

Predictive Analytics: practical 3

The OJ data set

The OJ data set from the ISLR package contains information on which of two brands of orange juice customers purchased¹ and can be loaded using

```
data(OJ, package = "ISLR")
```

After loading the caret and nclRpredictive package

```
library("caret")
library("nclRpredictive")
```

make an initial examination of the relationships between each of the predictors and the response²

```
par(mfrow = c(4, 5), mar = c(4, 0.5, 0.5, 0.5))
plot(Purchase ~ ., data = OJ)
```

¹ The response variable is Purchase.

² Use the plot function with a model formula or the pairs function.

Initial model building

- To begin, create a logistic regression model that takes into consideration the prices of the two brands of orange juice, PriceCH and PriceMM.³
- What proportion of purchases does this model get right?
- How does this compare to if we used no model?

³ Hint: Use the train function, with method = 'glm'. Look at the help page for the data set to understand what these variables represent.

Visualising the boundary

The nclRpredictive package contains following code produces a plot of the decision boundary as seen in figure 1.

```
boundary_plot(m1, OJ$PriceCH, OJ$PriceMM, OJ$Purchase,
              xlab="Price CH", ylab="Price MM")
```

Run the boundary code above, and make sure you get a similar plot.

- What happens if we add an interaction term? How does the boundary change?
- Try adding polynomial terms.

Using all of the predictors

- Fit a logistic regression model using all of the predictors.
- Is there a problem?

We can view the most recent warning messages by using the warnings function

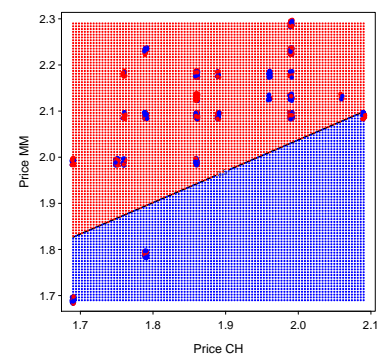


Figure 1: Examining the decision boundary for orange juice brand purchases by price.

```
warnings()
```

This suggests some rank-deficient fit problems,

- Look at the final model, you should notice that a number of parameters have not been estimated

The help page

```
?ISLR::OJ
```

gives further insight: the PriceDiff variable is a linear combination of SalePriceMM and SalePriceCH so we should remove this. In addition the StoreID and STORE variable are different encodings of the same information so we should remove one of these too. We also have DiscCH and DiscMM which are the differences between PriceCH and SalePriceCH and PriceMM and SalePriceMM respectively and ListPriceDiff is a linear combination of these prices. Removing all of these variables allows the model to be fit and all parameters to be estimated.⁴

⁴ This is to highlight that we need to understand what we have in our data.

```
OJsub = OJ[, !(colnames(OJ) %in% c("STORE", "SalePriceCH",
  "SalePriceMM", "PriceDiff", "ListPriceDiff"))]
OJsub$Store7 = as.numeric(OJsub$Store7) - 1
m_log = train(Purchase ~ ., data = OJsub, method = "glm")
```

The problem of linear combinations of predictors can be shown with this simple theoretical example. Suppose we have a response y and three predictors x_1 , x_2 and the linear combination $x_3 = (x_1 + x_2)$. On fitting a linear model we try to find estimates of the parameters in the equation

$$y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_3 (x_1 + x_2).$$

However we could just as easily rewrite this as

$$\begin{aligned} y &= \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_3 (x_1 + x_2) \\ &= \beta_0 + (\beta_1 + \beta_3) x_1 + (\beta_2 + \beta_3) x_2 \\ &= \beta_0 + \beta_1^* x_1 + \beta_2^* x_2. \end{aligned}$$

This leads to a rank-deficient model matrix, essentially we can never find the value of the β_3 due to the fact we have the linear combination of predictors.

We could achieve the same using the `caret` package function `findLinearCombos`. The function takes a model matrix as an argument. We can create such a matrix using the `model.matrix` function with our formula object

```
remove = findLinearCombos(model.matrix(Purchase ~ ., data = OJ))
```

The output list has a component called `remove` suggesting which variables should be removed to get rid of linear combinations

```
(badvar = colnames(OJ)[remove$remove])

## [1] "SalePriceMM" "SalePriceCH" "PriceDiff"
## [4] "ListPriceDiff" "STORE"

OJsub = OJ[, -remove$remove]
```

- How accurate is this new model using more predictors?]
- What are the values of sensitivity and specificity?
- What does this mean?

ROC curves

If we were interested in the area under the ROC curve, we could retrain the model using the `twoClassSummary` function as an argument to a train control object. Alternatively we can use the `pROC` package

```
library("pROC")
```

This also allows us to view the ROC curve, via

```
curve = roc(response = OJsub$Purchase,
  predictor = predict(m_log, type = "prob")[, "CH"])
## this makes CH the event of interest
plot(curve, legacy.axes = TRUE)
```

Other classification models

- Try fitting models using the other classification algorithms we have seen so far. To begin with, just have two covariates and use the `boundary_plot` function to visualise the results
- How do they compare?
- How does varying the number of nearest neighbours in a KNN affect the model fit?

The KNN algorithm described in the notes can also be used for regression problems. In this case the predicted response is the mean of the k nearest neighbours.

- Try fitting the KNN model for the regression problem in practical 1.
- How does this compare to the linear regression models?

Resampling methods

- Fit a KNN regression model to the cars2010 data set with FE as the response.
- Estimate test error using the validation set approach explored at the beginning of the chapter

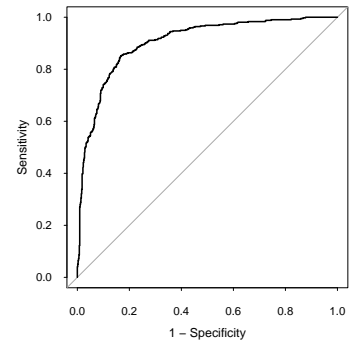


Figure 2: An example of a ROC curve for the logistic regression classifier. We can overlay ROC curves by adding the `add = TRUE` argument.

We have seen LDA, QDA, KNN and logistic regression. Tomorrow we will cover support vector machines and neural nets; we can visualise the results in the same way.

The data set can be loaded `data("FuelEconomy", package = "AppliedPredictiveModeling")`.

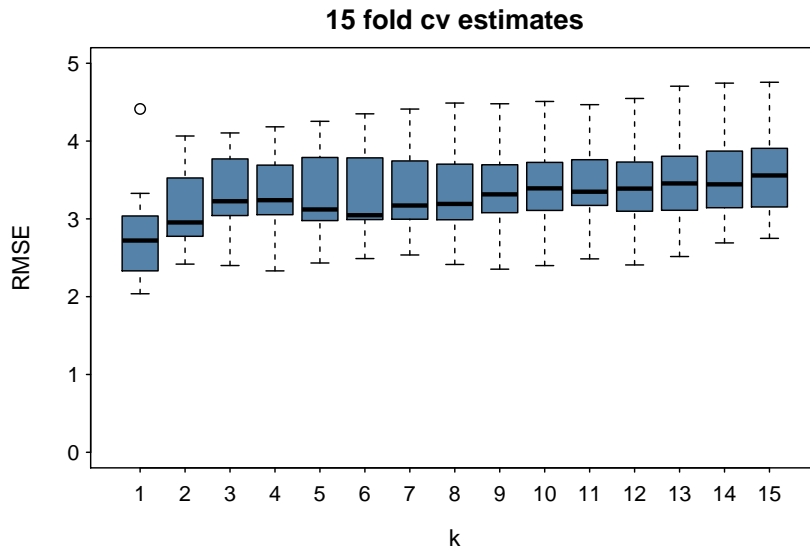


Figure 3: 15 fold cross validation estimates of RMSE in a K nearest neighbours model against number of nearest neighbours.

- Using the same validation set, estimate the performance of the k nearest neighbours algorithm for different values of k .
- Which model is chosen as the best when using the validation set approach?
- Create new `trainControl` objects to specify the use of 5 fold and 10 fold cross validation as well as bootstrapping to estimate test MSE.
- Go through the same training procedure attempting to find the best KNN model.
- How do the results vary based on the method of estimation?
- Are the conclusions always the same?

If we add the `returnResamp = "all"` argument in the `trainControl` function we can plot the resampling distributions, see figure 3.

```
tc = trainControl(method = "cv", number = 15, returnResamp = "all")
m = train(FE ~ ., data = cars2010, method = "knn", tuneGrid = data.frame(k = 1:15),
  trControl = tc)
boxplot(RMSE ~ k, data = m$resample)
```

We can overlay the information from each method using `add = TRUE`. In addition we could compare the computational cost of each of the methods. The output list from a `train` object contains timing information which can be accessed

```
m$time
```

- Which method is the most computationally efficient?

An example with more than two classes

The `Glass` data set in the `mlbench` package is a data frame containing examples of the chemical analysis of 7 different types of glass. The

goal is to be able to predict which category glass falls into based on the values of the 9 predictors.

```
data(Glass, package = "mlbench")
```

A logistic regression model is typically not suitable for more than 2 classes, so try fitting the other models using a training set that consists of 90% of the available data.

The function `createDataPartition` can be used here, see notes for a reminder.

Advanced

So far we have only used default functions and metrics to compare the performance of models, however we are not restricted to doing this. For example, training of classification models is typically more difficult when there is an imbalance in the two classes in the training set. Models trained from such data typically have high specificity but poor sensitivity or vice versa. Instead of training to maximise accuracy using data from the training set we could try to maximise according to some other criteria, namely sensitivity and specificity being as close to perfect as possible (1,1).

This section is intended for users who have a more in depth background to R programming. Attendance to the Programming in R course should be adequate background.

To add our function we need to make sure we mirror the structure of those included in `caret` already. The following code creates a new function that could be used to summarise a model

We can view a functions code by typing its name with no brackets.

```
fourStats = function(data, lev = NULL, model = NULL) {
  # This code will use the area under the ROC curve and the
  # sensitivity and specificity values from the built in
  # twoClassSummary function
  out = twoClassSummary(data, lev = levels(data$obs), model = NULL)
  # The best possible model has sensitivity of 1 and
  # specificity of 1. How far are we from that value?
  coords = matrix(c(1, 1, out["Spec"], out["Sens"]), ncol = 2,
    byrow = TRUE)
  # return the distance measure together with the output
  # from two class summary
  c(Dist = dist(coords)[1], out)
}
```

we could then use this in the `train` function

```
data(Sonar, package = "mlbench")
mod = train(Class ~ ., data = Sonar,
  method = "knn",
  # Minimize the distance to the perfect model
  metric = "Dist",
  maximize = FALSE,
  tuneLength = 20,
  trControl =
  trainControl(method = "cv", classProbs = TRUE,
    summaryFunction = fourStats))
```

The plot function

```
plot(mod)
```

will then show the profile of the resampling estimates of our chosen statistic against the tuning parameters, see figure 4.

- Have a go at writing a function that will allow a regression model to be chosen by the absolute value of the largest residual and try using it to fit a couple of models.

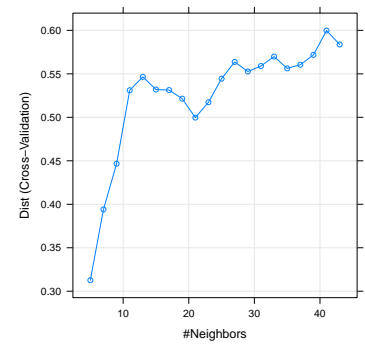


Figure 4: Plot of the distance from a perfect classifier measured by sensitivity and specificity against tuning parameter for a k nearest neighbour model.