

How to recode variables

```
dat$Species = as.factor(ifelse(iris$Species=="virginica",1,0))  
# to recode cleanly, you could use for instance:  
dat$Species = car::recode(dat$Species, "0='other'; 1='virginica'")  
# or:  
levels(dat$Species) = c("other","virginica")
```

Classification

1-. K-Nearest Neighbors (KNN) (01_Example Chp3 Exercise bank)

Note: KNN strongly depends on K chosen

- Small K: Overfitting (low bias/large variance)
- Large K: Underfitting (high bias/low variance)

So we need to select K to achieve a trade-off

Note: It is important to scale the data

```
library(class) # It has function knn
```

Splitting training & test (necessary for knn)

```
x_train, x_test, y_train, y_test
```

Passing them to knn

```
K = alpha # Number of neighbors
```

```
ko = knn(x_train, x_test, y_train, K)
```

Note: the training variable for the knn should be numeric

Note: it predicts automatically (i.e. not necessary to apply function predict)

Confusion matrix

1-. Using library(caret) (Recommended)

```
library(caret)
```

```
confusionMatrix(data = dat, reference = y.test) # they should have  
same levels to be compared!!
```

It gives us:

- 1-. Confusion Matrix
- 2-. Accuracy rate (also failure rate i.e. $1 - \text{Accuracy}$)
- 3-. A 95% CI for the **accuracy rate**
- 4-. Sensitivity and Specificity (using attribute \$class)

2-. Using table

```
tb = table(pred, y_test)  
tb  
  
# Calculating accuracy or failure rate  
sum(diag(tb))/sum(tb)  
  
# How to calculate specificity  
spec = tb[1,1]/sum(tb[,1])  
  
# Sensitivity  
sens = tb[2,2]/sum(tb[,2])
```

How to find the suitable K that maximizes the accuracy rate:

We will perform a grid search using different values of K

```
Kmax = 30 (for instance)  
acc = numeric(Kmax)  
for(k in 1:Kmax){  
  # Fitting knn  
  ko = knn(x.train, x.test, y.train, k)  
  # Building table  
  tb = table(ko, y.test)  
  # Storing error rates
```

```

    acc[k] = sum(diag(tb))/sum(tb)
}

# We can find the minimum or plot them

plot(acc, t = 'b', pch = ..., cex = ...)

or

k.best = which.max(acc)

```

2-. Logistic Regression (02_Exercise Chp 3)

Note: if Y is a binary classification Logistic Regression should be used as a REFERENCE (i.e. when Y has more than one class, doesn't work well...)

```

# How to code it

glm(interest ~., data = dat, subset = train, family = binomial(link =
logit))

```

Note: We will classify in terms of a cut-off (threshold)
(remember binomial classifies successes and failures)

Predicting with it:

1-. Obtaining a vector of TRUE/FALSE

```

Pred_vector = (predict(fit, newdata=data[-x_train,],
    type = "response") > Threshold )

```

2-. Obtaining the probability associated with each row

```

Pred_numeric = predict(fit, newdata=dat[-is,], type="response")

```

Boxplot

We can plot a boxplot to appreciate the overlap between classes. **Why?**

If there **is no overlap** we can ensure that these classes behave differently, and so they can be classified.

```
boxplot(pred_numeric, y_test)
```

Table

```
Tb = table(pred_vector , y.test)
```

We can perform a grid search to find a balance in the trade-off between sensibility and specificity (ROC CURVE ANALYSIS)

```
alpha = seq(0.05, 0.95, by = 0.05)
err = numeric(length(alpha))
for (i in 1:length(alpha)){
  pred.y = as.numeric(pred_numeric>alpha[i])
  tb = table(pred.y, y.test)
  err[i] = (1-sum(diag(tb))/sum(tb))
}
```

3-. ROC CURVE (06_exercise Chp 3 and 05_Exercise)

Useful to find a trade-off between specificity and sensitivity

1-. If alpha is small (Highly sensitive):

- \hat{P}_i is likely to be above the cut-off
- \hat{Z}_i is likely to be 1
- Also likely to detect "false alarms"

1-. If alpha is large (Highly specificity/not very sensitive):

- \hat{P}_i is likely to be below the cut-off
- \hat{Z}_i is likely to be 0

Ahead of anything we will introduce the concepts of sensitivity and specificity in terms of the confusion matrix.

- 2x2 confusion matrix (i.e. only two classes)
- 3x3 Confusion Matrix (i.e. 3 classes)

	Predicted class POSITIVE (spam 📧)	Predicted class NEGATIVE (normal 📧)	
Actual class POSITIVE (spam 📧)	TRUE POSITIVE (TP) 📧📧 320	FALSE NEGATIVE (FN) 📧📧 43	$\text{Sensitivity} = \frac{TP}{TP + FN} = \frac{320}{320 + 43} = 0.882$
Actual class NEGATIVE (normal 📧)	FALSE POSITIVE (FP) 📧📧 20	TRUE NEGATIVE (TN) 📧📧 538	$\text{Specificity} = \frac{TN}{FP + TN} = \frac{538}{20 + 538} = 0.964$

Recall: we can **calculate them** using

- ConfusionMatrix from caret
- Table

How to calculate specificity

spec = tb[1,1]/sum(tb[,1])

Sensitivity

sens = tb[2,2]/sum(tb[,2])

	Predicted class POSITIVE (spam 📧)	Predicted class NEGATIVE (ad 📧)	Predicted class NEGATIVE (normal 📧)
Actual class POSITIVE (spam 📧)	TRUE POSITIVES 📧📧 27	FALSE NEGATIVES 📧📧 286	40
Actual class NEGATIVE (ad 📧)	1	37	9
Actual class NEGATIVE (normal 📧)	FALSE POSITIVES 📧📧 5	16	TRUE NEGATIVES 500

We will focus as well in **the Area under the curve** (ROC curve of course)

Idea: the more we get 1 the better our model is

Library(pROC)

Roc.g = roc(y.test, glm.p #needs probabilities here)\$auc

plot(roc.g) # will give you the graph

How to plot it

plot(spec, sens,

xlim = c(1,0),

type = 'b')

abline(h = 1, v = 1)

4-. Linear Discriminant Analysis (LDA) (03_Exercise Chp3)

Note: Natural reference technique for classification problems WITH MORE THAN 3 CLASSES (Y RESPONSE)

First of all we need to check the assumptions of:

- **Normality**
- **Equal variance**

Library (MAAS)

Look code in exercise 03_Exercise Chpt3

How to assess normality (FOR EACH CLASS , SEPARATELY):

- 1-. Boxplot (informal):** we can assess normality here, looking if the boxplots of each class and attribute are symmetric.
- 2-. Histogram (specifically and formal):** we need to address normality here as you know: paying attention to skews, symmetry, tails..
- 3-. QQ-plots:** looking at substantial departures and if the fit a straight line..
- 4-. Shapiro Test (do not rely on these too much):** if the p-value is large is normal and if not is not normal..

How to assess equal variance

- 1-. Barlett's test:** if p is large then equal variance if p is small not equal variance. **We do not need to differentiate classes over here**

```
for(j in 1:4){print( bartlett.test(dat[,j]~dat$Species)$p.value )}
```

Note: in this exercise in particular the assumptions were not verified but we continued fitting lda...

Fitting LDA

```
lda.o = lda(Species~., data=dat)
(lda.o)
```

Gives us:

- Probability for each class
- Group means (if numerical)
- Coefficient of linear discriminant

How to get predict

```
lda.p = predict(lda.o, newdata=dat.test)
```

```
names(lda.p)
```

1. **Lda.p\$class**: contains the classes predicted
2. **Lda.p\$posterior** : contains an array of probabilities

Confusionmatrix

```
(tb = table(lda.p$class, dat.test$Species))
```

```
Accuracy = sum(diag(tb))/sum(tb)
```

```
# or
```

```
confusionMatrix(lda.p$class, reference = dat.test[, 'Species'])
```

5-. Quadratic Discriminator Analysis (QDA)

Note: more robust than LDA when LDA assumptions fail

```
# QDA:
```

```
qda.o = qda(Species~., data=dat.train)
```

```
qda.p = predict(qda.o, newdata=dat.test)
```

```
(tb = table(qda.p$class, dat.test$Species))
```

```
sum(diag(tb))/sum(tb)
```

```
# or
```

```
confusionMatrix(qda.p$class, dat.test[, 'Species'])
```

6-. Decision Trees (01_02_Exercise Chp 4)

Note: Pruning might be required in some situations since trees tend to overfit (i.e. low bias large variance)

Note: as the trees grow more, the more overfitting you will have

Library(tree)

How to code a tree

```
tree.out = tree(High~., data = dat, subset = i.train,  
                na.action = na.pass # if you need to omit NAs)
```

Summary

summary(tree.out) gives you:

1. **Misclassification** error
2. **Names of variables used**
3. Number of terminal nodes/leaf nodes

Plot a tree

```
plot(tree.out) # Will plot the edges and structure of tree  
text(tree.out, pretty = 0) # will set the names on top of each split
```

Pruning a tree

Note: we need to set a seed (if wanted) to get same results

Note: pruning reduces overfitting

Note: FUN = prune.misclass - classification

FUN = Prune.tree - regression

```
cv.CS = cv.tree(tree.out, FUN=prune.misclass)
```

names(cv.CS)

- size:

number of terminal nodes in each tree in the cost-complexity pruning sequence.


```
# - deviance:
# total deviance of each tree in the cost-complexity pruning sequence.
# - k:
# the value of the cost-complexity pruning parameter of each tree in
the sequence.
```

Plotting size vs deviance

```
plot(cv.CS$size, cv.CS$dev, t='b')
abline(v = cv.CS$size[which.min(cv.CS$dev)]) # Optimal pruning
```

Plotting k vs deviance

```
plot(cv.CS$k, cv.CS$dev, t='b')
```

How to implement the pruning :

1. use `which.min(cv.CS$dev)` to get the location of the optimum

```
opt.size = cv.CS$size[which.min(cv.CS$dev)]
```

2. retrieve the corresponding tree size
3. pass this information on to pruning function

Note: `prune.tree` for regression

```
ptree = prune.misclass(tree.out, best=opt.size)
```

And now we could plot the ptree as explained above.

Predicting with trees

We can use:

1. Class: to get the classes
2. Vector: to get the probabilities

```
tree.pred = predict(tree.out, CS.test, type="class")
```

```
tbl = table(tree.pred, High.test)
```

7-. Random Forests (04_Exercise Chp 4)

Note: random forests are important since with them we can rule out some attributes with ease. (i.e. using variable importance)

```
library(randomForest)
```

Coding a random Forest

```
rf.out = randomForest(High~., CS)
```

Predicting with a forest

We can use:

1. **Class:** vector with predicted classes
2. **Prob:** vector with probabilities

```
rf.yhat = predict(rf.out, CS, type="class")
```

Note: we can get the fitted values passing the original dataframe to the function predict

Matrix for the OOB observations: (it has the class error associated)

```
(tb.rf2 = rf.out$confusion)
```

Ex:

	No	Yes	class.error
No	209	27	0.1144068
Yes	50	114	0.3048780

Bagging

Note: Bagging can work even better than randomForests!! Remember: it decorrelates the trees (i.e. great reduction in variance , central limit theorem)

How to code and predict with bagging

```
bag.out = randomForest(High~., CS, mtry=P)
```

P: numbers of attributes to be considered usually root(ncol())

```
bag.yhat = predict(bag.out, CS, type="class")
```

Note: we can get here too the predicted values of the training set..

Variable importance (07_Exercise Chp 4):

Note: we can have an overview of which variables are the most influential for the reference (i.e. which variables should be dropped)

```
rf = randomForest(High~., data = CS)
rf$importance
```

We can **plot** it

```
varImpPlot(rf, pch=15, main="Ensemble method 1")
```

8-. Gradient Boosting (07_Exercise Chp 4)

Watch out: it needs numerical variable as response variables!!

Note: we can get even better results than randomFORESTS

Note: the main idea is rule out useless variables

Library(gbm)

How to code it:

```
gb.out = gbm(High~., data=CS,
              distribution="bernoulli", # use "gaussian" instead for
regression
              n.trees=5000, # size of the ensemble
              interaction.depth=1) # depth of the trees, 1 = stumps
```

Inspect output:

```
par(mar=c(4.5,6,1,1))
summary(gb.out, las=1) Gives you variable importance
plot(gb.out, i="Price") Graph of Price
plot(gb.out, i="ShelveLoc") Graph of ShelveLoc
```

Predict with it

```
gb.p = (predict(gb.out, newdata=CS.test, n.trees=5000, type =
"response")) > 0.5
```

Roc Analysis

Note: for gbm we do not need to pass into roc function a vector of probabilities...

```
roc.gb = roc(response=CS.test$High, predictor=gb.p)
```

USING CARET

```
library(caret)
```

Coding it

```
gb.out = train(Salary~., data=dat.train, method='gbm',  
distribution='bernoulli')
```

Note: distribution = "gaussian" if we want to use regression

Predicting

```
gb.fitted = predict(gb.out) # corresponding fitted values
```

```
gb.pred = predict(gb.out, dat.validation)
```

Confusion Matrix

```
confusionMatrix(reference=dat.validation$Salary, data=gb.pred,  
mode="everything")
```