# Performance Assessment

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# 1 Create data partitions

```
library(caret)
data("RailTrail")
set.seed(4711)
```

## 1.1 Train/Test-split

```
part = createDataPartition(RailTrail$volume, times = 2, p = 2/3)
part

## $Resample1
## [1] 1 3 5 7 8 9 10 11 12 14 15 16 17 18 19 20 21 23 24 25 26 27 28 29 30
## [26] 34 35 39 41 42 43 45 46 47 48 49 50 51 52 53 54 56 57 58 59 61 62 65 66 67
## [51] 68 70 71 73 75 79 80 84 87 88 89 90
##
## $Resample2
## [1] 2 3 4 5 6 7 8 9 10 11 15 17 18 20 21 22 25 27 28 29 30 31 33 34 35
## [26] 36 38 39 40 42 43 44 45 46 47 48 49 52 56 57 58 60 66 67 68 69 70 71 72 73
## [51] 74 75 77 78 79 80 81 82 83 84 87 88

train = RailTrail[part$Resample1,]
test = RailTrail[-part$Resample1,]
```

#### 1.2 Cross-Validation

createFolds(RailTrail\$volume, k = 5)

```
## $Fold1
## [1] 4 13 16 17 25 28 31 32 34 38 51 52 53 57 59 60 65 85
##
## $Fold2
## [1] 2 12 15 21 22 27 30 39 40 49 55 66 69 80 81 84 86
##
## $Fold3
## [1] 3 5 6 8 11 19 24 37 44 47 58 61 63 64 75 77 79 82 83 87
## $Fold4
## [1] 7 9 10 18 20 35 43 45 46 48 50 54 62 68 70 71 78 88 90
##
## $Fold5
## [1] 1 14 23 26 29 33 36 41 42 56 67 72 73 74 76 89
With repetitions:
createMultiFolds(RailTrail$volume, k = 2, times = 3)
## $Fold1.Rep1
## [1] 2 3 6 7 8 13 14 17 19 23 24 25 26 31 33 34 35 37 38 43 47 51 53 54 56
## [26] 58 62 63 67 68 69 71 72 73 74 75 76 80 81 82 83 84 86 89
## $Fold2.Rep1
## [1] 1 4 5 9 10 11 12 15 16 18 20 21 22 27 28 29 30 32 36 39 40 41 42 44 45
## [26] 46 48 49 50 52 55 57 59 60 61 64 65 66 70 77 78 79 85 87 88 90
##
## $Fold1.Rep2
## [1] 1 2 3 13 15 16 19 21 24 25 27 28 34 36 37 38 40 41 42 47 48 50 53 56 57
## [26] 58 59 60 63 64 65 66 68 71 72 73 74 80 82 84 85 86 87 88
## $Fold2.Rep2
## [1] 4 5 6 7 8 9 10 11 12 14 17 18 20 22 23 26 29 30 31 32 33 35 39 43 44
## [26] 45 46 49 51 52 54 55 61 62 67 69 70 75 76 77 78 79 81 83 89 90
##
## $Fold1.Rep3
## [1] 2 4 8 13 14 17 18 20 21 25 27 28 29 31 32 34 38 41 42 44 45 47 48 49 51
## [26] 53 54 56 57 58 59 60 63 64 65 68 71 72 74 75 77 82 84 90
##
## $Fold2.Rep3
## [1] 1 3 5 6 7 9 10 11 12 15 16 19 22 23 24 26 30 33 35 36 37 39 40 43 46
## [26] 50 52 55 61 62 66 67 69 70 73 76 78 79 80 81 83 85 86 87 88 89
```

#### 1.3 Bootstrap

```
createResample(RailTrail$volume, times = 3)
```

```
## $Resample1
              1 2 3 4 5 5 6 7 7 9 10 11 11 11 12 14 15 17 19 20 22 23 24
  [1]
       1 1
## [26] 25 26 29 30 30 31 31 32 33 33 35 35 36 39 39 40 40 40 41 43 45 46 47 48
## [51] 49 50 51 51 51 54 54 54 55 56 59 59 61 61 64 64 67 68 68 72 73 74 76 76 76
## [76] 76 77 78 80 81 82 83 83 83 83 86 86 87 88 90
##
## $Resample2
## [1] 3 4 5
                 6 6 7 9 9 12 15 16 18 18 19 20 22 23 24 25 26 27 29 29 31 32
## [26] 34 35 36 36 41 41 41 42 42 43 44 45 45 46 46 47 47 48 48 51 52 52 53 56 57
## [51] 58 58 59 60 60 61 61 62 62 63 63 64 65 65 68 68 70 70 70 70 70 71 71 74 76
## [76] 77 78 79 80 81 81 82 82 83 85 85 86 87 88 88
## $Resample3
       1 1 1 1 3 4 6 6 9 9 11 11 15 15 16 16 17 18 18 19 19 19 20 21 21
## [26] 22 25 25 25 28 29 30 30 30 31 33 34 35 36 39 40 42 42 42 42 45 47 48 48 49
## [51] 51 51 51 52 53 53 54 54 55 55 55 56 56 57 57 58 59 60 61 61 64 65 65 68 69
## [76] 72 73 74 74 75 75 75 77 77 77 82 85 86 87 87
```

# 2 Regression

## 2.1 Create train/test samples

```
part = createDataPartition(RailTrail$volume, times = 2, p = 2/3)
train = RailTrail[part$Resample1,]
test = RailTrail[-part$Resample1,]
```

#### 2.2 Train

```
model_lm = lm(volume ~ hightemp, data = train)
model_knnreg = gknn(volume ~ hightemp, data = train)
```

#### 2.3 Predict test set data

```
pred_lm = predict(model_lm, test)
pred_knnreg = predict(model_knnreg, test)
```

#### 2.4 Evaluate

```
rbind(lm = postResample(pred_lm, test$volume),
    knn = postResample(pred_knnreg, test$volume))
```

```
## RMSE Rsquared MAE
## lm 126.5919 0.18265927 93.62582
## knn 154.8042 0.06529704 117.16369
```

# 3 Classification

## 3.1 Create train/test samples

Bootstrap

```
ind = createResample(iris$Species, times = 1)
train = iris[ind$Resample1,] ## 150 cases!
test = iris[-ind$Resample1,] ## only those not in train set
nrow(train)

## [1] 150

nrow(test)
## [1] 60
```

#### 3.2 Train models

```
model_nb = naiveBayes(Species ~ ., data = train)
model_knn = gknn(Species ~ ., data = train)
```

#### 3.3 Predict test set data

```
pred_nb = predict(model_nb, test)
pred_knn = predict(model_knn, test, type = "class")
```

#### 3.4 Evaluate

```
rbind(nb = postResample(pred_nb, test$Species),
     knn = postResample(pred_knn, test$Species))

## Accuracy Kappa
## nb 0.9333333 0.8984772
## knn 0.9333333 0.8984772
```

## 4 Performance Evaluation for Classifiers

## 4.1 Confusion Matrix for true/predicted values

```
confusionMatrix(pred_knn, test$Species, mode = "prec_recall")
## Confusion Matrix and Statistics
##
               Reference
## Prediction
                setosa versicolor virginica
                    22
##
     setosa
                                 0
                     0
                                13
##
     versicolor
                                           1
##
     virginica
                     0
                                 3
                                          21
## Overall Statistics
##
                  Accuracy: 0.9333
                    95% CI : (0.838, 0.9815)
##
##
       No Information Rate: 0.3667
##
       P-Value [Acc > NIR] : < 2.2e-16
##
##
                     Kappa: 0.8985
##
   Mcnemar's Test P-Value : NA
##
## Statistics by Class:
##
##
                        Class: setosa Class: versicolor Class: virginica
## Precision
                                1.0000
                                                  0.9286
                                                                    0.8750
                                1.0000
                                                  0.8125
                                                                    0.9545
## Recall
## F1
                                1.0000
                                                  0.8667
                                                                    0.9130
## Prevalence
                                0.3667
                                                  0.2667
                                                                    0.3667
## Detection Rate
                                0.3667
                                                   0.2167
                                                                    0.3500
## Detection Prevalence
                                0.3667
                                                  0.2333
                                                                    0.4000
## Balanced Accuracy
                                1.0000
                                                  0.8949
                                                                    0.9378
confusionMatrix(pred_knn, test$Species)
## Confusion Matrix and Statistics
##
##
               Reference
## Prediction
                setosa versicolor virginica
##
     setosa
                    22
                                 0
##
     versicolor
                     0
                                13
                                           1
                     0
                                          21
                                 3
##
     virginica
##
## Overall Statistics
##
##
                  Accuracy: 0.9333
##
                    95% CI : (0.838, 0.9815)
```

##

No Information Rate: 0.3667

```
P-Value [Acc > NIR] : < 2.2e-16
##
##
##
                     Kappa: 0.8985
##
##
   Mcnemar's Test P-Value : NA
##
## Statistics by Class:
##
##
                         Class: setosa Class: versicolor Class: virginica
## Sensitivity
                                1.0000
                                                   0.8125
                                                                     0.9545
## Specificity
                                1.0000
                                                   0.9773
                                                                     0.9211
## Pos Pred Value
                                1.0000
                                                   0.9286
                                                                     0.8750
## Neg Pred Value
                                1.0000
                                                   0.9348
                                                                     0.9722
## Prevalence
                                                                     0.3667
                                0.3667
                                                   0.2667
## Detection Rate
                                0.3667
                                                   0.2167
                                                                     0.3500
## Detection Prevalence
                                0.3667
                                                   0.2333
                                                                     0.4000
## Balanced Accuracy
                                1.0000
                                                   0.8949
                                                                     0.9378
```

## 4.2 Confusion matrix for a given fourfold-table

```
pred = c(T, T, F, F, T, T, F, F, T, F)
true = c(T, T, F, F, F, F, T, T, F)
tab = table(pred, true)
confusionMatrix(tab, positive = "TRUE")
```

```
## Confusion Matrix and Statistics
##
##
          true
##
  pred
           FALSE TRUE
##
     FALSE
               4
                    1
               2
##
     TRUE
                    3
##
##
                  Accuracy: 0.7
##
                    95% CI: (0.3475, 0.9333)
##
       No Information Rate: 0.6
##
       P-Value [Acc > NIR] : 0.3823
##
##
                     Kappa : 0.4
##
##
    Mcnemar's Test P-Value : 1.0000
##
##
               Sensitivity: 0.7500
               Specificity: 0.6667
##
##
            Pos Pred Value: 0.6000
##
            Neg Pred Value: 0.8000
##
                Prevalence: 0.4000
##
            Detection Rate: 0.3000
##
      Detection Prevalence: 0.5000
##
         Balanced Accuracy: 0.7083
##
##
          'Positive' Class : TRUE
##
```

## 5 Calibration plots for probability-based classifiers

#### 5.1 Bank marketing data

Bank data: Response to marketing campaign for some bank product (term deposit)

```
dat = read.table("bank.csv", sep = ";", header = TRUE, stringsAsFactors = TRUE)
head(dat)
##
                 job marital education default balance housing loan
                                                                       contact day
     age
## 1
      30
          unemployed married
                                primary
                                                    1787
                                                              no
                                                                   no cellular
## 2
      33
            services married secondary
                                                    4789
                                                             yes
                                                                  yes cellular
                                             no
## 3
      35
          management single
                              tertiary
                                             no
                                                    1350
                                                             yes
                                                                   no cellular
## 4
      30
          management married tertiary
                                                    1476
                                                                  yes
                                                                       unknown
                                                                                  3
                                             no
                                                             yes
                                                                                  5
      59 blue-collar married secondary
                                                             yes
                                                                       unknown
          management single
                              tertiary
                                             no
                                                     747
                                                              no
                                                                   no cellular
##
     month duration campaign pdays previous poutcome
## 1
       oct
                 79
                           1
                                 -1
                                           0
                                              unknown no
## 2
                220
                                339
       may
                            1
                                              failure no
                                              failure no
## 3
       apr
                185
                                330
                            1
                                           1
## 4
       jun
                199
                            4
                                 -1
                                              unknown no
## 5
       may
                226
                            1
                                -1
                                           0
                                              unknown no
## 6
       feb
                141
                                176
                                              failure no
summary(dat)
```

```
##
                              job
                                           marital
                                                            education
                                                                         default
         age
##
    Min.
           :19.00
                    management:969
                                       divorced: 528
                                                        primary: 678
                                                                         no:4445
##
    1st Qu.:33.00
                    blue-collar:946
                                                                         yes: 76
                                       married:2797
                                                        secondary:2306
    Median :39.00
                    technician:768
                                       single :1196
                                                        tertiary:1350
##
   Mean
           :41.17
                                :478
                                                        unknown: 187
                    admin.
##
    3rd Qu.:49.00
                    services
                                :417
##
    Max.
           :87.00
                    retired
                                :230
##
                    (Other)
                               :713
##
       balance
                    housing
                                loan
                                                contact
                                                                  day
##
           :-3313
                    no :1962
                               no:3830
                                           cellular :2896
                                                                   : 1.00
    Min.
                                                             Min.
                    yes:2559
                                           telephone: 301
                                                             1st Qu.: 9.00
##
    1st Qu.:
               69
                                yes: 691
    Median: 444
                                           unknown:1324
                                                             Median :16.00
           : 1423
                                                                    :15.92
##
    Mean
                                                             Mean
##
    3rd Qu.: 1480
                                                             3rd Qu.:21.00
                                                                    :31.00
##
    Max.
           :71188
                                                             Max.
##
##
        month
                      duration
                                      campaign
                                                         pdays
##
           :1398
                         : 4
                                   Min.
                                         : 1.000
                                                           : -1.00
    may
                   Min.
                                                     Min.
                                                     1st Qu.: -1.00
                                   1st Qu.: 1.000
##
    jul
           : 706
                   1st Qu.: 104
           : 633
                   Median: 185
                                   Median : 2.000
                                                    Median : -1.00
##
    aug
                           : 264
                                         : 2.794
##
    jun
           : 531
                   Mean
                                   Mean
                                                    Mean
                                                            : 39.77
##
    nov
           : 389
                   3rd Qu.: 329
                                   3rd Qu.: 3.000
                                                     3rd Qu.: -1.00
##
    apr
           : 293
                   Max.
                          :3025
                                   Max.
                                          :50.000
                                                    Max.
                                                            :871.00
    (Other): 571
##
##
       previous
                         poutcome
                                        У
                                      no:4000
   Min.
         : 0.0000
                      failure: 490
```

```
## 1st Qu:: 0.0000 other : 197 yes: 521
## Median : 0.0000 success: 129
## Mean : 0.5426 unknown:3705
## 3rd Qu:: 0.0000
## Max. :25.0000
## = createDataPartition(dat$y, times = 1, p = 2/3)
train = dat[part$Resample1,]
test = dat[-part$Resample1,]
```

### 5.2 Fit NaiveBayes-Model

Mcnemar's Test P-Value: 8.832e-07

```
head(train)
##
    age
                job marital education default balance housing loan contact day
## 2 33
           services married secondary
                                                 4789
                                                          yes yes cellular
                                           no
## 3 35 management single tertiary
                                                 1350
                                                               no cellular 16
                                           no
                                                          yes
## 4 30 management married tertiary
                                                 1476
                                                          yes
                                                               yes unknown
                                           no
     59 blue-collar married secondary
                                                                no unknown
                                                                              5
## 5
                                           no
                                                    0
                                                          yes
## 6 35 management single tertiary
                                           no
                                                  747
                                                          no
                                                                no cellular 23
## 8 39 technician married secondary
                                           no
                                                  147
                                                          yes
                                                                no cellular
##
    month duration campaign pdays previous poutcome y
## 2
               220
                          1
                              339
                                         4 failure no
      may
                                         1 failure no
               185
                              330
## 3
                          1
      apr
                                         0 unknown no
## 4
      jun
               199
                          4
                               -1
## 5
      may
               226
                          1
                               -1
                                         0 unknown no
## 6
      feb
               141
                          2
                              176
                                         3
                                            failure no
## 8
      may
               151
                               -1
                                         0 unknown no
model = naiveBayes(y ~ ., data = train)
## Performance on test set
confusionMatrix(predict(model, test), test$y, positive = "yes")
## Confusion Matrix and Statistics
##
##
            Reference
## Prediction
               no yes
##
         no 1175
##
         yes 158
                    92
##
##
                 Accuracy : 0.8413
                   95% CI: (0.8219, 0.8594)
##
##
      No Information Rate: 0.8851
##
      P-Value [Acc > NIR] : 1
##
##
                    Kappa: 0.3462
##
```

```
##
##
               Sensitivity: 0.53179
##
               Specificity: 0.88147
##
           Pos Pred Value : 0.36800
##
            Neg Pred Value: 0.93551
##
                Prevalence: 0.11487
##
           Detection Rate: 0.06109
     Detection Prevalence: 0.16600
##
##
         Balanced Accuracy: 0.70663
##
##
          'Positive' Class : yes
##
```

Note: model useless since accuracy ~ NIR

## 5.3 Calibrate classifier using ROC

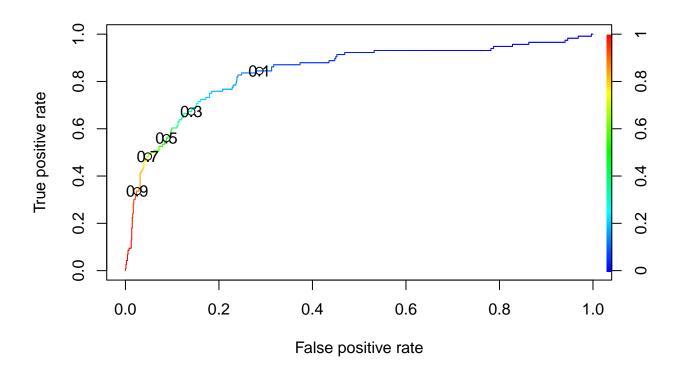
Create probabilities for predictions on validation set:

```
part = createDataPartition(train$y, times = 1, p = 2/3)
train_sub = train[part$Resample1,]
validation = train[-part$Resample1,]
model = naiveBayes(y ~ ., data = train_sub)

## use "yes" column
prob = predict(model, validation, type = "raw")[,"yes"]
```

#### 5.4 ROC-curve

```
predobj = prediction(prob, validation$y, label.ordering = c("no", "yes"))
perf = performance(predobj, "tpr", "fpr")
plot(perf, colorize = TRUE, print.cutoffs.at = seq(0.1, 1, 0.2))
```



```
## AUC-value:
performance(predobj, "auc")@y.values

## [[1]]
## [1] 0.841453
```

Choose Cutoff 0.2 and compute performance again on test set:

```
pred = predict(model, test, type = "raw")[,2] > 0.2
confusionMatrix(table(pred, test$y == "yes"), positive = "TRUE")
```

```
## Confusion Matrix and Statistics
##
##
           FALSE TRUE
## pred
##
     FALSE
            1046
                    49
##
     TRUE
             287
                  124
##
##
                   Accuracy : 0.7769
##
                     95% CI : (0.755, 0.7977)
       No Information Rate: 0.8851
##
##
       P-Value [Acc > NIR] : 1
##
##
                      Kappa : 0.3137
```

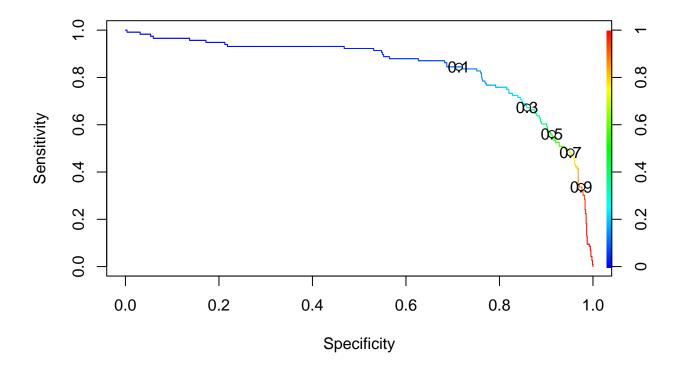
```
##
    Mcnemar's Test P-Value : <2e-16
##
##
##
               Sensitivity: 0.71676
               Specificity: 0.78470
##
##
            Pos Pred Value : 0.30170
##
            Neg Pred Value : 0.95525
                Prevalence: 0.11487
##
##
            Detection Rate: 0.08234
##
      Detection Prevalence : 0.27291
##
         Balanced Accuracy: 0.75073
##
##
          'Positive' Class : TRUE
##
```

Better tradeoff between sensitivity and specificity.

## 5.5 Sensitivity-Specificity-Curve

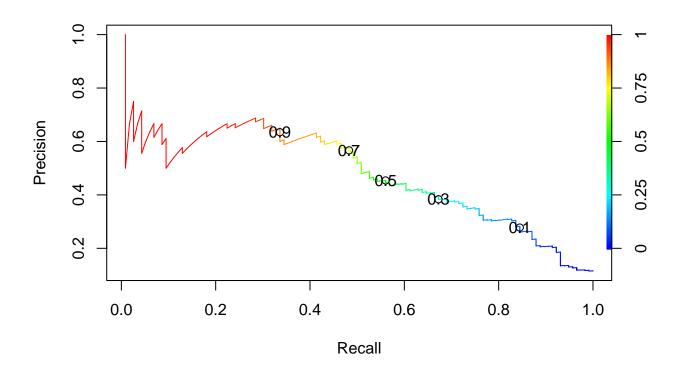
Actually, same than ROC-curve (X-axis flipped)

```
perf = performance(predobj, "sens", "spec")
plot(perf, colorize = TRUE, print.cutoffs.at = seq(0.1, 1, 0.2))
```



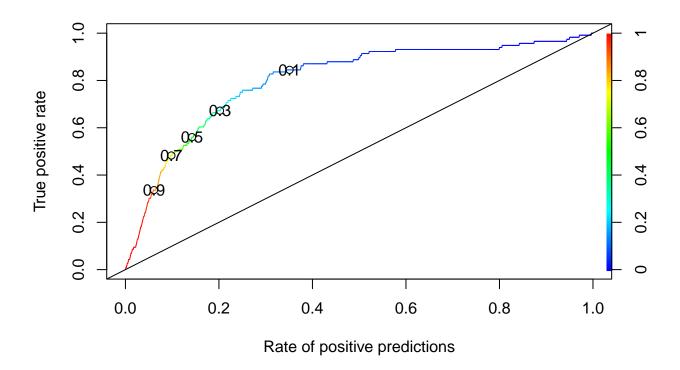
## 5.6 Recall-Precision-Curve

```
perf = performance(predobj, "prec", "rec")
plot(perf, colorize = TRUE, print.cutoffs.at = seq(0.1, 1, 0.2))
```



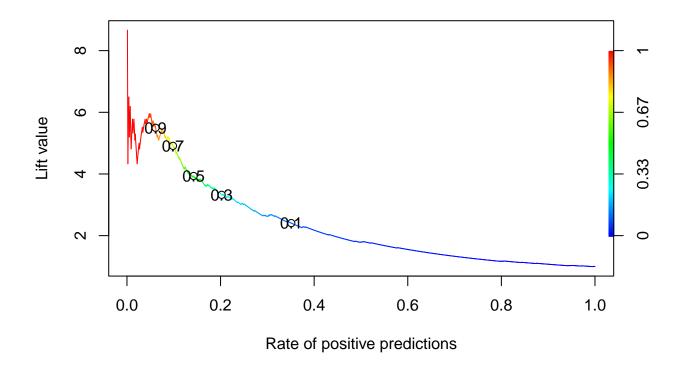
# 5.7 Cumulative Response Curve

```
perf = performance(predobj, "tpr", "rpp")
plot(perf, colorize = TRUE, print.cutoffs.at = seq(0.1, 1, 0.2))
abline(a = 0, b = 1)
```



# 5.8 Lift chart

```
perf = performance(predobj, "lift", "rpp")
plot(perf, colorize = TRUE, print.cutoffs.at = seq(0.1, 1, 0.2))
```



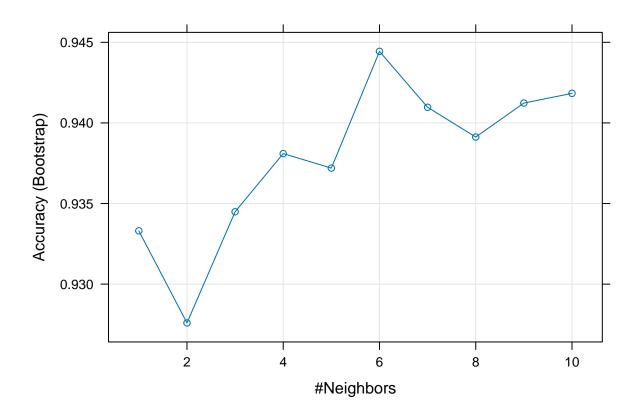
# 6 Tuning hyperparameters

**Note:** In the following examples, we use the whole data set for tuning for simplicity. In real applications, create training/test sets first and perform tuning only on *training* set, using part of it as *validation* set!

```
set.seed(4711)
model_knn = train(Species ~ ., data = iris, "knn",
                  preProcess = c("scale", "center"),
                  trControl = trainControl(method = "boot"),
                  tuneGrid = data.frame(k = 1:10))
model_knn
## k-Nearest Neighbors
##
## 150 samples
##
     4 predictor
##
     3 classes: 'setosa', 'versicolor', 'virginica'
##
## Pre-processing: scaled (4), centered (4)
## Resampling: Bootstrapped (25 reps)
## Summary of sample sizes: 150, 150, 150, 150, 150, 150, ...
## Resampling results across tuning parameters:
##
##
         Accuracy
                    Kappa
     k
```

```
0.9333046 0.8989173
##
##
      2
        0.9275919 0.8903665
         0.9344876 0.9008575
##
##
        0.9380984
                    0.9061775
##
         0.9371970
                    0.9048937
##
        0.9444377
                    0.9159108
##
         0.9409696
                    0.9106566
                    0.9078966
##
         0.9391245
##
      9
         0.9412302
                    0.9110822
##
     10
        0.9418332
                    0.9119600
##
## Accuracy was used to select the optimal model using the largest value.
## The final value used for the model was k = 6.
```

### plot(model\_knn)



The tuning was performed on the 25 bootstrap samples.

Average confusion matrix for best model:

```
confusionMatrix(model_knn)
```

```
## Bootstrapped (25 reps) Confusion Matrix
##
## (entries are percentual average cell counts across resamples)
##
```

```
##
              Reference
## Prediction setosa versicolor virginica
     setosa
##
                  34.4
                            0.0
                                        0.0
##
     versicolor
                  0.1
                             29.4
                                        3.0
##
    virginica
                   0.0
                              2.5
                                       30.6
##
  Accuracy (average): 0.9447
Trick to get measures:
tab = trunc(confusionMatrix(model_knn)$table)
confusionMatrix(tab)
## Confusion Matrix and Statistics
##
##
              Reference
## Prediction setosa versicolor virginica
##
    setosa
                   34
                               0
                                          2
                    0
##
     versicolor
                               29
##
    virginica
                     0
                                2
                                         30
##
## Overall Statistics
##
##
                  Accuracy : 0.9588
##
                    95% CI: (0.8978, 0.9887)
##
      No Information Rate: 0.3505
##
      P-Value [Acc > NIR] : < 2.2e-16
##
##
                     Kappa: 0.9381
##
## Mcnemar's Test P-Value : NA
##
## Statistics by Class:
##
##
                        Class: setosa Class: versicolor Class: virginica
## Sensitivity
                              1.0000
                                                 0.9355
                                                                  0.9375
## Specificity
                               1.0000
                                                 0.9697
                                                                  0.9692
## Pos Pred Value
                                                                  0.9375
                               1.0000
                                                 0.9355
## Neg Pred Value
                              1.0000
                                                 0.9697
                                                                  0.9692
## Prevalence
                               0.3505
                                                 0.3196
                                                                  0.3299
## Detection Rate
                               0.3505
                                                 0.2990
                                                                  0.3093
## Detection Prevalence
                               0.3505
                                                 0.3196
                                                                  0.3299
## Balanced Accuracy
                               1.0000
                                                 0.9526
                                                                  0.9534
Use best model:
```

```
predict(model_knn, iris[1:5,-5])
```

```
## [1] setosa setosa setosa setosa
## Levels: setosa versicolor virginica
```

## 7 Automatic sampling, training & tuning

See ?models for a list of available models in caret.

### 7.1 Fitting models

```
set.seed(4711) # set seed for all models!
model_lm = train(volume ~ hightemp, method = "lm", data = RailTrail)
model_lm
## Linear Regression
## 90 samples
  1 predictor
##
## No pre-processing
## Resampling: Bootstrapped (25 reps)
## Summary of sample sizes: 90, 90, 90, 90, 90, 90, ...
## Resampling results:
##
##
    RMSE
              Rsquared
     105.9944 0.3320082 79.12959
##
## Tuning parameter 'intercept' was held constant at a value of TRUE
set.seed(4711) # use same seed for all models!
model_knn = train(volume ~ hightemp, method = "knn", data = RailTrail,
                 preProcess = c("scale", "center"),
                 tuneGrid = data.frame(k = 1:10))
model_knn
## k-Nearest Neighbors
##
## 90 samples
   1 predictor
##
## Pre-processing: scaled (1), centered (1)
## Resampling: Bootstrapped (25 reps)
## Summary of sample sizes: 90, 90, 90, 90, 90, 90, ...
## Resampling results across tuning parameters:
##
        RMSE
##
                  Rsquared
                             MAE
##
      1 133.1976 0.1943992
                             100.10263
##
      2 125.4203 0.2437184
                              92.65906
##
      3 120.4376 0.2652129
                             88.75831
##
      4 116.7899 0.2778544
                              86.00548
     5 113.5367 0.3026275
##
                              83.61075
##
     6 110.2958 0.3233051
                              81.02598
##
     7 107.6897 0.3483983
                             79.06783
##
     8 106.2128 0.3570732
                             77.90331
     9 105.1751 0.3642035 77.37585
##
```

```
## 10 104.2709 0.3741905 76.84947 ## ## RMSE was used to select the optimal model using the smallest value. ## The final value used for the model was k = 10.
```

## 7.2 Model comparison

### 7.2.1 side-by-side

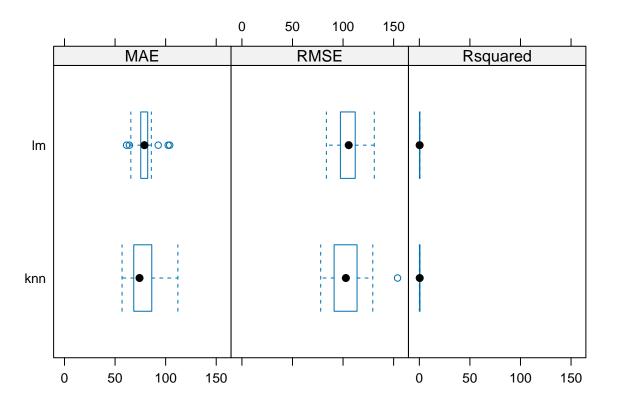
```
res = resamples(list(knn = model_knn, lm = model_lm))
```

#### summary(res)

```
##
## Call:
## summary.resamples(object = res)
## Models: knn, lm
## Number of resamples: 25
##
## MAE
##
           Min. 1st Qu.
                           Median
                                      Mean 3rd Qu.
## knn 56.90604 68.48944 74.17990 76.84947 86.29575 112.1055
## lm 61.37323 75.39249 79.01849 79.12959 82.26355 103.9788
##
## RMSE
##
           Min. 1st Qu.
                           Median
                                      Mean 3rd Qu.
## knn 77.90514 91.13558 102.7691 104.2709 113.8434 153.8869
## lm 83.50299 97.36886 105.5822 105.9944 112.0109 130.8544
##
## Rsquared
##
             Min.
                    1st Qu.
                               Median
                                           Mean
                                                  3rd Qu.
                                                               Max. NA's
## knn 0.01455077 0.2914759 0.3593974 0.3741905 0.4808125 0.6055482
## lm 0.09209436 0.2747304 0.3036938 0.3320082 0.4092167 0.5794341
                                                                        0
```

Compare graphically:

```
bwplot(res)
```



## 7.2.2 Pairwise:

t-test for differences:

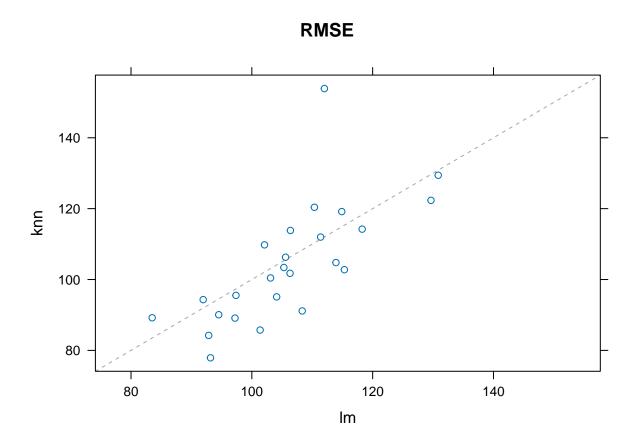
```
summary(diff(res))
```

```
##
## Call:
## summary.diff.resamples(object = diff(res))
## p-value adjustment: bonferroni
## Upper diagonal: estimates of the difference
## Lower diagonal: p-value for HO: difference = 0
##
## MAE
##
       knn
              lm
              -2.28
## knn
##
  lm 0.2348
##
## RMSE
##
       knn
              lm
## knn
              -1.723
## lm 0.4705
##
## Rsquared
```

```
## knn lm
## knn 0.04218
## lm 0.05598
```

Correlation plot:

```
xyplot(res, metric = "RMSE")
```



RMSE will highly correlate if classifiers have similar performance.

## 7.3 Use on SLURM cluster

In order to use caret on a cluster, it suffices to create a cluster and to register it for the doParallel package before calling train:

```
library(slurmR)
cl = makeSlurmCluster(84)

library(doParallel)
registerDoParallel(cl)
```

At the end, do not forget to clean up:

stopCluster(cl)