}_k$$

The decision boundaries are defined by:

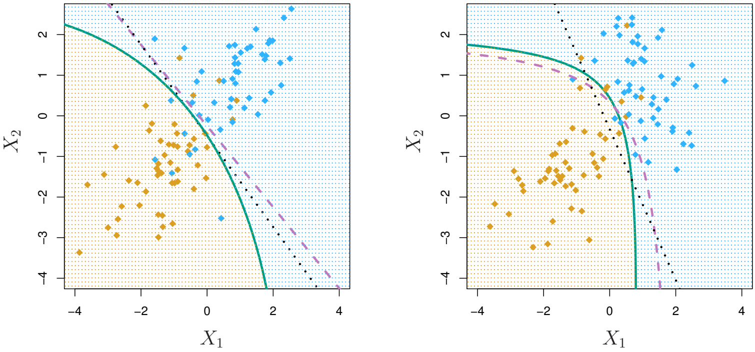
$$\log \hat{\pi}_k - \frac{1}{2}\hat{\mu}_k^T \hat{\mathbf{\Sigma}}^{-1}\hat{\mu}_k + x^T \hat{\mathbf{\Sigma}}^{-1}\hat{\mu}_k = \log \hat{\pi}_\ell - \frac{1}{2}\hat{\mu}_\ell^T \hat{\mathbf{\Sigma}}^{-1}\hat{\mu}_\ell + x^T \hat{\mathbf{\Sigma}}^{-1}\hat{\mu}_\ell$$

These are the solid lines in the following image:



Quadratic discriminant analysis (QDA)

The assumption that the inputs of every class have the same covariance $\mathbf{\Sigma}$ can be quite restrictive:



Boundaries for Bayes (dashed), LDA (dotted), and QDA (solid).

Quadratic discriminant analysis (QDA)

In **quadratic discriminant analysis** we estimate a mean $\hat{\mu}_k$ and a covariance matrix $\hat{\mathbf{\Sigma}}_k$ for each class separately.

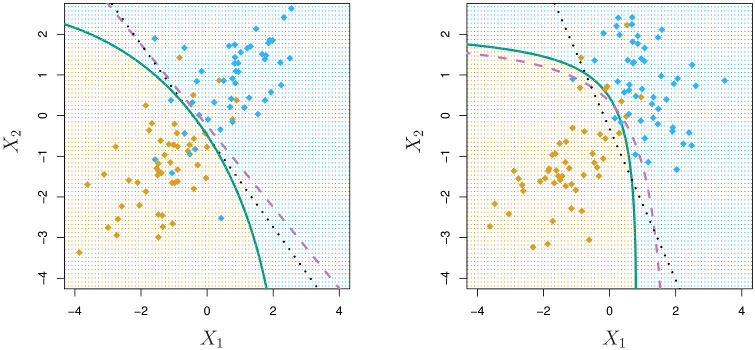
Given an input, it is easy to derive an objective function:

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

This objective is now quadratic in x and so are the decision boundaries.

Quadratic discriminant analysis (QDA)

- Bayes boundary (– – –)
- LDA (· · · · · ·)
- QDA (——).



Evaluating a classification method

We have talked about the 0-1 loss:

$$\frac{1}{m}\sum_{i=1}^{m}\mathbf{1}(y_i \neq \hat{y}_i).$$

It is possible to make the wrong prediction for some classes more often than others. The 0-1 loss doesn't tell you anything about this.

A much more informative summary of the error is a **confusion matrix**:

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

Example. Predicting `default`

Used LDA to predict credit card default in a dataset of 10K people.

Predicted "yes" if $P(\texttt{default} = \text{yes}|X) > 0.5$.

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

- The error rate among people who do **not** default (false positive rate) is very low.
- However, the error rate among people who **do** default (false negative rate) is 76%.
- False negatives may be a bigger source of concern!
- One possible solution: Change the threshold.

Example. Predicting `default`

Changing the threshold to 0.2 makes it easier to classify to "yes".

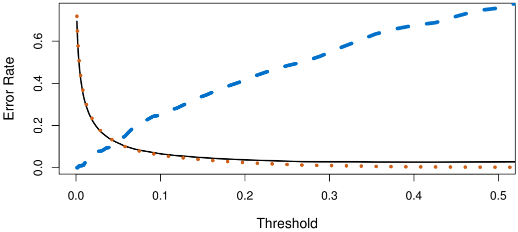
Predicted "yes" if $P(\texttt{default} = \text{yes}|X) > 0.2$.

		True default status		
		No	Yes	Total
Predicted default status	No	$9,432$	138	$9,570$
	Yes	235	195	430
	Total	$9,667$	333	$10,000$

Note that the rate of false positives became higher! That is the price to pay for fewer false negatives.

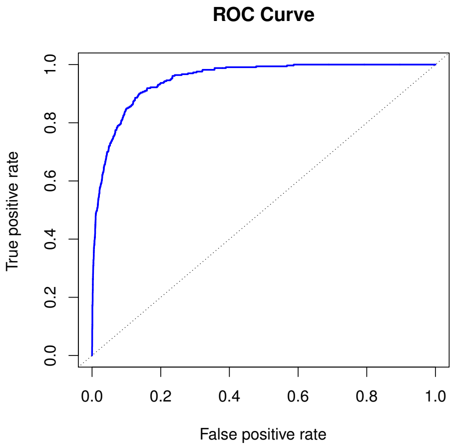
Example. Predicting `default`

Let's visualize the dependence of the error on the threshold:



- – – – False negative rate (error for defaulting customers)
- · · · · False positive rate (error for non-defaulting customers)
- —— 0-1 loss or total error rate.

Example. The ROC curve



- Displays the performance of the method for any choice of threshold.
- The area under the curve (AUC) measures the quality of the classifier:
  - 0.5 is the AUC for a random classifier
  - The closer AUC is to 1, the better.

Next time

- Comparison of logistic regression, LDA, QDA, and KNN classification.
- Start Chapter 5: Resampling.