Machine Learning for Biostatistics

Module 3

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Contents

Resampling methods

Introduction

This module will cover **bootstrap** and **cross-validation**. These are two important techniques that are useful to study sample variability, evaluate model performance and choosing *tuning* parameters in many of the methods covered in this unit.

We will switch the order presented in the book *Introduction to Statistical Learning* and start with bootstrap and then proceed to cross-validation.

By the end of this module you should be able to:

1. Be able to compute standard errors for different statistics through bootstrapping
2. Compute model performance statistics by cross-validation
3. Use cross-validation to select *tuning* parameters such as the number of neighbours in KNN

Dataset used in the examples

The file bmd.csv contains 169 records of bone densitometries (measurement of bone mineral density). The following variables were collected:

- id – patient's number
- age – patient's age
- fracture – hip fracture (fracture / no fracture)
- weight_kg – weight measured in Kg
- height_cm – height measure in cm
- waiting_time – time the patient had to wait for the densitometry (in minutes)
- bmd – bone mineral density measure in the hip

The file SBI.csv contains the records of 2349 children admitted to the emergency room with fever and tested for serious bacterial infection (sbi). The following

variables were collected:

- id – patient's number
- fever_hours – duration of the fever in hours
- age – child's age
- sex – child's sex (M / F)
- wcc – white cell count
- prevAB – previous antibiotics (Yes / No)
- sbi – serious bacterial infection (Not Applicable / UTI / Pneum / Bact)
- pct – procalcitonin
- crp – c-reactive protein

Slides

You can download the slides used in the videos for resampling methods:

- Slides

Chapter 1

Bootstrap

1.1 Introduction

Bootstrap was proposed by Efron in 1979 and it mimics the sampling process by sampling with replacement the original sample. This process replicates the sample variation and allows the calculation of standard errors. It can also be used to refine more complex machine learning algorithms, as we will see later.

From the original sample of size n, we create many (e.g. 10,000) samples of size n by sampling from the original sample with replacement. Notice that the replacement allows the same value to be included multiple times in the same sample. This is why you can create many different samples. For each of the bootstrapped samples we compute the statistics of interest. The standard deviation of all these computed statistics, is the standard error.

1.2 Readings

Read the following chapter of *An introduction to statistical learning*:

- 5.2 The Bootstrap

1.3 Practice session

Task - Confidence intervals with bootstrap

We will be using the bmd.csv dataset to plot the histogram, compute the median and 95% confidence interval for the "waiting_time"

Let's first read the data and create the variable BMI that will be used later.

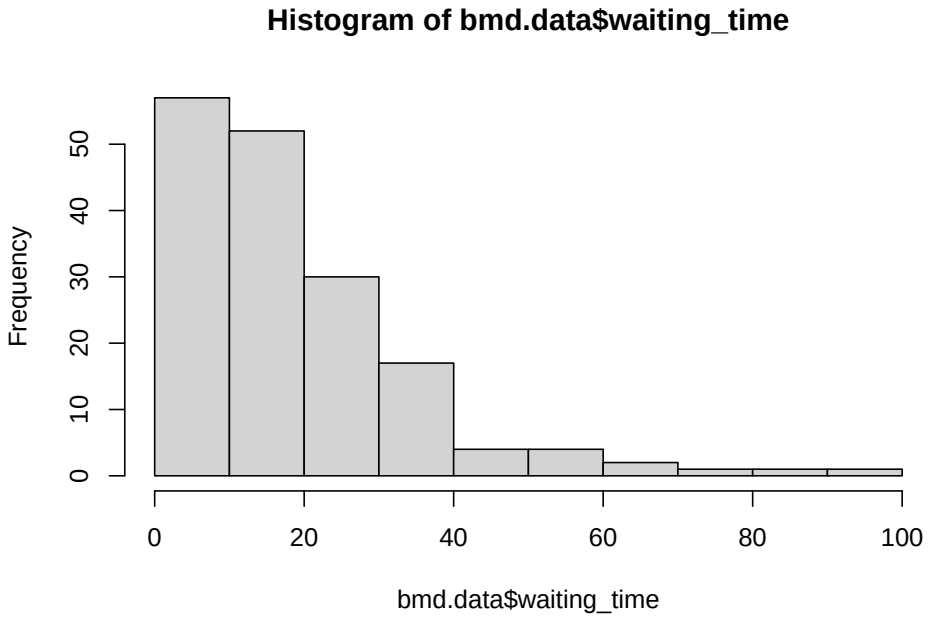
```
library(caret) #library for Machine Learning
```

```
## Warning: package 'ggplot2' was built under R version 4.3.3
```

```
library(boot)  #library for bootstrap
library(pROC)  #library for the ROC curve
library(Rmisc) #CI() function to compute conf interval
set.seed(1974)

#the option stringsAsFactors = TRUE in the command below converts
#string variables as sex into factor variables
bmd.data <- read.csv("https://www.dropbox.com/s/c6mhgatkotuze8o/bmd.csv?dl=1",
                     stringsAsFactors = TRUE)
#computes the BMI
bmd.data$bmi <- bmd.data$weight_kg / (bmd.data$height_cm/100)^2
```

Let's plot the histogram for *waiting time* and compute the median

```
hist(bmd.data$waiting_time)
```




```
median(bmd.data$waiting_time)
```

```
## [1] 14
```

And now use the function **boot()**, from the library **boot**, to bootstrap the median. We will also compute it manually

```
#using the boot function
median(bmd.data$waiting_time)
```

```
## [1] 14
```

```
samplemedian <- function(x, d) { #need to define the function to use bootstrap
  return(median(x[d]))           #d is the index for the bootstrap
}
bootresults <- boot(bmd.data$waiting_time, statistic=samplemedian, R=10000)
# get 95% confidence interval
boot.ci(bootresults, type="perc")
```

```
## BOOTSTRAP CONFIDENCE INTERVAL CALCULATIONS
## Based on 10000 bootstrap replicates
##
## CALL :
## boot.ci(boot.out = bootresults, type = "perc")
##
## Intervals :
## Level     Percentile
## 95%   (13, 18 )
## Calculations and Intervals on Original Scale
```

```
#manual bootstrap
median.bs <- NA
for (i in 1:10000){ # change to 10000
  sample.bs    <- sample(bmd.data$waiting_time, 169, replace = TRUE)
  median.bs[i] <- median(sample.bs)
}
median(median.bs)  #median (could use mean) of all the bootstrapped medians
```

```
## [1] 14
```

```
sd(median.bs)      #Std error of the median
```

```
## [1] 1.34752
```

```
quantile(median.bs, c(0.025, 0.975))  #95% empirical confidence interval
```

```
##  2.5% 97.5%
##    12    18
```

TRY IT YOURSELF:

1) Compute the mean for *waiting_time* and the usual 95% confidence interval using the **CI()** function.

See the solution code

```
#library(Rmisc) #CI() function to compute the conf interval for the mean
CI(bmd.data$waiting_time)
```

2) Compute the 95% confidence interval for the mean using the boot function

See the solution code

```
CI(bmd.data$waiting_time)

samplemean <- function(x, d) { #need to define the function to use bootstrap
  return(mean(x[d]))           #d is the index for the bootstrap
}

bootresults <- boot(bmd.data$waiting_time, statistic=samplemean, R=10000)
boot.ci(bootresults, type="perc")
```

1.4 Exercises

Solve the following exercises:

The diabetes data were provided by Hastie and Tibshirani (1990, p. 6). The observations arise from a study of the factors affecting patterns of insulin-dependent diabetes mellitus in 43 children (Sockett et al., 1987). The aim was to investigate the dependence of serum C-peptide on other factors, better to understand the patterns of residual insulin secretion.

The response, *cpep*, is the log of C-peptide concentration at diagnosis, and the selected covariates are *age*, the child's age at diagnosis, and *base*, minus their base deficit. Base deficit is a measure of acidity.

1) Calculate the Pearson correlation coefficient between *cpep* and *base* with the respective 95% confidence interval obtained by the Fisher's z-transformation (the usual way of getting the confidence interval for the Pearson's correlation)
   Note: you can use the function CIr in the "psychometric" package

2) Write your own function to compute the 95% confidence interval for the above correlation, using bootstrap.

3) Use the function *boot()* from the *boot* package to compute the 95% confidence interval through bootstrap

4) Plot the histogram with the correlations obtained in the bootstrap samples.

See the solution code

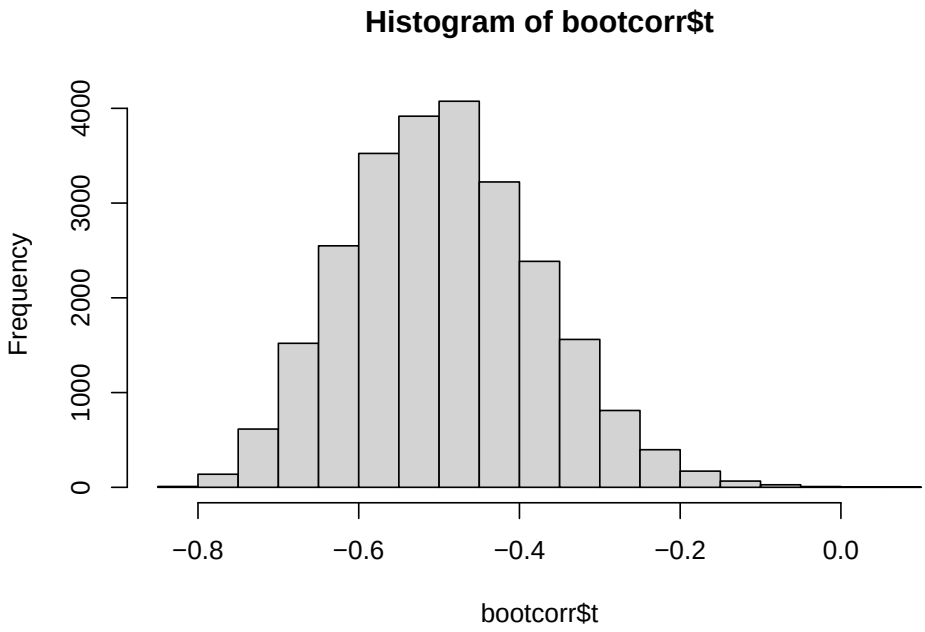
```
#install.packages("psychometric") # install package with function for
                                  # the correlation confidence interval
#install.packages("boot")          # install package for bootstrap function
```

```
library(boot)
library(psychometric)
```

```
## Warning: package 'dplyr' was built under R version 4.3.1
```

```
## Warning: package 'purrr' was built under R version 4.3.3
```

```
set.seed(1001)
myData <- read.csv("https://www.dropbox.com/s/6rc00ealjtyp3qi/diabetes.csv?dl=1")

sample.size <- dim(myData)[1] #nr of observations

#1 - the Person correlation
  cor(myData$base, myData$cpep)
  CIr( r = cor(myData$base, myData$cpep),   #conf interval using
       n = sample.size, level = .95)        # Fisher's z-transformations

#2 - Bootstrap
  n.boot   <- 25000  #choose how many bootstraps
  cor.boot <- NULL # to store the bootstrap correlations

  #manually implementing bootstrap
  for (i in 1:n.boot) {
    id.bs <- sample.int(sample.size,   #bootstrap the
                        sample.size,   #original sample
                        replace = TRUE)
    cor.boot[i] <- cor(myData[id.bs, ])[2,3]  #Compute correlation
                                              #between
   }
   quantile(cor.boot, c(0.025, 0.975))  #95% confidence interval

#3 - Using the boot() function
  sample.corr <- function(data, d) {
    return(cor(data$base[d], data$cpep[d]))   #d is the index for the bootstrap
  }

  bootcorr <- boot(myData,
                   statistic=sample.corr,
                   R=n.boot)
  # get 95% confidence interval
  boot.ci(bootcorr, type="perc")

#4 - Histogram
  #the correlations for the bootstrap samples
  #are stored in bootcorr$t
  hist(bootcorr$t)
```




```
#or
#hist(cor.boot)
```

Chapter 2

Cross-validation

2.1 Introduction

When assessing the performance of a model in the same data that was used to fit the model, we will be overestimating the model performance. A better strategy is to initially split the data and use one part to fit the model and the other one to test it. In machine learning terminology the data used to fit the model is called the **training data** and the data used to assess the model performance is called **testing data**.

The cross-validation is a repetition of the process above but each time we use a different split of the data. This will result in several measures of performance obtained in each split combination. The final performance statistics is obtained by averaging all results of the different splits.

2.2 Readings

Read the following chapter of *An introduction to statistical learning*:

- 5.1 Cross-validation

2.3 Practice session

Task 1 - Cross-validated MSE and R^2

We will be using the bmd.csv dataset to fit a linear model for *bmd* using *age*, *sex* and *bmi*, and compute the cross-validated MSE and R^2. We will fit the model with main effects using 10 times a 5-fold cross-validation.

We will use the tools from the **caret** package. This is a powerful package that wraps several methods for regression and classification: manual

```
library(e1071)
library(caret) #library for Machine Learning
library(boot)  #library for bootstrap
library(pROC)  #library for the ROC curve
library(Rmisc) #CI() function to compute the conf interval for the mean
set.seed(1974)
#the option stringsAsFactors = TRUE in the command below converts
#string variables as sex into factor variables
bmd.data <- read.csv("https://www.dropbox.com/s/c6mhgatkotuze8o/bmd.csv?dl=1",
                     stringsAsFactors = TRUE)
#computes the BMI
bmd.data$bmi <- bmd.data$weight_kg / (bmd.data$height_cm/100)^2
```

```
trC.lm <- trainControl(                  #defines the CV procedure
                method = "repeatedcv",   #multiple CV
                number = 5,              #5-fold CV
                repeats = 10)            #repeats the cross validation 10 times

#fits the linear model with CV defined above
model.lm <- train(bmd ~ age + sex + bmi,
                  data = bmd.data,
                  method = "lm",
                  trControl = trC.lm)

model.lm
```

```
## Linear Regression
##
## 169 samples
##   3 predictor
##
## No pre-processing
## Resampling: Cross-Validated (5 fold, repeated 10 times)
## Summary of sample sizes: 136, 135, 134, 135, 136, 136, ...
## Resampling results:
##
##   RMSE      Rsquared  MAE
##   0.137992  0.331976  0.1044175
##
## Tuning parameter 'intercept' was held constant at a value of TRUE
```

```
summary(model.lm$finalModel)
```

```
##
## Call:
```

```
## lm(formula = .outcome ~ ., data = dat)
##
## Residuals:
##      Min       1Q   Median       3Q      Max
## -0.38207 -0.07669 -0.00654  0.07888  0.51256
##
## Coefficients:
##               Estimate Std. Error t value Pr(>|t|)
## (Intercept)  0.6063945  0.0834051   7.270 1.36e-11 ***
## age         -0.0041579  0.0008625  -4.821 3.23e-06 ***
## sexM         0.0949602  0.0213314   4.452 1.56e-05 ***
## bmi          0.0155913  0.0024239   6.432 1.30e-09 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 0.138 on 165 degrees of freedom
## Multiple R-squared:  0.3254, Adjusted R-squared:  0.3131
## F-statistic: 26.53 on 3 and 165 DF,  p-value: 4.677e-14
```

TRY IT YOURSELF:

1) Refit the same model and evaluate the MSE and R^2 using leave one out (**method = "LOOCV"**)

See the solution code

```
trC.lm.loocv <- trainControl(
                 method = "LOOCV") # leave on out CV

model.lm2 <- train(bmd ~ age + sex + bmi,
                data = bmd.data, method = "lm",
                trControl = trC.lm.loocv)

model.lm2
summary(model.lm2$finalModel)
```

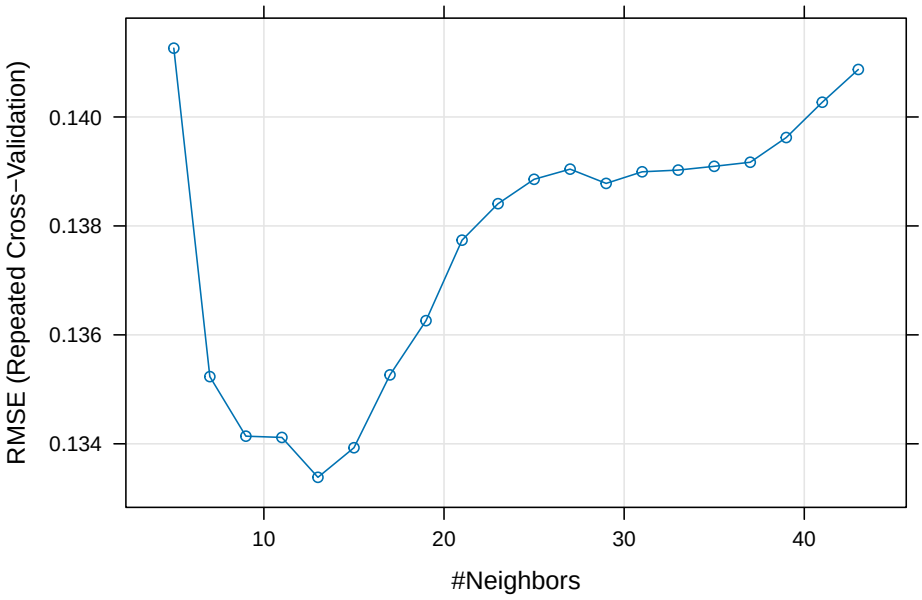
2) Fit a k nearest neighbour regression for BMD using AGE, SEX and BMI, and choose the k (number of neighbours) by 10-fold cross-validation repeated 10 times. Also, obtain the MSE and R^2.

NOTE1: you need the make sure all the predictors are in the same scale. You can either use the 'scale() function or add `preProcess = c("center","scale")` to the `train()` function.

NOTE2: you can either use `tuneLength = 20` to define the number of neighbours or `tuneGrid=expand.grid(k=seq(1,43,2))`

See the solution code

```
trC.knn <- trainControl(
                  method = "repeatedcv", # multiple CV
                  number = 10,  #10-fold CV
                  repeats = 10)

model.knn <- train(bmd ~ age + sex + bmi,
                 data = bmd.data, method = "knn",
                 trControl = trC.knn,
                 preProcess = c("center","scale"),
                 tuneLength = 20)   #instead of tuneLength, we could have
                                    #used tuneGrid=expand.grid(k=1:40)
# Model Summary
model.knn
model.knn$results

#results in each cv-fold
model.knn$resample
plot(model.knn)
```



Task 2 - ROC cross-validation

We want to fit the following model **logit(fracture)** ~ **age + sex + bmi +bmd** and assess its performance by computing the area under the ROC curve using cross-validation

```
#caret does not like the category "no fracture"
#because of the space
#We are creating a new label for the categories
bmd.data$fract <- ifelse (bmd.data$fracture =="fracture", "F", "NF")
bmd.data$fract <- as.factor(bmd.data$fract)

trC <- trainControl(
            method = "cv",     #just 1 CV
            number = 10,       #10-fold CV
            classProbs = TRUE,
            summaryFunction = twoClassSummary,
            savePred =TRUE)  #to be used in the confusion matrix

model.LR <- train(fract ~ age + sex + bmi + bmd ,
                data = bmd.data, method = "glm",
                family="binomial",
                trControl = trC,
                metric = "ROC")


# Model Summary
model.LR
```

```
## Generalized Linear Model
##
## 169 samples
##   4 predictor
##   2 classes: 'F', 'NF'
##
## No pre-processing
## Resampling: Cross-Validated (10 fold)
## Summary of sample sizes: 152, 152, 152, 152, 152, 152, ...
## Resampling results:
##
##   ROC        Sens  Spec
##   0.8980303  0.72  0.9166667
```

```
model.LR$results
```

```
##   parameter       ROC Sens      Spec     ROCSD    SensSD     SpecSD
## 1      none 0.8980303 0.72 0.9166667 0.1362458 0.1686548 0.09622504
```

```
#results in each cv-fold
model.LR$resample
```

```
##          ROC Sens      Spec Resample
## 1  0.9500000  0.6 1.0000000   Fold01
```

```
## 2  0.7500000  0.6 0.9166667   Fold02
## 3  0.9666667  0.6 0.9166667   Fold03
## 4  0.9000000  0.8 1.0000000   Fold04
## 5  0.5666667  0.6 0.6666667   Fold05
## 6  0.9666667  1.0 0.9166667   Fold06
## 7  0.9636364  0.6 1.0000000   Fold07
## 8  0.9833333  0.8 0.9166667   Fold08
## 9  0.9333333  0.6 0.9166667   Fold09
## 10 1.0000000  1.0 0.9166667   Fold10
```

```
#Confusion matrix cross-validated
confusionMatrix(model.LR)
```

```
## Cross-Validated (10 fold) Confusion Matrix
##
## (entries are percentual average cell counts across resamples)
##
##           Reference
## Prediction    F   NF
##         F  21.3  5.9
##         NF  8.3 64.5
##
##  Accuracy (average) : 0.858
```

```
#Confusion matrix for the final model
pred.LR  <- predict(model.LR)
confusionMatrix(data=pred.LR, reference=bmd.data$fract)
```

```
## Confusion Matrix and Statistics
##
##           Reference
## Prediction   F  NF
##         F   35   9
##         NF  15 110
##
##                Accuracy : 0.858
##                  95% CI : (0.7961, 0.9068)
##     No Information Rate : 0.7041
##     P-Value [Acc > NIR] : 2.272e-06
##
##                   Kappa : 0.6469
##
##  Mcnemar's Test P-Value : 0.3074
##
##             Sensitivity : 0.7000
##             Specificity : 0.9244
##          Pos Pred Value : 0.7955
```

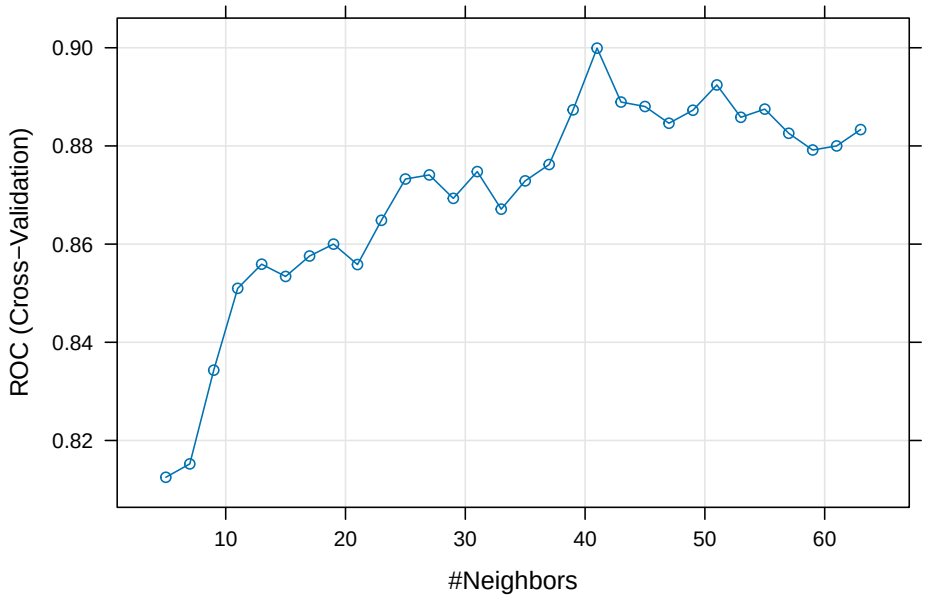
```
##          Neg Pred Value : 0.8800
##              Prevalence : 0.2959
##          Detection Rate : 0.2071
##    Detection Prevalence : 0.2604
##       Balanced Accuracy : 0.8122
##
##        'Positive' Class : F
##
```

TRY IT YOURSELF

1) Use the KNN algorithm to predict **fracture** based on the same variables of the logistic model above, by choosing the k using cross-validation and compute the area under the ROC.

See the solution code

```
trC.knn <- trainControl(
            method = "cv",     #just 1 CV
            number = 10,       #10-fold CV
            classProbs = TRUE,
            summaryFunction = twoClassSummary,
            savePred =TRUE)  #to be used in the confusion matrix

model.knn <- train(fract ~ age + sex + bmi + bmd ,
                data = bmd.data, method = "knn",
                trControl = trC.knn,
                tuneLength = 30,
                preProcess = c("center","scale"),
                metric = "ROC")


# Model Summary
model.knn
plot(model.knn)
```




```
model.knn$results

#results in each cv-fold
model.knn$resample

#Confusion matrix cross-validated
confusionMatrix(model.knn)

#Confusion matrix for the final model
pred.knn  <- predict(model.knn)
confusionMatrix(data=pred.knn, reference=bmd.data$fract)
```

Task 3 - Classification

Read the dataset SBI.csv and create a prediction model for the outcome "sbi" using "age", "pct", "crp", "wcc" and "fever_hours" as predictors (you can read.

Let's first read the data in

```
sbi.data     <-
  read.csv("https://www.dropbox.com/s/wg32uj43fsy9yvd/SBI.csv?dl=1",
           stringsAsFactors = TRUE)
summary(sbi.data)
```

```
##        X                id          fever_hours          age        sex
##  Min.   :   1.0   Min.   :   495   Min.   :  0.00   Min.   :0.010   F:1013
##  1st Qu.: 587.8   1st Qu.:133039   1st Qu.: 24.00   1st Qu.:0.760   M:1335
##  Median :1174.5   Median :160016   Median : 48.00   Median :1.525
```

```
##  Mean   :1174.5   Mean   :153698   Mean   :  80.06   Mean   :1.836
##  3rd Qu.:1761.2   3rd Qu.:196030   3rd Qu.:  78.00   3rd Qu.:2.752
##  Max.   :2348.0   Max.   :229986   Max.   :3360.00   Max.   :4.990
##       wcc          prevAB                sbi            pct
##  Min.   : 0.2368   No :1370   Bact         :  34   Min.   :  0.00865
##  1st Qu.: 7.9000   Yes: 978   NotApplicable:1752   1st Qu.:  0.16000
##  Median :11.6000              Pneu         : 251   Median :  0.76000
##  Mean   :12.6431              UTI          : 311   Mean   :  3.74354
##  3rd Qu.:16.1000                                   3rd Qu.:  4.61995
##  Max.   :58.7000                                   Max.   :156.47000
##       crp
##  Min.   :  0.00
##  1st Qu.: 11.83
##  Median : 30.97
##  Mean   : 48.41
##  3rd Qu.: 66.20
##  Max.   :429.90
```

We will try different approaches starting with linear discriminant analysis

```
trCtrl.lda <- trainControl(method = "repeatedcv",
                           number = 10,  #10-fold CV
                           repeats = 10,
                           classProbs = TRUE,
                           savePredictions = TRUE)
model.lda <- train(sbi ~ crp+pct+age+wcc+fever_hours,
                   data=sbi.data,
                   method="lda",
                   trControl = trCtrl.lda,
                   metric="Accuracy" )

model.lda$results
```

```
##   parameter  Accuracy      Kappa AccuracySD    KappaSD
## 1      none 0.7478769 0.09311667 0.01071987 0.04376718
```

```
confusionMatrix(predict(model.lda), sbi.data$sbi)
```

```
## Confusion Matrix and Statistics
##
##                Reference
## Prediction      Bact NotApplicable Pneu  UTI
##   Bact             5             5    7    6
##   NotApplicable   28          1722  238  273
##   Pneu             0             3    2    1
##   UTI              1            22    4   31
##
## Overall Statistics
```

```
##
##                Accuracy : 0.7496
##                  95% CI : (0.7315, 0.767)
##     No Information Rate : 0.7462
##     P-Value [Acc > NIR] : 0.3623
##
##                   Kappa : 0.0985
##
##  Mcnemar's Test P-Value : <2e-16
##
## Statistics by Class:
##
##                      Class: Bact Class: NotApplicable Class: Pneu Class: UTI
## Sensitivity             0.147059              0.98288   0.0079681    0.09968
## Specificity             0.992221              0.09564   0.9980925    0.98675
## Pos Pred Value          0.217391              0.76161   0.3333333    0.53448
## Neg Pred Value          0.987527              0.65517   0.8936806    0.87773
## Prevalence              0.014480              0.74617   0.1068995    0.13245
## Detection Rate          0.002129              0.73339   0.0008518    0.01320
## Detection Prevalence    0.009796              0.96295   0.0025554    0.02470
## Balanced Accuracy       0.569640              0.53926   0.5030303    0.54321
```

Now, let's try the logistic regression

```
trCtrl.lr <- trainControl(method = "repeatedcv",
                          number = 10,  #10-fold CV
                          repeats = 10,
                          classProbs = TRUE,
                          savePredictions = TRUE)
model.lr <- train(sbi ~ crp+pct+age+wcc+fever_hours,
                  data=sbi.data,
                  method="multinom",
                  trControl = trCtrl.lr,
                  tuneLength=1)
```

```
model.lr$results
```

```
##   decay  Accuracy      Kappa  AccuracySD    KappaSD
## 1     0 0.7516195 0.09927548 0.008932933 0.04049479
```

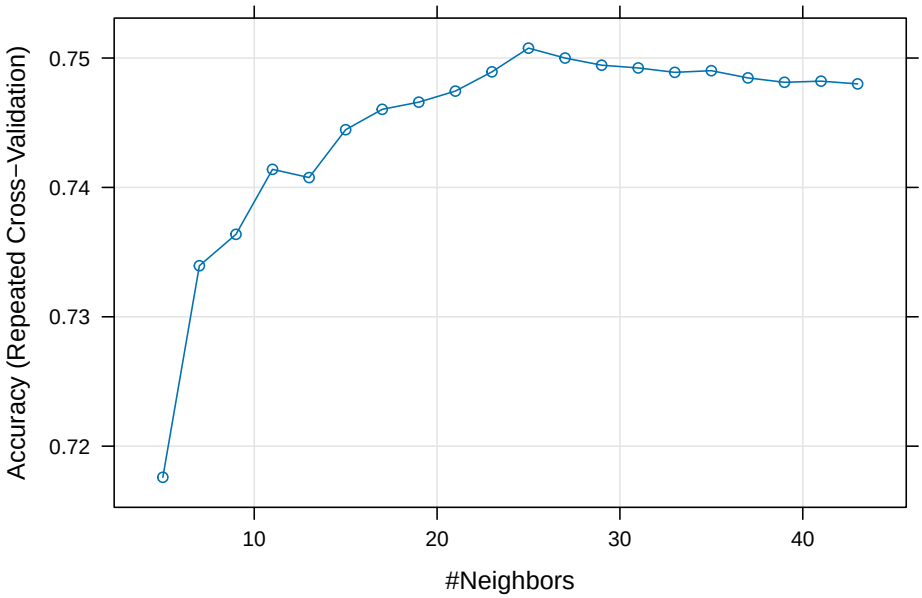
```
confusionMatrix(predict(model.lr), sbi.data$sbi)
```

```
## Confusion Matrix and Statistics
##
##                Reference
## Prediction      Bact NotApplicable Pneu  UTI
##   Bact             0             1    1    0
##   NotApplicable   27          1727  241  270
```

```
##   Pneu             1             2    2    4
##   UTI              6            22    7   37
##
## Overall Statistics
##
##                Accuracy : 0.7521
##                  95% CI : (0.7341, 0.7695)
##     No Information Rate : 0.7462
##     P-Value [Acc > NIR] : 0.2618
##
##                   Kappa : 0.101
##
##  Mcnemar's Test P-Value : <2e-16
##
## Statistics by Class:
##
##                      Class: Bact Class: NotApplicable Class: Pneu Class: UTI
## Sensitivity            0.0000000              0.98573   0.0079681    0.11897
## Specificity            0.9991357              0.09732   0.9966619    0.98282
## Pos Pred Value         0.0000000              0.76247   0.2222222    0.51389
## Neg Pred Value         0.9855072              0.69880   0.8935442    0.87961
## Prevalence             0.0144804              0.74617   0.1068995    0.13245
## Detection Rate         0.0000000              0.73552   0.0008518    0.01576
## Detection Prevalence   0.0008518              0.96465   0.0038330    0.03066
## Balanced Accuracy      0.4995678              0.54152   0.5023150    0.55089
```

And finally, knn.

```
trCtrl.knn <- trainControl(method = "repeatedcv",
                           number = 10,  #10-fold CV
                           repeats = 10,
                           classProbs = TRUE,
                           savePredictions = TRUE)
model.knn <- train(sbi ~ crp+pct+age+wcc+fever_hours,
                   data=sbi.data,
                   method="knn",
                   trControl = trCtrl.knn,
                   preProcess = c("center","scale"),
                   tuneLength=20)

plot(model.knn)
```




```
model.knn
```

```
## k-Nearest Neighbors
##
## 2348 samples
##    5 predictor
##    4 classes: 'Bact', 'NotApplicable', 'Pneu', 'UTI'
##
## Pre-processing: centered (5), scaled (5)
## Resampling: Cross-Validated (10 fold, repeated 10 times)
## Summary of sample sizes: 2114, 2114, 2113, 2114, 2113, 2112, ...
## Resampling results across tuning parameters:
##
##   k   Accuracy   Kappa
##    5  0.7175953  0.12171412
##    7  0.7339458  0.12278852
##    9  0.7363738  0.10479303
##   11  0.7413980  0.10979312
##   13  0.7407610  0.09426706
##   15  0.7444609  0.09148660
##   17  0.7460360  0.08657437
##   19  0.7465912  0.08561247
##   21  0.7474448  0.08364397
##   23  0.7489325  0.08502779
##   25  0.7507663  0.08610948
##   27  0.7500005  0.07935699
##   29  0.7494477  0.07417419
```

```
##   31  0.7492342  0.07113888
##   33  0.7488938  0.06312317
##   35  0.7490229  0.05901425
##   37  0.7484635  0.05259630
##   39  0.7481255  0.04619287
##   41  0.7482135  0.04377731
##   43  0.7480011  0.04061429
##
## Accuracy was used to select the optimal model using the largest value.
## The final value used for the model was k = 25.
```

```
confusionMatrix(predict(model.knn), sbi.data$sbi)
```

```
## Confusion Matrix and Statistics
##
##                Reference
## Prediction      Bact NotApplicable Pneu  UTI
##   Bact             0             1    0    0
##   NotApplicable   29          1727  244  264
##   Pneu             0             1    2    1
##   UTI              5            23    5   46
##
## Overall Statistics
##
##                Accuracy : 0.756
##                  95% CI : (0.7381, 0.7732)
##     No Information Rate : 0.7462
##     P-Value [Acc > NIR] : 0.1429
##
##                   Kappa : 0.1154
##
##  Mcnemar's Test P-Value : NA
##
## Statistics by Class:
##
##                      Class: Bact Class: NotApplicable Class: Pneu Class: UTI
## Sensitivity            0.0000000              0.98573   0.0079681    0.14791
## Specificity            0.9995678              0.09899   0.9990463    0.98380
## Pos Pred Value         0.0000000              0.76281   0.5000000    0.58228
## Neg Pred Value         0.9855134              0.70238   0.8937713    0.88321
## Prevalence             0.0144804              0.74617   0.1068995    0.13245
## Detection Rate         0.0000000              0.73552   0.0008518    0.01959
## Detection Prevalence   0.0004259              0.96422   0.0017036    0.03365
## Balanced Accuracy      0.4997839              0.54236   0.5035072    0.56585
```

2.4 Exercises

1) What are the advantages and disadvantages of k-fold cross- validation relative to the validation set approach? And LOOCV?

See the solution

The validation set approach is conceptually simple and easily implemented as you are simply partitioning the existing training data into two sets. However, there are two drawbacks: (1.) the estimate of the test error rate can be highly variable depending on which observations are included in the training and validation sets. (2.) the validation set error rate may tend to overestimate the test error rate for the model fit on the entire data set.

LOOCV is a special case of k-fold cross-validation with $k = n$. Thus, LOOCV is the most computationally intense method since the model must be fit n times. Also, LOOCV has higher variance, but lower bias, than k-fold CV.

2) Load the dataset *PimaIndiansDiabetes* in the package *mlbench* (you might need to install this package). This dataset consists of 768 observations of 9 variables: 8 variables which will be used as model predictors (number of times pregnant, plasma glucose concentration, diastolic blood pressure (mm Hg), triceps skin fold thickness (in mm), 2-hr serum insulin measure, body mass index, a diabetes pedigree function, and age) and 1 outcome variable (whether or not the patient has diabetes).
Use the KNN algorithm to predict diabetes using all the predictors available. Choose the number of neighbours using cross-validation

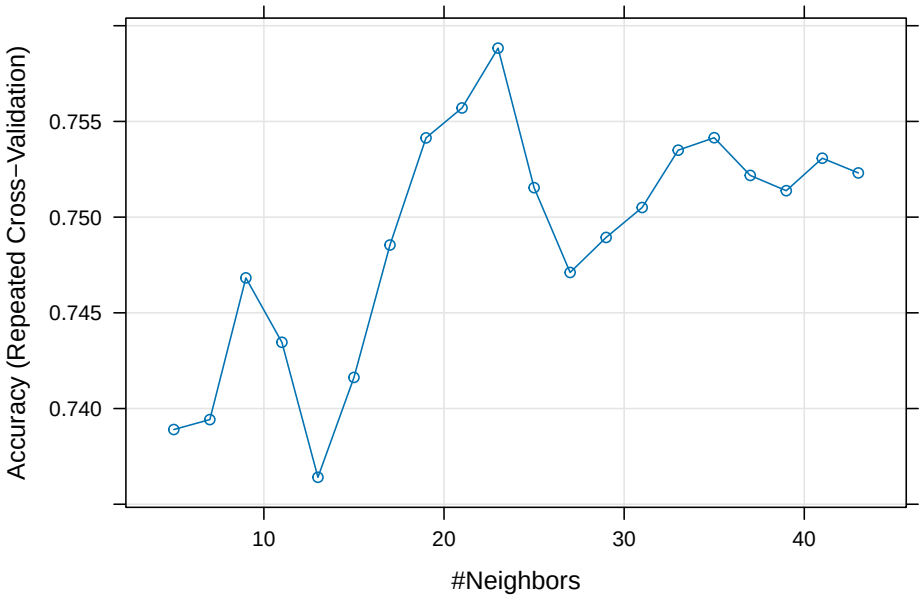
See the solution code

```
#install.packages("mlbench")
library(mlbench)
library(caret)
library(class)
set.seed(1999)

data(PimaIndiansDiabetes)


trCtrl.knn.diab <- trainControl(method = "repeatedcv",
                           number = 10,  #10-fold CV
                           repeats = 10,
                           classProbs = TRUE,
                           savePredictions = TRUE)

model.knn.diab  <- train(diabetes ~ .,
                   data = PimaIndiansDiabetes,
                   method="knn",
                   trControl = trCtrl.knn.diab,
```

```
                    tuneLength=20,
                    preProcess = c("center","scale"))
model.knn.diab
```

```
## k-Nearest Neighbors
##
## 768 samples
##   8 predictor
##   2 classes: 'neg', 'pos'
##
## Pre-processing: centered (8), scaled (8)
## Resampling: Cross-Validated (10 fold, repeated 10 times)
## Summary of sample sizes: 691, 691, 691, 691, 691, 692, ...
## Resampling results across tuning parameters:
##
##   k   Accuracy   Kappa
##    5  0.7389029  0.4053295
##    7  0.7394224  0.4047962
##    9  0.7468267  0.4180659
##   11  0.7434604  0.4096912
##   13  0.7364081  0.3904171
##   15  0.7416251  0.3977650
##   17  0.7485424  0.4127157
##   19  0.7541388  0.4228489
##   21  0.7557040  0.4227617
##   23  0.7588295  0.4297422
##   25  0.7515396  0.4093277
##   27  0.7471087  0.3962969
##   29  0.7489388  0.3985084
##   31  0.7505024  0.4013708
##   33  0.7534979  0.4066469
##   35  0.7541490  0.4071122
##   37  0.7521787  0.4003432
##   39  0.7513807  0.3975556
##   41  0.7530776  0.3995618
##   43  0.7523086  0.3964125
##
## Accuracy was used to select the optimal model using the largest value.
## The final value used for the model was k = 23.
```

```
plot(model.knn.diab)
```


Accuracy (Repeated Cross−Validation)
0.740
0.745
0.750
0.755
10
20
30
40
#Neighbors