Lecture 9: Classification, LDA

Reading: Chapter 4

STATS 202: Data mining and analysis

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Slide credits: Sergio Bacallado

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:

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

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

$$\hat{P}(Y = k \mid X = x) = \frac{\hat{P}(X = x \mid Y = k)\hat{P}(Y = k)}{\hat{P}(X = x)}$$

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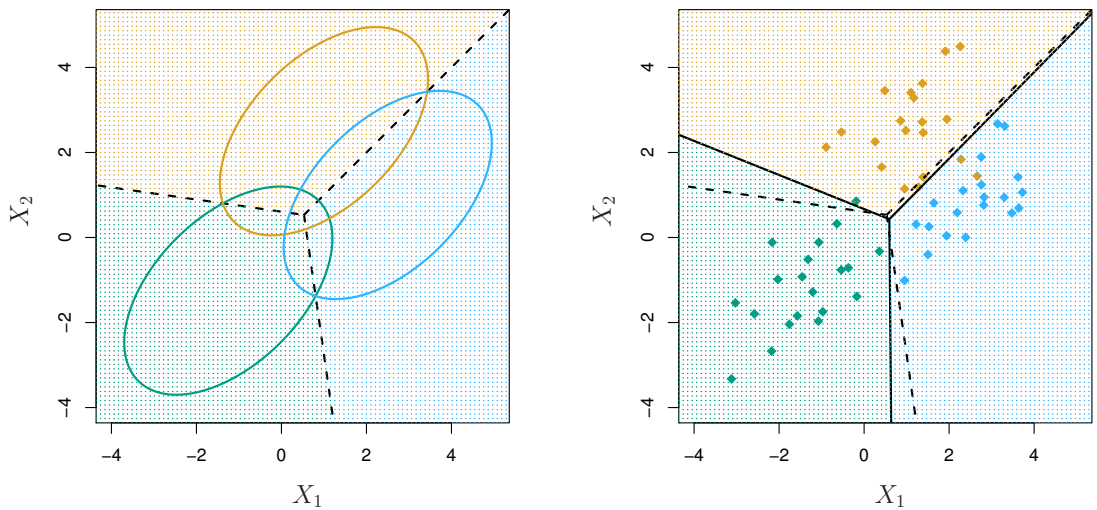
Instead of estimating $P(Y \mid X)$, we will estimate:

1. We model $\hat{P}(X = x \mid Y = k) = \hat{f}_k(x)$ as a *Multivariate Normal Distribution*:



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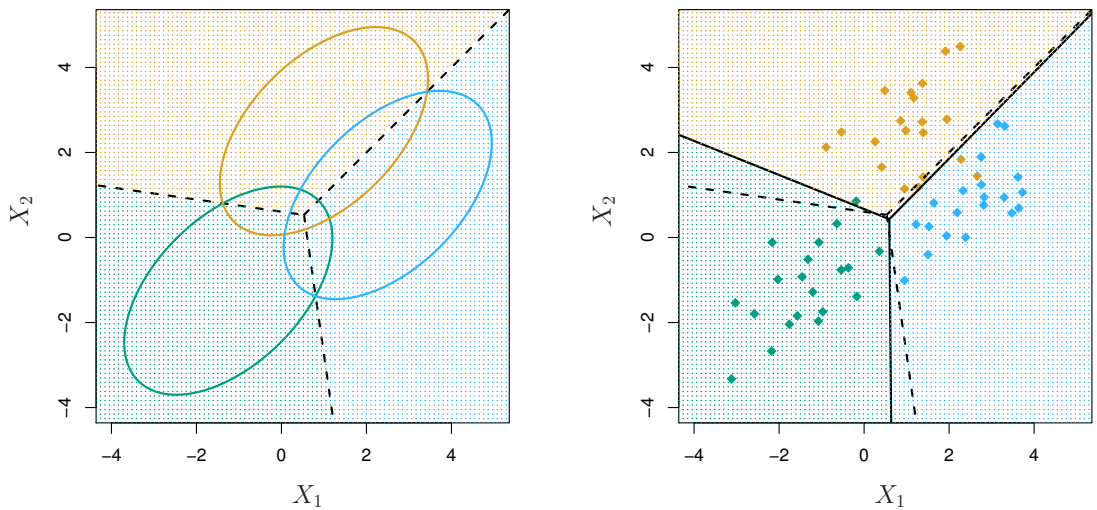

2. $\hat{P}(Y = k) = \hat{\pi}_k$ is estimated by the fraction of training samples of class k.

LDA has linear decision boundaries

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

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Then, what is the Bayes classifier?

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Now, expanding $f_k(x)$:

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

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

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and take the logarithm of both sides:

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So we want to find the maximum of this over k.

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Goal, maximize the following over k:

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We define the objective:

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

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

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What is the decision boundary? It is the set of points in which 2 classes do just as well:

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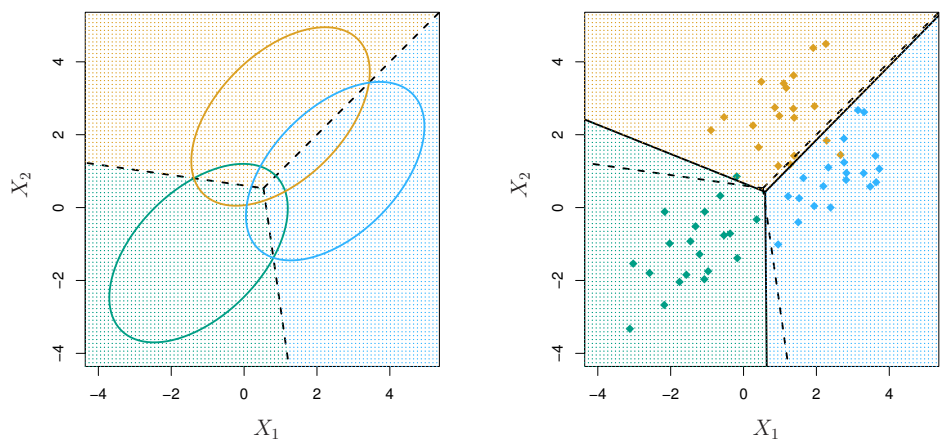
This is a linear equation in x.



Estimating π_k

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

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

Estimating the parameters of $f_k(x)$

Estimate the center of each class μ_k:

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

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- One predictor ($p = 1$):

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- 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:

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

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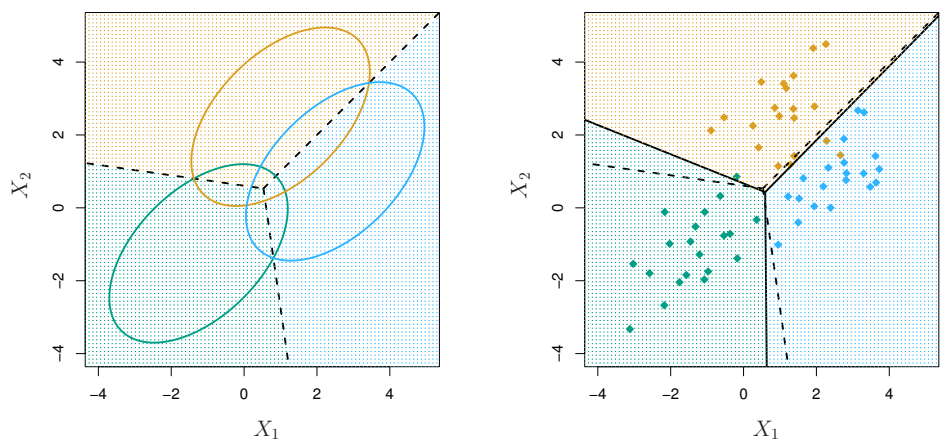
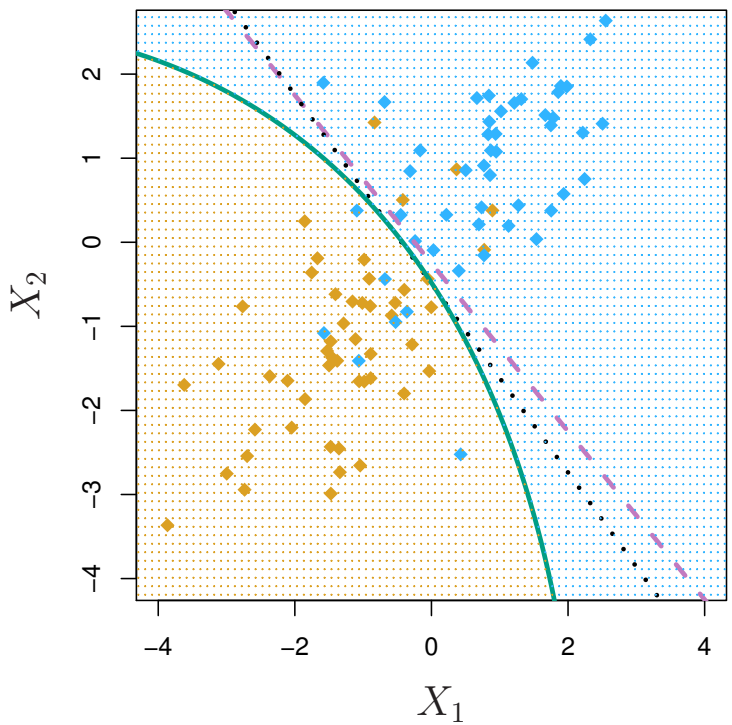
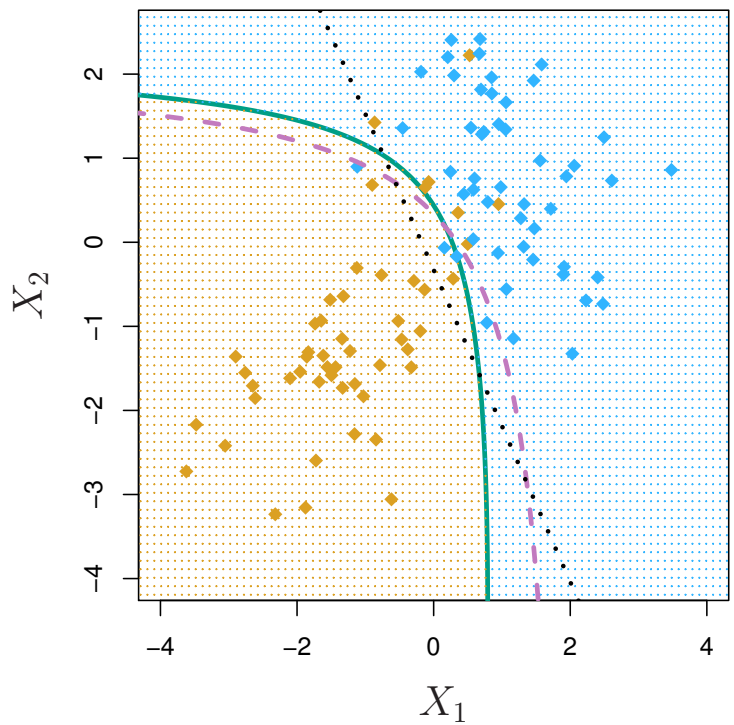
Solid lines in:



Quadratic discriminant analysis (QDA)

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





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

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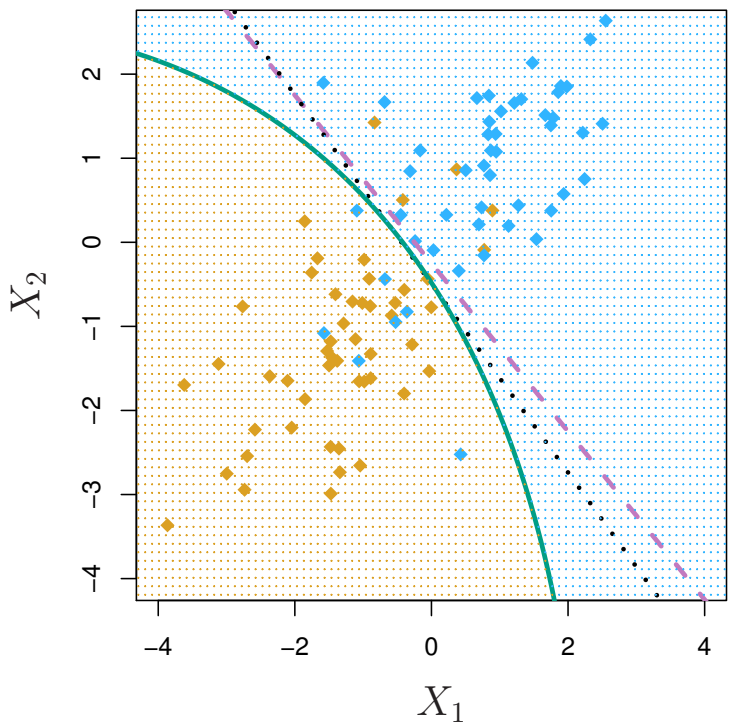
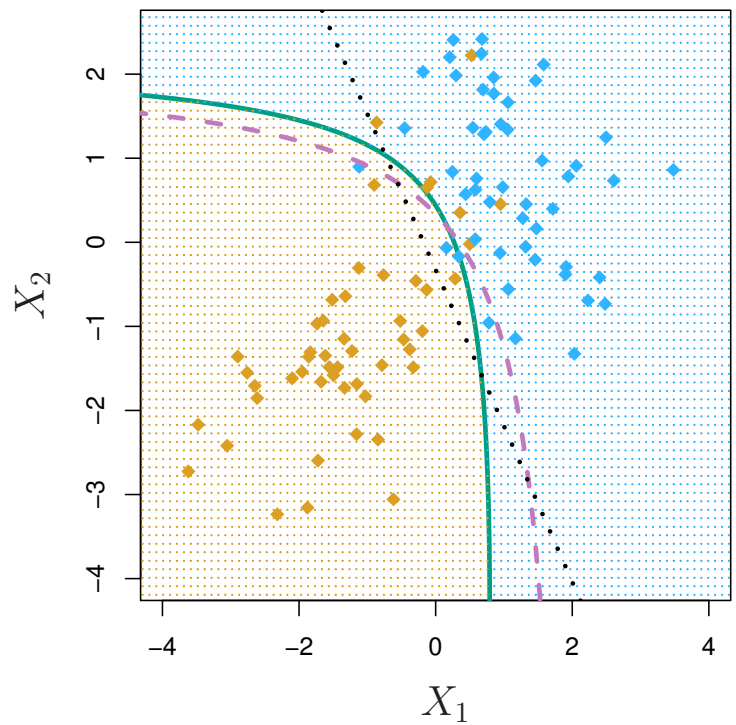
This objective is now quadratic in x and so are the decision boundaries.

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.

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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
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	Yes	23	81	104
	Total	9,667	333	10,000

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- However, the rate of false negatives is 76%.
- It is possible that false negatives are a bigger source of concern!
- One possible solution: Change the threshold.

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

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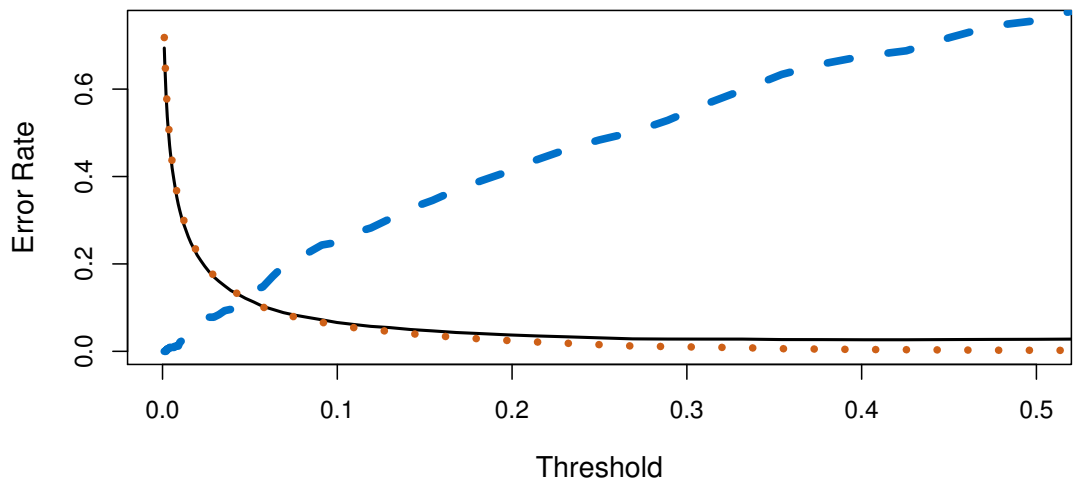
Note that the rate of false positives became higher! That is the price to pay for fewer false negatives.

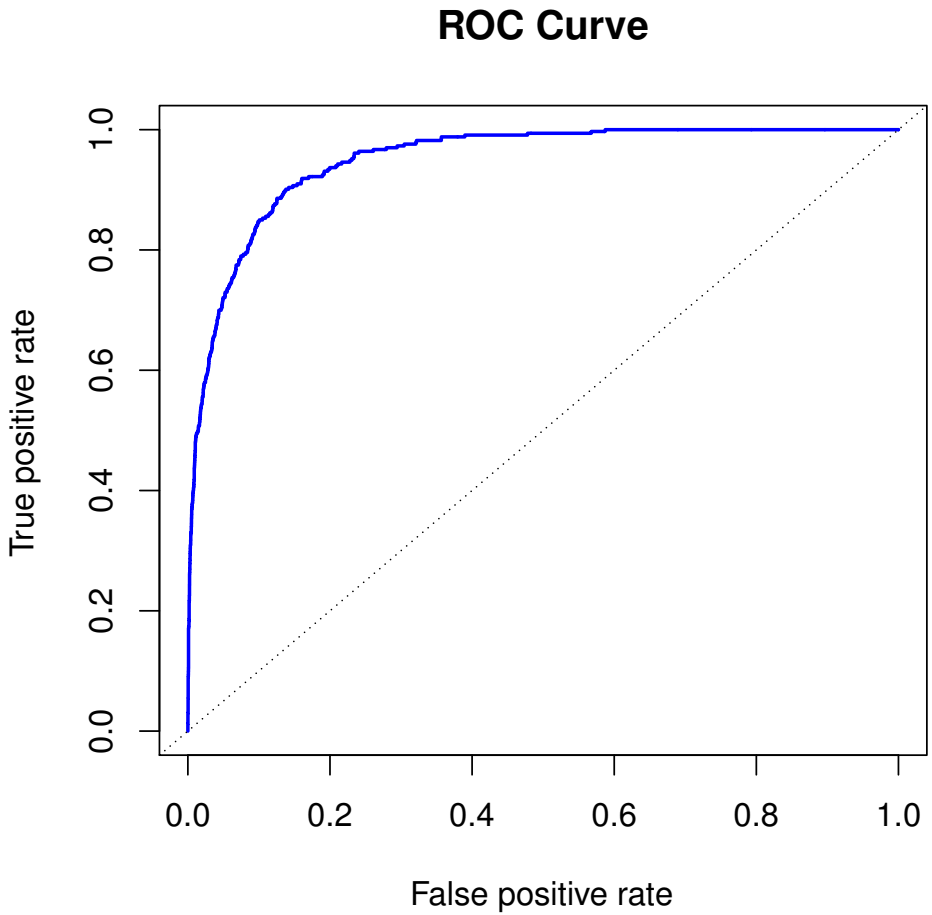
Example. Predicting `default`

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



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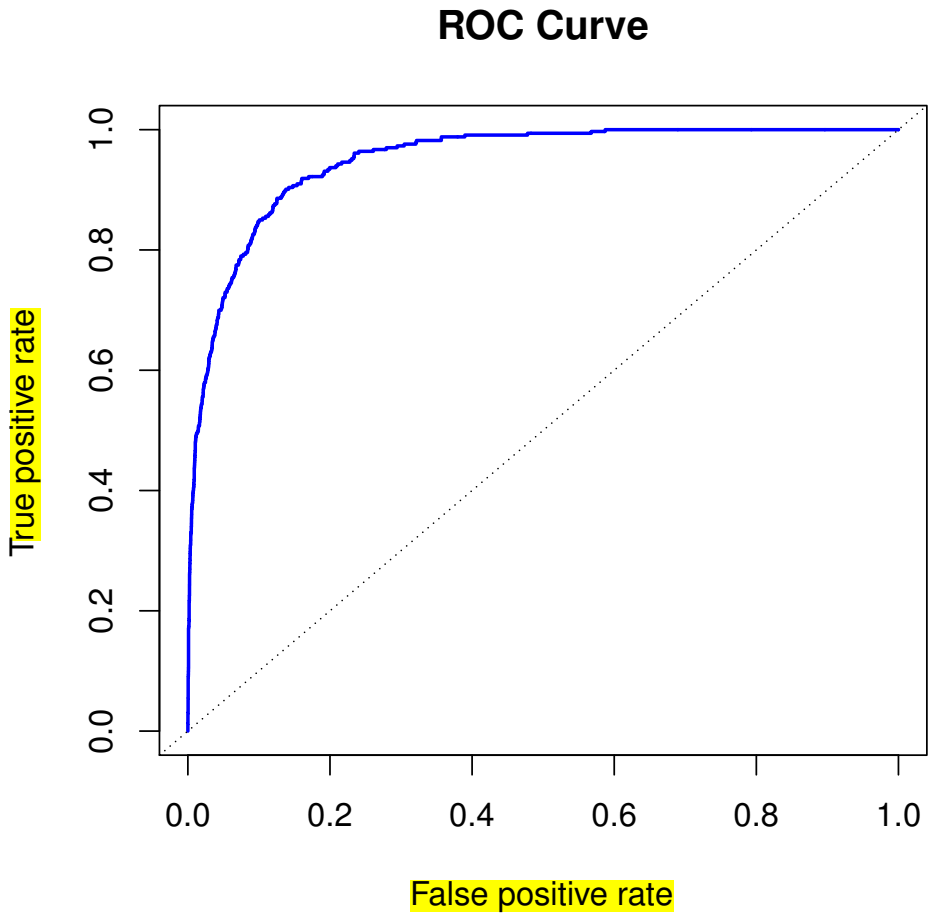

- Displays the performance of the method for any choice of threshold.
- The area under the curve (AUC) measures the quality of the classifier:
  - 0.5 is the AUC for a random classifier
  - The closer AUC is to 1, the better.

Next time

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