Day 5: Classification

ME314: Introduction to Data Science and Machine Learning

LSE Methods Summer Programme 2019

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Day 5 Outline

Classification

- Logistic Regression
- Maximum Likelihood
- Multiple logistic regression
- Logistic regression with more than two classes
- Naive Bayes Classifier
- Logistic Regression versus LDA

Characterizing performance of classifiers

- Confusion matrix
- Sensitivity and specificity
- Performance measures for classifiers: Zoo

Classification

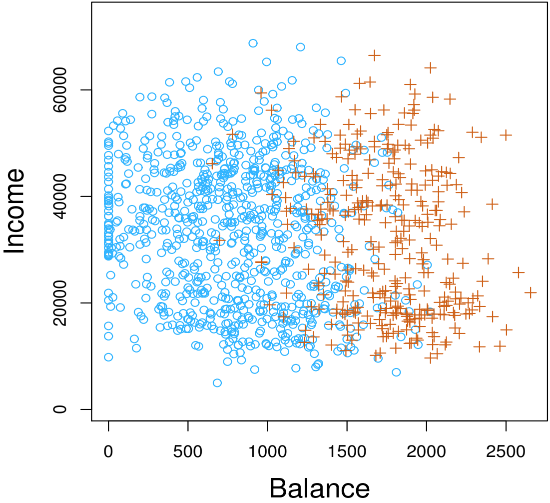
Classification

- 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. $\mathcal{C}(\mathcal{X}) \in \mathcal{C}$.

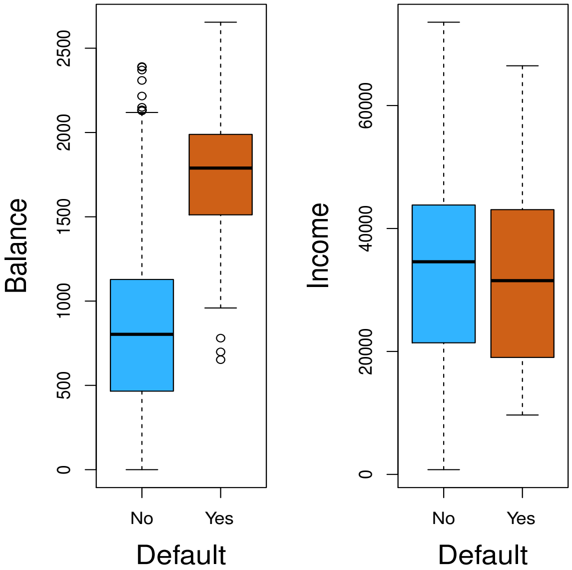
Classification

- 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



Example: Credit Card Default



Can we use Linear Regression?

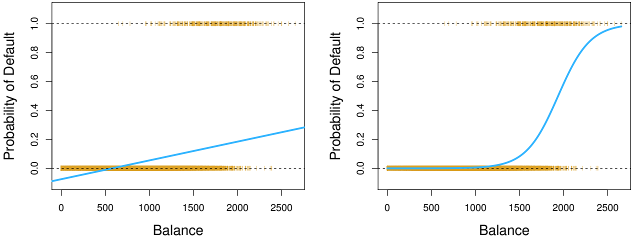
Suppose for the Default classification task that we code

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

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

- 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.
- Since in the population $E(Y|X = x) = Pr(Y = 1|X = x)$, we might think that regression is perfect for this task.
- However, linear regression might produce probabilities less than zero or bigger than one. Logistic regression is more appropriate.

Linear versus Logistic Regression



- 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*. Logistic regression uses the form

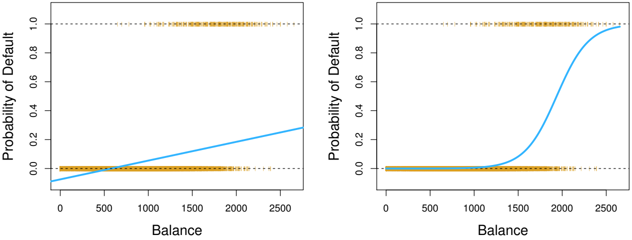
$$p(X) = \frac{e^{\beta_0 + \beta_1 X}}{1 + e^{\beta_0 + \beta_1 X}}.$$

  ($e \approx 2.71828$ 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



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

Maximum Likelihood

- We use maximum likelihood to estimate the parameters.

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

- 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.

```
> library(ISLR)
> data("Default")
> names(Default)

[1] "default" "student" "balance" "income"

> logistic <- glm(Default$default ~ Default$balance, family = binomial)
```

```
> summary(logistic)

Call:
glm(formula = Default$default ~ Default$balance, family = binomial)

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 ***
Default$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?

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

```
> logistic2 <- glm(Default$default ~ Default$student, family = binomial)
> summary(logistic2)

Call:
glm(formula = Default$default ~ Default$student, family = binomial)

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 ***
Default$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)

$$\widehat{Pr}(default = Yes|student = Yes) = \frac{e^{-3.5041+0.4049\times 1}}{1+e^{-3.5041+0.4049\times 1}} = 0.0431$$

$$\widehat{Pr}(default = Yes|student = No) = \frac{e^{-3.5041+0.4049\times 0}}{1+e^{-3.5041+0.4049\times 0}} = 0.0292$$

Logistic regression with several variables

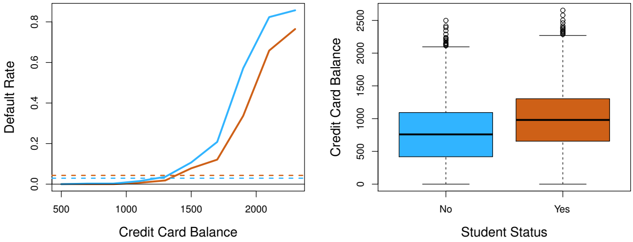
$$log\left(\frac{p(X)}{1-p(X)}\right) = \beta_0 + \beta_1 X_1 + \ldots + \beta_p X_p$$

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

```
> logistic3 <- glm(Default$default ~ Default$balance + Default$income + Default$student, family = binomial)
> summary(logistic3)

Call:
glm(formula = Default$default ~ Default$balance + Default$income +
    Default$student, family = binomial)

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 ***
Default$balance    5.737e-03  2.319e-04  24.738  < 2e-16 ***
Default$income     3.033e-06  8.203e-06   0.370  0.71152
Default$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
AIC: 1579.5

Number of Fisher Scoring iterations: 8

>
```

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

Confounding



- 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.

Example: South African Heart Disease

- 160 cases of MI (myocardial infarction) and 302 controls (all male in age range 15-64), from Western Cape, South Africa in early 80s.
- Overall prevalence very high in this region: 5.1%.
- Measurements on seven predictors (risk factors), shown in scatterplot matrix.
- Goal is to identify relative strengths and directions of risk factors.
- This was part of an intervention study aimed at educating the public on healthier diets.

```
> library(ElemStatLearn)
> data("SAheart")
> names(SAheart)
 [1] "sbp"       "tobacco"   "ldl"       "adiposity" "famhist"
 [7] "obesity"   "alcohol"   "age"       "chd"
```

```
> pairs(SAheart)
```

```
> heartfit <- glm(chd ~ . , data = SAheart, family = binomial)
> summary(heartfit)

Call:
glm(formula = chd ~ ., family = binomial, data = SAheart)

Deviance Residuals:
    Min       1Q   Median       3Q      Max
-1.7781  -0.8213  -0.4387   0.8889   2.5435

Coefficients:
                 Estimate Std. Error z value Pr(>|z|)
(Intercept)    -6.1507209  1.3082600  -4.701 2.58e-06 ***
sbp             0.0065040  0.0057304   1.135 0.256374
tobacco         0.0793764  0.0266028   2.984 0.002847 **
ldl             0.1739239  0.0596617   2.915 0.003555 **
adiposity       0.0185866  0.0292894   0.635 0.525700
famhistPresent  0.9253704  0.2278940   4.061 4.90e-05 ***
typea           0.0395950  0.0123202   3.214 0.001310 **
obesity        -0.0629099  0.0442477  -1.422 0.155095
alcohol         0.0001217  0.0044832   0.027 0.978350
age             0.0452253  0.0121298   3.728 0.000193 ***
---
Signif. codes:  0 ‘***’ 0.001 ‘**’ 0.01 ‘*’ 0.05 ‘.’ 0.1 ‘ ’ 1

(Dispersion parameter for binomial family taken to be 1)

    Null deviance: 596.11  on 461  degrees of freedom
Residual deviance: 472.14  on 452  degrees of freedom
AIC: 492.14

Number of Fisher Scoring iterations: 5
```

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 symmetric form

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

- Here there is a linear function for each class.
- Multiclass logistic regression is also referred to as multinomial regression.

Naive Bayes Classifier

- Naive Bayes (NB) classifier especially appropriate when the dimension p of the feature space is high, making density estimation unattractive.
- Assumes that given a class $G = j$, the features X_k are independent:

$$f_j(X) = \prod_{k=1}^{p} f_{jk}(X_k).$$

- While this assumption is pretty heroic and generally not true, it significantly simplifies the estimation.
- The individual class-conditional marginal densities f_{jk} can each be estimated separately.
- If a component X_j of X is discrete, then an appropriate histogram estimate can be used. This provides a seamless way of mixing variable types in a feature vector.

Naive Bayes Classifier

- Despite these strong assumptions, NB classifiers often outperform far more sophisticated alternatives.
- Although the individual class density estimates may be biased, this bias might not hurt the posterior probabilities as much, especially near the decision regions.
- In fact, the problem may be able to withstand considerable bias for the savings in variance such a “naive” assumption earns.

Logistic Regression versus LDA

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

$$log\left(\frac{p_1(x)}{1-p_1(x)}\right) = log\left(\frac{p_1(x)}{p_2(x)}\right) = c_0 + c_1x_1 + \cdots + c_px_p$$

- 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 No	Default Yes	Status 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

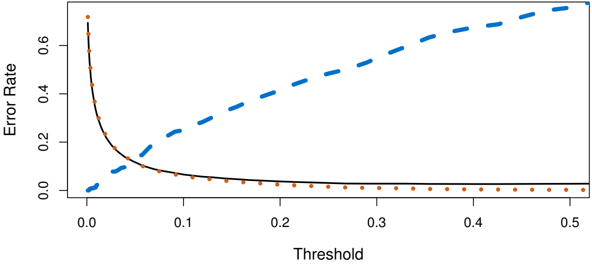
$$\widehat{Pr}(Default = Yes | Balance, Student) \geq 0.5$$

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

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

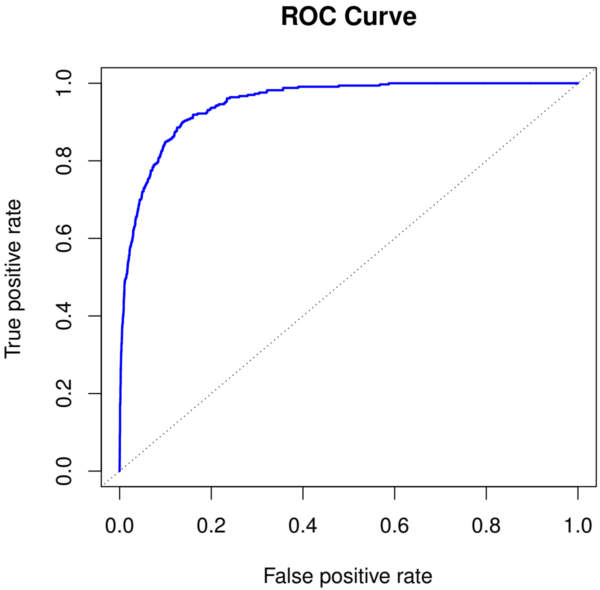
and vary *threshold*.

Varying the *threshold*



- 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



ROC Curve
True positive rate
False positive rate
0.0
0.2
0.4
0.6
0.8
1.0

Characterizing performance of classifiers

		Predicted - or Null	class + 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 $K > 2$.
- Naive Bayes is useful when p is very large.
- See Section 4.5 for some comparisons of logistic regression, LDA and KNN.