Week 3: Classification

PUBLG088: Advanced Quantitative Methods

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Week 3 Outline

1. Classification
   - Logistic Regression
   - Maximum Likelihood
   - Multiple logistic regression
   - Logistic regression with more than two classes
2. Discriminant Analysis
   - Bayes theorem for classification
   - Linear Discriminant Analysis when $p > 1$
   - Quadratic Discriminant Analysis
   - Logistic Regression versus LDA
3. Characterizing performance of classifiers
   - Confusion matrix
   - Sensitivity and specificity
   - Performance measures for classifiers: Zoo

Classification

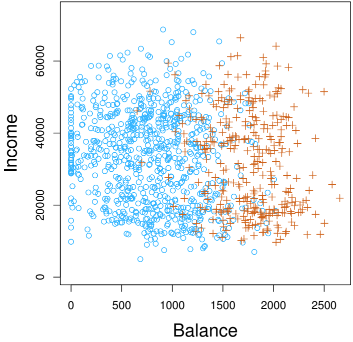
Classification

- Qualitative variables take values in an unordered set $\mathcal{C}$, such as: *eye color* $\in$ {*brown,blue,green*}*; email* $\in$ {*spam, ham*}.
- Given a feature vector X and a qualitative response Y taking values in the set $\mathcal{C}$, the classification task is to build a function $\mathcal{C}(\mathcal{X})$ that takes as input the feature vector X and predicts its value for Y; i.e. $\mathcal{C}(\mathcal{X}) \in \mathcal{C}$.

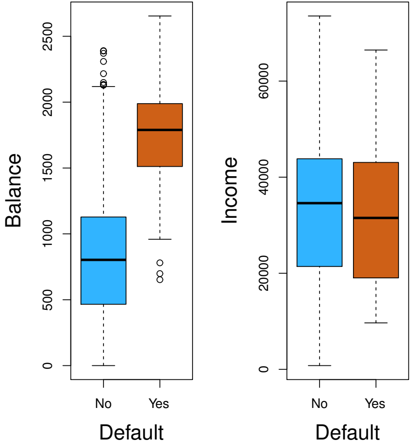
Classification

- Often we are more interested in estimating the probabilities that X belongs to each category in $\mathcal{C}$.
- For example, it is more valuable to have an estimate of the probability that an insurance claim is fraudulent, than a classification fraudulent or not.

Example: Credit Card Default



Source: James et al. 2013



Source: James et al. 2013

Can we use Linear Regression?

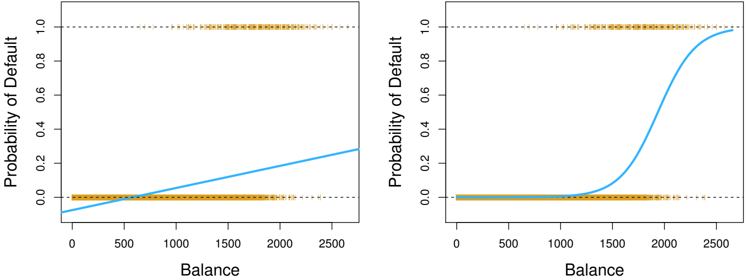
Suppose for the Default classification task that we code

$$Y = \begin{cases} 0 & \text{if } No \\ 1 & \text{if } Yes. \end{cases}$$

Can we simply perform a linear regression of Y on X and classify as Yes if $\hat{Y} > 0.5$?

- In this case of a binary outcome, linear regression does a good job as a classifier, and is equivalent to linear discriminant analysis which we discuss later.
- However, linear regression might produce probabilities less than zero or bigger than one. Logistic regression is more appropriate.

Linear versus Logistic Regression



Source: James et al. 2013

- The orange marks indicate the response Y, either 0 or 1.
- Linear regression does not estimate $Pr(Y = 1|X)$ well.
- Logistic regression seems well suited to the task.

Linear Regression continued

- Now suppose we have a response variable with three possible values. A patient presents at the emergency room, and we must classify them according to their symptoms.

$$Y = \begin{cases} 1 & \text{if } \textit{stroke}; \\ 2 & \text{if } \textit{drug overdose}; \\ 3 & \text{if } \textit{epileptic seizure}. \end{cases}$$

- This coding suggests an ordering, and in fact implies that the difference between *stroke* and *drug overdose* is the same as between *drug overdose* and *epileptic seizure*.
- Linear regression is not appropriate here.
- Multiclass Logistic Regression or Discriminant Analysis are more appropriate.

Logistic Regression

- Let's write $p(X) = Pr(Y = 1|X)$ for short and consider using *balance* to predict *default*. Using a *logistic function*, we can get $p(X)$ between 0 and 1.

$$p(X) = \frac{e^{\beta_0+\beta_1 X}}{1 + e^{\beta_0+\beta_1 X}}.$$

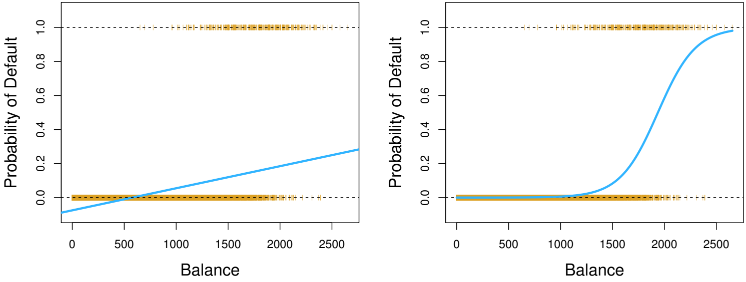
  ($e \approx 2.71828$ is a mathematical constant [Euler's number.])

- It is easy to see that no matter what values β_0, β_1 or X take, $p(X)$ will have values between 0 and 1.
- A bit of rearrangement gives

$$log\left(\frac{p(X)}{1 - p(X)}\right) = \beta_0 + \beta_1 X.$$

- This monotone transformation is called the log odds or logit transformation of $p(X)$.

Linear versus Logistic Regression



Source: James et al. 2013

- Logistic regression ensures that our estimate for $p(X)$ lies between 0 and 1.

Maximum Likelihood

- We use maximum likelihood to estimate the parameters.

$$\ell(\beta_0, \beta_1) = \prod_{i:y_i=1} p(x_i) \prod_{i:y_i=0} (1 - p(x_i)).$$

- This likelihood gives the probability of the observed zeros and ones in the data.
- We pick β_0 and β_1 to maximize the likelihood of the observed data.
- Most statistical packages can fit linear logistic regression models by maximum likelihood. In R we use the *glm* function.

```r
library(ISLR)
data(Default)
logit1 <- glm(default ~ balance, data = Default, family = binomial)
summary(logit1)
```

```
##
## Call:
## glm(formula = default ~ balance, family = binomial, data = Default)
##
## Deviance Residuals:
##     Min       1Q   Median       3Q      Max
## -2.2697  -0.1465  -0.0589  -0.0221   3.7589
##
## Coefficients:
##               Estimate Std. Error z value Pr(>|z|)
## (Intercept) -1.065e+01  3.612e-01  -29.49   <2e-16 ***
## balance      5.499e-03  2.204e-04   24.95   <2e-16 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## (Dispersion parameter for binomial family taken to be 1)
##
##     Null deviance: 2920.6  on 9999  degrees of freedom
## Residual deviance: 1596.5  on 9998  degrees of freedom
## AIC: 1600.5
##
## Number of Fisher Scoring iterations: 8
```

Making Predictions

- What is our estimated probability of *default* for someone with a balance of $1000?

$$\hat{p}(X) = \frac{e^{\hat{\beta}_0 + \hat{\beta}_1 X}}{1 + e^{\hat{\beta}_0 + \hat{\beta}_1 X}} = \frac{e^{-10.6513 + 0.0055 \times 1000}}{1 + e^{-10.6513 + 0.0055 \times 1000}} = 0.006$$

- With a balance of $2000?

$$\hat{p}(X) = \frac{e^{\hat{\beta}_0 + \hat{\beta}_1 X}}{1 + e^{\hat{\beta}_0 + \hat{\beta}_1 X}} = \frac{e^{-10.6513 + 0.0055 \times 2000}}{1 + e^{-10.6513 + 0.0055 \times 2000}} = 0.586$$

```r
logit2 <- glm(default ~ student, data = Default, family = binomial)
summary(logit2)
```

```
##
## Call:
## glm(formula = default ~ student, family = binomial, data = Default)
##
## Deviance Residuals:
##     Min       1Q   Median       3Q      Max
## -0.2970  -0.2970  -0.2434  -0.2434   2.6585
##
## Coefficients:
##             Estimate Std. Error z value Pr(>|z|)
## (Intercept) -3.50413    0.07071  -49.55  < 2e-16 ***
## studentYes   0.40489    0.11502    3.52 0.000431 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## (Dispersion parameter for binomial family taken to be 1)
##
##     Null deviance: 2920.6  on 9999  degrees of freedom
## Residual deviance: 2908.7  on 9998  degrees of freedom
## AIC: 2912.7
##
## Number of Fisher Scoring iterations: 6
```

Making Predictions (binary variable)

$$\hat{p}(default = Yes|student = Yes) = \frac{e^{-3.5041+0.4049\times1}}{1+e^{-3.5041+0.4049\times1}} = 0.0431$$

$$\hat{p}(default = Yes|student = No) = \frac{e^{-3.5041+0.4049\times0}}{1+e^{-3.5041+0.4049\times0}} = 0.0292$$

Logistic regression with several variables

$$log\left(\frac{p(X)}{1-p(X)}\right) = \beta_0 + \beta_1 X_1 + \ldots + \beta_p X_p$$

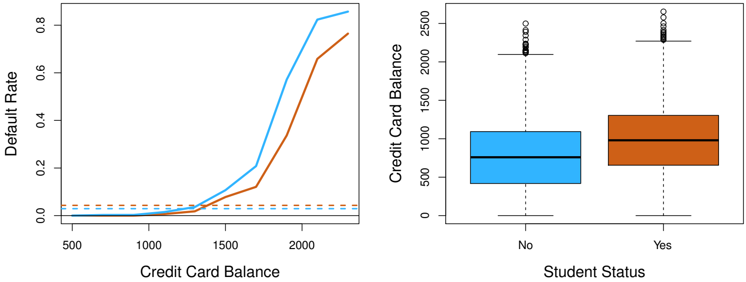
$$p(X) = \frac{e^{\beta_0+\beta_1 X_1+\ldots+\beta_p X_p}}{1+e^{\beta_0+\beta_1 X_1+\ldots+\beta_p X_p}}$$

```r
logit3 <- glm(default ~ balance + income + student,
              data = Default,
              family = binomial)
summary(logit3)
```

```
##
## Call:
## glm(formula = default ~ balance + income + student, family = binomial,
##     data = Default)
##
## Deviance Residuals:
##     Min       1Q   Median       3Q      Max
## -2.4691  -0.1418  -0.0557  -0.0203   3.7383
##
## Coefficients:
##               Estimate Std. Error z value Pr(>|z|)
## (Intercept) -1.087e+01  4.923e-01 -22.080  < 2e-16 ***
## balance      5.737e-03  2.319e-04  24.738  < 2e-16 ***
## income       3.033e-06  8.203e-06   0.370  0.71152
## studentYes  -6.468e-01  2.363e-01  -2.738  0.00619 **
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## (Dispersion parameter for binomial family taken to be 1)
##
##     Null deviance: 2920.6  on 9999  degrees of freedom
## Residual deviance: 1571.5  on 9996  degrees of freedom
```

- Why is coefficient for *student* negative, while it was positive before?

Multiple logistic regression



Source: James et al. 2013

- Students tend to have higher balances than non-students, so their marginal default rate is higher than for non-students.
- But for each level of balance, students default less than non-students.
- Multiple logistic regression can tease this out.

Logistic regression with more than two classes

- So far we have discussed logistic regression with two classes.
- It is easily generalized to more than two classes.
- One version (used in the R package *glmnet*) has the form:

$$Pr(Y = k|X) = \frac{e^{\beta_{0k}+\beta_{1k}X_1+\ldots+\beta_{pk}X_p}}{\sum_{\ell=1}^{K} e^{\beta_{0\ell}+\beta_{1\ell}X_1+\ldots+\beta_{p\ell}X_p}}$$

- Multiclass logistic regression is also referred to as multinomial regression.

Discriminant Analysis

Discriminant Analysis

- Here the approach is to model the distribution of X in each of the classes separately, and then use Bayes theorem to flip things around and obtain $Pr(Y|X)$.
- When we use normal (Gaussian) distributions for each class, this leads to linear or quadratic discriminant analysis.
- However, this approach is quite general, and other distributions can be used as well. Here, we will focus on normal distributions.

Bayes theorem for classification

- Thomas Bayes was a famous mathematician whose name represents a big subfield of statistical and probabilistic modeling.
- Here we focus on a simple result, known as Bayes theorem:

$$Pr(Y = k|X = x) = \frac{Pr(X = x|Y = k) \cdot Pr(Y = k)}{Pr(X = x)}$$

- One writes this slightly differently for discriminant analysis:

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

where

  - $f_k(x) = Pr(X = x|Y = k)$ is the density for X in class k. Here we will use normal densities for these, separately in each class.
  - $\pi_k = Pr(Y = k)$ is the marginal or prior probability for class k.

Why discriminant analysis?

- 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 popular when we have more than two response classes, because it also provides low-dimensional views of the data.

Linear Discriminant Analysis when $p = 1$

- The Gaussian density has the form

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

- Here μ_k is the mean, and σ_k^2 the variance (in class k). We will assume that all the $\sigma_k = \sigma$ are the same.
- Plugging this into Bayes formula, we get a rather complex expression for $p_k(x) = Pr(Y = k|X = x)$:

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

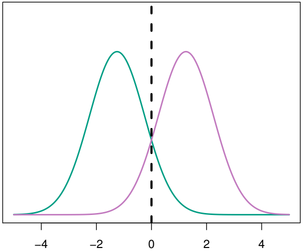
Discriminant functions

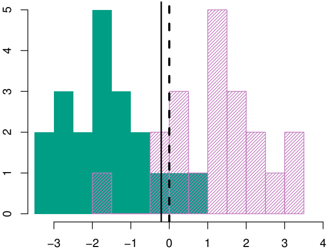
- To classify at the value $X = x$, we need to see which of the $p_k(x)$ is largest. Taking logs, and discarding terms that do not depend on k, we see that this is equivalent to assigning x to the class with the largest discriminant score:

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

- Note that $\delta_k(x)$ is a linear function of x.
- If there are $K = 2$ classes and $\pi_1 = \pi_2 = 0.5$, then one can see that the decision boundary is at

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





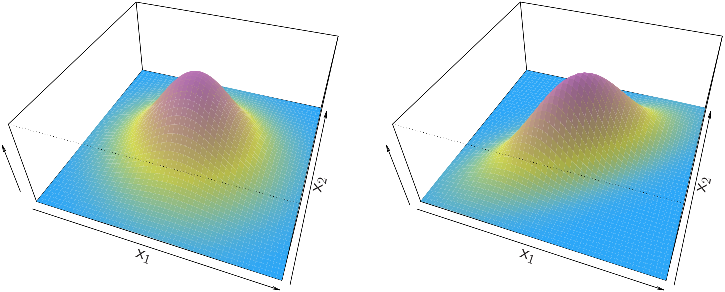
Source: James et al. 2013

- Example with $\mu_1 = -1.25,\ \mu_2 = 1.25,\ \sigma_1^2 = \sigma_2^2 = 1$.
- Typically we don't know these parameters; we just have the training data.
- In that case we simply estimate the parameters and plug them into the rule.

Estimating the parameters

- $\hat{\pi}_k = \frac{n_k}{n}$;
- $\hat{\mu}_k = \frac{1}{n_k} \sum_{i: y_i = k} x_i$;
- $\hat{\sigma}^2 = \frac{1}{n-K} \sum_{k=1}^{K} \sum_{i: y_i = k} (x_i - \hat{\mu}_k)^2 = \sum_{k=1}^{K} \frac{n_k - 1}{n-K} \cdot \hat{\sigma}_k^2$
- where $\hat{\sigma}_k^2 = \frac{1}{n_k - 1} \sum_{i: y_i = k} (x_i - \hat{\mu}_k)^2$ is the usual formula for the estimated variance in the kth class.

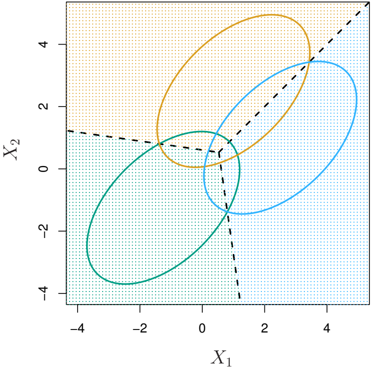
Linear Discriminant Analysis when $p > 1$

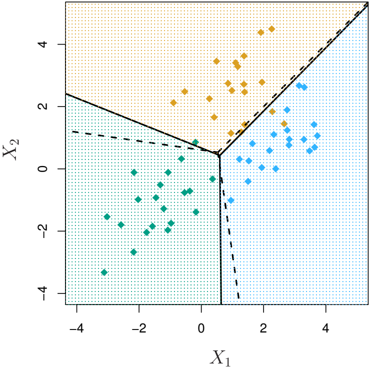


Source: James et al. 2013

- Density: $f(x) = \frac{1}{(2\pi)^{p/2}|\Sigma|^{1/2}} e^{-\frac{1}{2}(x-\mu)^T\Sigma^{-1}(x-\mu)}$
- Discriminant function: $\delta_k(x) = x^T\Sigma^{-1}\mu_k - \frac{1}{2}\mu_k^T\Sigma^{-1}\mu_k + log\pi_k$
- Despite its complex form, $\delta_k(x) = c_{k0} + c_{k1}x_1 + c_{k2}x_2 + \cdots + c_{kp}x_p$ – a linear function.

Illustration: $p = 2$ and $K = 3$ classes





Source: James et al. 2013

- Here $\pi_1 = \pi_2 = \pi_3 = 1/3$.
- The dashed lines are known as the Bayes decision boundaries.
- Were they known, they would yield the fewest misclassification errors, among all possible classifiers.

From $\delta_k(x)$ to probabilities

- Once we have estimates $\delta_k(x)$, we can turn these into estimates for class probabilities:

$$\widehat{Pr}(Y = k|X = x) = \frac{e^{\hat{\delta}_k(x)}}{\sum_{\ell=1}^{K} e^{\hat{\delta}_\ell(x)}}.$$

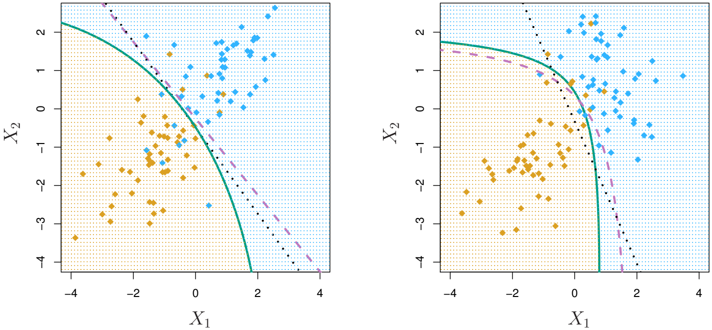
- So classifying to the largest $\hat{\delta}_k(x)$ amounts to classifying to the class for which $\widehat{Pr}(Y = k|X = x)$ is largest.
- When $K = 2$, we classify to class 2 if $\widehat{Pr}(Y = 2|X = x) \geq 0.5$, else to class 1.

Other forms of Discriminant Analysis

$$Pr(Y = k|X = x) = \frac{\pi_k f_k(x)}{\sum_{\ell=1}^{K} \pi_\ell f_\ell(x)}$$

- 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.
  - Many other forms, by proposing specific density models for $f_k(x)$, including nonparametric approaches.

Quadratic Discriminant Analysis



Source: James et al. 2013

- $\delta_k(x) = -\frac{1}{2}(x-\mu_k)^T\Sigma_k^{-1}(x-\mu_k) + log\pi_k$
- Because the Σ_k are different, the quadratic terms matter.

Logistic Regression versus LDA

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

$$log\left(\frac{p_1(x)}{1-p_1(x)}\right) = log\left(\frac{p_1(x)}{p_2(x)}\right) = c_0 + c_1 x_1 + \cdots + c_p x_p$$

- So it has the same form as logistic regression.
- The difference is in how the parameters are estimated.
  - Logistic regression uses the conditional likelihood based on $Pr(Y|X)$ (known as discriminative learning).
  - LDA uses the full likelihood based on $Pr(X, Y)$ (known as generative learning).
  - Despite these differences, in practice the results are often very similar.
- Note: logistic regression can also fit quadratic boundaries like QDA, by explicitly including quadratic terms in the model.

Characterizing performance of classifiers

Confusion matrix and error rates (from LDA)

		True Default Status		
		No	Yes	Total
Predicted	No	9644	252	9896
Default Status	Yes	23	81	104
	Total	9667	333	10000

- (23 + 252) / 10000 errors — a 2.75% misclassification rate.
- Some caveats:
  - This is training error, and we may be overfitting. Not a big concern here since $n = 10000$ and $p = 4$.
  - If we classified to the prior – always to class *No* in this case – we would make 333/10000 errors, or only 3.33%.
  - Of the true *No*'s, we make $23/9667 = 0.2\%$ errors; of the true *Yes*'s, we make $252/333 = 75.7\%$ errors!

Types of errors

- False positive rate: The fraction of negative examples that are classified as positive – 0.2% in example.
- False negative rate: The fraction of positive examples that are classified as negative – 75.7% in example.

Sensitivity and specificity

- Performance of a classifier is often characterized in terms of sensitivity and specificity.
- Here, the sensitivity is the percentage of true defaulters that are identified. It is 24.3% in our case.
- The specificity is the percentage of non-defaulters that are correctly identified. Here it is $(1 - 23/9,667) \cdot 100 = 99.8\%$
- The true positive rate is the sensitivity of our classifier.
- The false positive rate is *one minus* the specificity of our classifier.

Errors and threshold

- We produced the confusion matrix above by classifying to class *Yes* if

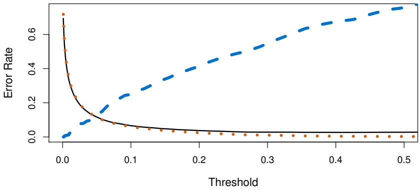
$$\widehat{Pr}(Default = Yes|Balance, Student) \geq 0.5$$

- We can change the two error rates by changing the threshold from 0.5 to some other value in [0,1]:

$$\widehat{Pr}(Default = Yes|Balance, Student) \geq threshold,$$

and vary *threshold*.

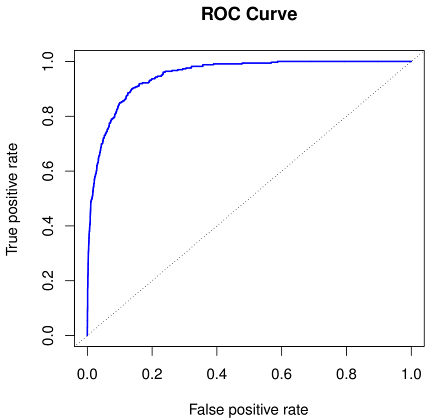
Varying the *threshold*



Source: James et al. 2013

- Error rates are shown as a function of the threshold value for the posterior probability that is used to perform the assignment.
- The black solid line displays the overall error rate.
- The blue dashed line represents the fraction of defaulting customers that are incorrectly classified (False Negative).
- The orange dotted line indicates the fraction of errors among the non-defaulting customers (False Positive).
- In order to reduce the false negative rate, we may want to reduce the threshold to 0.1 or less.

ROC curve



Source: James et al. 2013

- The ROC plot displays both simultaneously.
- Sometimes we use the AUC or area under the curve to summarize the overall performance.

Characterizing performance of classifiers

		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*	

- "+" is "disease" or alternative (non-null) hypothesis (here, those who default);
- "-" is "non-disease" or the null hypothesis (here, those who do not default).

Performance measures for classifiers

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*	

- The denominators for the false positive and true positive rates are the actual population counts in each class.
- The denominators for the positive predictive value and the negative predictive value are the total predicted counts for each class.

Summary

- Logistic regression is very popular for classification, especially when $K = 2$.
- LDA is useful when n is small, or the classes are well separated, and Gaussian assumptions are reasonable. Also when $K > 2$.
- See Section 4.5 for some comparisons of logistic regression, LDA and KNN.

Acknowledgements

Some of the figures in this presentation are taken from "An Introduction to Statistical Learning, with applications in R" (Springer, 2013) with permission from the authors: G. James, D. Witten, T. Hastie and R. Tibshirani

References

James, Gareth et al. (2013). *An Introduction to Statistical Learning*. Vol. 103, p. 440. ISBN: 1461471389. DOI: 10.1007/978-1-4614-7138-7. arXiv: arXiv:1011.1669v3.