Predictive Analytics

Solutions to Hands On Exercises

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Mar, 2019

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Hands on LDAs - the Vehicle data set

The data set `Vehicle` is available in package **mlbench**. Load it and explore its help page to grab a minimal understanding of the data and then answer the following questions:

1. Obtain a random split of the data into two sub-sets using the proportion 80%-20%. solution
2. Obtain a linear discriminant using the larger set. solution
3. Obtain the predictions of the obtained model on the smaller set. solution
4. Obtain a confusion matrix of the predictions and calculate the respective accuracy. solution

Solutions to Exercise 1

- Obtain a random split of the data into two sub-sets using the proportion 80%-20%. solution

```
data(Vehicle,package="mlbench")
idx.tr <- sample(1:nrow(Vehicle),as.integer(0.8*nrow(Vehicle)))
tr <- Vehicle[idx.tr,]
ts <- Vehicle[-idx.tr,]
```

Go Back

Solutions to Exercise 2

- Obtain a linear discriminant using the larger set.

```
library(MASS)
model <- lda(Class ~ .,tr)
```

Go Back

Solutions to Exercise 3

- Obtain the predictions of the obtained model on the smaller set.

```
preds <- predict(model,ts)
```

Go Back

Solutions to Exercise 4

- Obtain a confusion matrix of the predictions and calculate the respective accuracy.

```r
cm <- table(preds$class,ts$Class)
acc <- sum(diag(cm))/sum(cm)
cat("The accuracy is ",round(acc*100,2),"%.\n")

## The accuracy is  30 %.
```

Hands on Linear Regression - the Boston data set

The data set `Boston` is available in package **MASS**. Load it and explore its help page to grab a minimal understanding of the data and then answer the following questions:

1. Obtain a random split of the data into two sub-sets using the proportion 70%-30%. solution
2. Obtain a multiple linear regression model using the larger set. solution
3. Check the diagnostic information provided for the model. solution
4. Obtain the predictions of the obtained model on the smaller set. solution
5. Obtain the mean squared error of these predictions and also an error scatter plot. solution

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Solutions to Exercise 1

- Obtain a random split of the data into two sub-sets using the proportion 70%-30%. solution

```
data(Boston,package="MASS")
idx.tr <- sample(1:nrow(Boston),as.integer(0.7*nrow(Boston)
tr <- Boston[idx.tr,]
ts <- Boston[-idx.tr,]
```

Go Back

Solutions to Exercise 2

- Obtain a multiple linear regression model using the larger set.

```
model <- lm(medv ~ ., tr)
```

Go Back

Solutions to Exercise 3

- Check the diagnostic information provided for the model.

```
summary(model)
```

```
##
## Call:
## lm(formula = medv ~ ., data = tr)
##
## Residuals:
##     Min      1Q  Median      3Q     Max
## -10.776  -2.371  -0.664   1.906  25.349
##
## Coefficients:
##              Estimate Std. Error t value Pr(>|t|)
## (Intercept)  2.53e+01   5.93e+00    4.27  2.6e-05 ***
## crim        -6.74e-02   3.91e-02   -1.73  0.08534 .
## zn           4.96e-02   1.50e-02    3.29  0.00109 **
## indus        5.14e-04   6.43e-02    0.01  0.99364
## chas         3.28e+00   9.18e-01    3.57  0.00041 ***
## nox         -1.09e+01   4.07e+00   -2.67  0.00793 **
## rm           4.71e+00   4.96e-01    9.50  < 2e-16 ***
## age         -3.91e-02   1.45e-02   -2.69  0.00749 **
## dis         -1.60e+00   2.22e-01   -7.18  4.4e-12 ***
## rad          2.38e-01   7.48e-02    3.18  0.00162 **
## tax         -1.34e-02   4.15e-03   -3.22  0.00140 **
## ptratio     -8.23e-01   1.40e-01   -5.89  9.4e-09 ***
## black        1.39e-02   3.19e-03    4.34  1.9e-05 ***
## lstat       -3.93e-01   5.46e-02   -7.19  4.1e-12 ***
## ---
```

Solutions to Exercise 4

- Obtain the predictions of the obtained model on the smaller set.

```
preds <- predict(model,ts)
```

Go Back

Solutions to Exercise 5

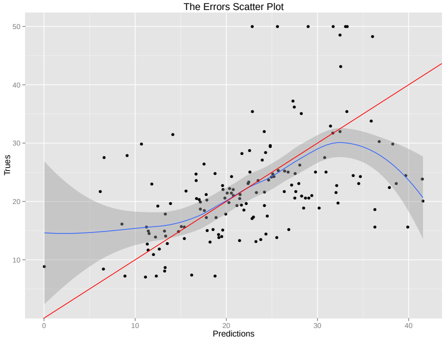
- Obtain the mean squared error of these predictions and also an error scatter plot.

```r
mse <- mean((preds-ts$medv)^2)
cat("The mean squared error is ",round(mse*100,2),"\n")

## The mean squared error is  6203
```

Solutions to Exercise 5 (cont.)

- Obtain the mean squared error of these predictions and also an error scatter plot.

```
library(ggplot2)
ggplot(data.frame(Predictions=preds,Trues=ts$medv),aes(x=Predictions,y=Trues)) +
    geom_point() + geom_smooth(method='loess') +
        geom_abline(slope=1, intercept=0,color="red") + ggtitle("The Errors Scatter Plot")
```



Hands on Tree-based Models - the Wines data

File `Wine.Rdata` contains two data frames with data on green wine quality: (i) `redWine` and (ii) `whiteWine`. Each of these data sets contains a series of tests with green wines (red and white). For each of these tests the values of several physicochemical variables together with a quality score assigned by wine experts (column `quality`).

1. Build a regression tree for the white wines data set solution
2. Obtain a graph of the obtained regression tree solution
3. Apply the tree to the data used to obtain the model and calculate the mean squared error of the predictions solution
4. Split the data set in two parts: 70% of the tests and the remaining 30%. Using the larger part to obtain a regression tree and apply it to the other part. Calculate again the mean squared error. Compare with the previous scores and comment. solution

Solutions Exercise 1

- Build a regression tree for the white wines data set

```r
load("Wine.Rdata")
library(DMwR2)
```

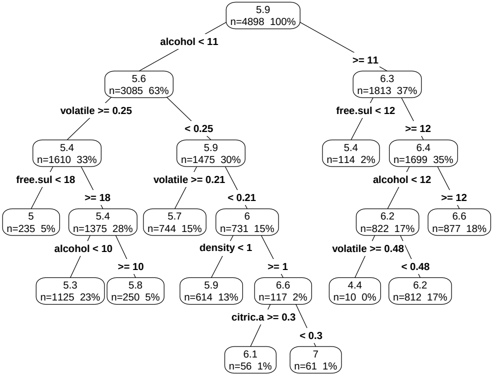
```r
ab <- rpartXse(quality ~ .,whiteWine)
```

Go back

Solutions Exercise 2

- Obtain a graph of the obtained regression tree

```
library(rpart.plot)
prp(ab,type=4,extra=101)
```



Solutions Exercise 3

- Apply the tree to the data used to obtain the model and calculate the mean squared error of the predictions

```
prevs <- predict(ab,whiteWine)
mse <- mean((whiteWine$quality - prevs)^2)
mse

## [1] 0.5382
```

Go back

Solutions Exercise 4

- Split the data set in two parts: 70% of the tests and the remaining 30%. Using the larger part to obtain a regression tree and apply it to the other part. Calculate again the mean squared error. Compare with the previous scores and comment.

```
xs <- sample(1:nrow(whiteWine),as.integer(0.7*nrow(whiteWine)))
train <- whiteWine[xs,]
test <- whiteWine[-xs,]
ab2 <- rpartXse(quality ~.,train)
prevs2 <- predict(ab2,test)
mse2 <- mean((test$quality - prevs2)^2)
c(before=mse,now=mse2)


##    before       now
## 0.5382229 0.6037395
```

Go back

Hands on SVMs

The file `Wine.Rdata` contains 2 data frames with data about the quality of “green” wines: i) `redWine` and ii) `whiteWine`. Each of these data sets has information on a series of wine tasting sessions to “green” wines (both red and white). For each wine sample several physico-chemical properties of the wine sample together with a quality score assigned by a committee of wine experts (variable `quality`).

1. Obtain and SVM for forecasting the quality of the red variant of “green” wines solution
2. Split the data set in two parts: one with 70% of the samples and the other with the remaining 30%. Obtain an SVM with the first part and apply it to the second. What was the resulting mean absolute error? solution
3. Using the `round()` function, round the predictions obtained in the previous question to the nearest integer. Calculate the error rate of the resulting integers when compared to the true values solution

Solutions to Exercise 1

- Obtain and SVM for forecasting the quality of the red variant of “green” wines

```r
load("Wine.Rdata")
library(e1071)
```

```r
s <- svm(quality ~ .,redWine)
```

Go back

Solutions to Exercise 2

- Split the data set in two parts: one with 70% of the samples and the other with the remaining 30%. Obtain an SVM with the first part and apply it to the second. What was the resulting mean absolute error?

```
xs <- sample(1:nrow(redWine),
               as.integer(0.7*nrow(redWine)))
train <- redWine[xs,]
test  <- redWine[-xs,]
s2 <- svm(quality ~.,train)
p2 <- predict(s2,test)
mae <- mean(abs(test$quality - p2))
mae

## [1] 0.4358064
```

Go back

Solutions to Exercise 3

- Using the `round()` function, round the predictions obtained in the previous question to the nearest integer. Calculate the error rate of the resulting integers when compared to the true values

```
pi2 <- round(p2)
mc <- table(pi2,test$quality)
mc

##
## pi2   3   4   5   6   7   8
##   5   2   9 165  60   1   0
##   6   0   4  41 114  36   4
##   7   0   0   2  18  23   1
```

Solutions to Exercise 3 (cont.)

```
pi3 <- factor(pi2,levels=levels(factor(test$quality)))
mc2 <- table(pi3,test$quality)
mc2


##
## pi3   3   4   5   6   7   8
##   3   0   0   0   0   0   0
##   4   0   0   0   0   0   0
##   5   2   9 165  60   1   0
##   6   0   4  41 114  36   4
##   7   0   0   2  18  23   1
##   8   0   0   0   0   0   0


err <- 1-sum(diag(mc2))/sum(mc2)
err


## [1] 0.3708333
```

Is this as bad as it looks like?

Go back

Hands on Linear Regression and Random Forests

the Algae data set

Load in the data set `algae` from package **DMwR2** and answer the following questions:

1. How would you obtain a random forest to forecast the value of alga *a4* solution
2. Repeat the previous exercise but now using a linear regression model. Try to simplify the model using the `step()` function. solution
3. Obtain the predictions of the two previous models for the data used to obtain them. Draw a scatterplot comparing these predictions solution
4. The data frame named `test.algae` contains a test set with some extra 140 water samples for which we want predictions. Use the previous two models to obtain predictions for `a4` on these new samples. Check what happened to the test cases with NA's. Fill-in the NA's on the test set and repeat the experiment. solution

Solutions to Exercise 1

- How would you obtain a random forest to forecast the value of alga *a4*

```
library(randomForest)
library(DMwR2)
data(algae)
algae <- algae[-c(62,199),]
algae <- knnImputation(algae)
rf.a4 <- randomForest(a4 ~.,algae[,c(1:11,15)])
```

Go back

Solutions to Exercise 2

- Repeat the previous exercise but now using a linear regression model. Try to simplify the model using the `step()` function.

```
lm.a4 <- lm(a4 ~ .,algae[,c(1:11,15)])
```

```
lm.a4 <- step(lm.a4)
```

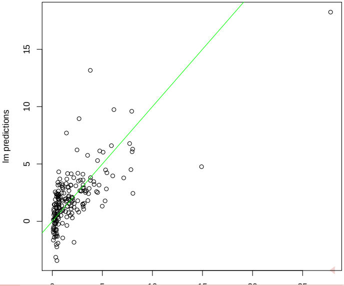
```
lm.a4

##
## Call:
## lm(formula = a4 ~ mxPH + mnO2 + NO3 + NH4 + PO4, data = algae[,
##     c(1:11, 15)])
##
## Coefficients:
## (Intercept)         mxPH         mnO2          NO3          NH4
##   25.155775    -2.564539    -0.307999    -0.466876     0.000932
##         PO4
##    0.009314
```

Go back

Solutions to Exercise 3

- Obtain the predictions of the two previous models for the data used to obtain them. Draw a scatterplot comparing these predictions

```
psrf <- predict(rf.a4,algae)
pslm <- predict(lm.a4,algae)
plot(psrf,pslm,xlab="Random forest predictions",ylab="lm predictions")
abline(0,1,col="green")
```



Solutions to Exercise 4

- The data frame named `test.algae` contains a test set with some extra 140 water samples for which we want predictions. Use the previous two models to obtain predictions for `a4` on these new samples.

```
prevs.rf <- predict(rf.a4,test.algae)
prevs.lm <- predict(lm.a4,test.algae)
summary(prevs.rf)

##     Min.  1st Qu.   Median     Mean  3rd Qu.     Max.     NA's
##  0.09421  0.83539  1.56449  2.12729  2.45076 21.66409       18

summary(prevs.lm) # notice the difference in the number of NA's. Why?

##    Min. 1st Qu.  Median    Mean 3rd Qu.    Max.    NA's
## -2.8201  0.5774  1.5603  2.2330  3.3549 28.6980       6
```

Solutions to Exercise 4 (cont.)

```
test.algae <- knnImputation(test.algae,distData=algae[,1:11])
prevs.rf <- predict(rf.a4,test.algae)
prevs.lm <- predict(lm.a4,test.algae)
```

Hands on Mars and Gradient Boosting

Load in the data set `Boston Housing` from package **MASS** and answer the following questions:

1. Split the data set into training and testing sets and obtain a MARS model and a GBM model with the training set. solution
2. Check the predictions of the models on the test set. Obtain their mean squared error. solution
3. Read the help pages of the two functions that obtain MARS and GBM and explore a few variants of these models and check the results in terms of the performance on the test set solution
4. Produce a barplot with the errors of the different variants you have considered. solution

Solutions to Exercise 1

- Split the data set into training and testing sets and obtain a MARS model and a GBM model with the training set.

```r
library(gbm)
library(earth)
data(Boston,package="MASS")
set.seed(1234)
trPerc <- 0.7
sp <- sample(1:nrow(Boston),as.integer(trPerc*nrow(Boston)))
tr <- Boston[sp,]
ts <- Boston[-sp,]
b <- gbm(medv ~ .,distribution='gaussian',data=tr,n.trees=5000,verbose=F)
m <- earth(medv ~ .,tr,degree=2)
```

Go back

Solutions to Exercise 2

- Check the predictions of the models on the test set. Obtain their mean squared error.

```
pb <- predict(b,ts,n.trees=5000)
mean((pb-ts$medv)^2)

## [1] 20.96

pm <- predict(m,ts)
mean((pm-ts$medv)^2)

## [1] 19.9
```

Go back

Solutions to Exercise 3

- Explore a few variants of these models and check the results in terms of the performance on the test set

```
varsb <- expand.grid(n.trees=c(5000,7500,15000),interaction.depth=c(1,2),
                     shrinkage=c(0.001,0.05))
varsm <- expand.grid(degree=c(1,2,3),thresh=c(0.001,0.05,0.01),
                     fast.k=c(20,30))
nvars <- nrow(varsb)
nreps <- 10
trPerc <- 0.7
res <- matrix(NA,nrow=nvars*2,ncol=2)
```

Solutions to Exercise 3 (cont.)

```
set.seed(1234)
for(v in 1:nvars) {
    errs <- matrix(NA,nrow=nreps,ncol=2)
    for(r in 1:nreps) {
        sp <- sample(1:nrow(Boston),as.integer(trPerc*nrow(Boston)))
        tr <- Boston[sp,]
        ts <- Boston[-sp,]
        b <- gbm(medv ~ .,distribution='gaussian',data=tr,
                 n.trees=varsb[v,"n.trees"],
                 interaction.depth=varsb[v,"interaction.depth"],
                 shrinkage=varsb[v,"shrinkage"],verbose=FALSE)
        pb <- predict(b,ts,n.trees=varsb[v,"n.trees"])
        m <- earth(medv ~ .,tr,
                   degree=varsm[v,"degree"],
                   thresh=varsm[v,"thresh"],
                   fast.k=varsm[v,"fast.k"]
                   )
        pm <- predict(m,ts)
        errs[r,1] <- mean((pb-ts$medv)^2)
        errs[r,2] <- mean((pm-ts$medv)^2)
    }
    res[v,] <- c(mean(errs[,1]),sd(errs[,1]))
    res[nvars+v,] <- c(mean(errs[,2]),sd(errs[,2]))
}
```

Go back

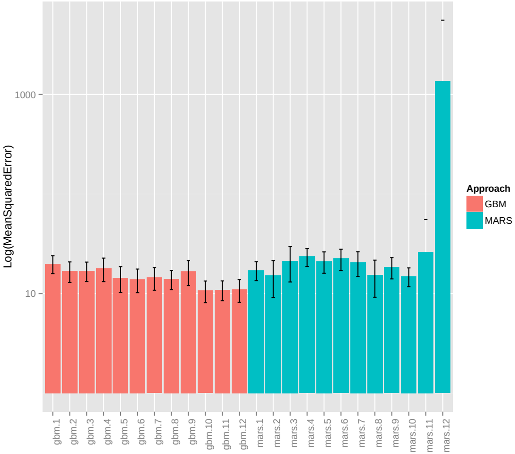
Solutions to Exercise 4

- Produce a barplot with the errors of the different variants you have considered.

```r
library(ggplot2)
colnames(res) <- c("AvgErr","SdErr")
results <- data.frame(System=c(paste("gbm",1:nvars,sep="."),
                          paste("mars",1:nvars,sep=".")),res)
results$Approach <- c(rep("GBM",nvars),rep("MARS",nvars))
results$System <- factor(results$System,levels=results$System)
ggplot(data=results,aes(x=System, y=AvgErr,fill=Approach)) +
    geom_bar(stat="identity") +
        geom_errorbar(aes(ymax = AvgErr + SdErr, ymin=AvgErr - SdErr), width=0.2) +
            theme(axis.text.x = element_text(angle = 90, hjust = 1),
                  axis.title.x = element_blank())
```

Solutions to Exercise 4 (cont.)

```
## Warning:  NaNs produced
## Warning:  Removed 4 rows containing missing values (geom_path).
## Warning:  Removed 4 rows containing missing values (geom_path).
```



Hands on Performance Estimation

the Algae data set

Load in the data set `algae` and answer the following questions:

1. Estimate the MSE of a regression tree for forecasting alga *a1* using 10-fold Cross validation. solution
2. Repeat the previous exercise this time trying some variants of random forests. Check what are the characteristics of the best performing variant. solution
3. Compare the results in terms of mean absolute error of the default variants of a regression tree, a linear regression model and a random forest, in the task of predicting alga a3. Use 2 repetitions of a 5-fold Cross Validation experiment. solution
4. Carry out an experiment designed to select what are the best models for each of the seven harmful algae. Use 10-fold Cross Validation. For illustrative purposes consider only the default variants of regression trees, linear regression and random forests. solution

Solutions to Exercise 1

- Estimate the MSE of a regression tree for forecasting alga *a1* using 10-fold Cross validation.

```r
library(DMwR)
library(performanceEstimation)
data(algae)
algae <- algae[-c(62,199),]
res.a1 <- performanceEstimation(
    PredTask(a1 ~ .,algae[,1:12],"algaA1"),
    Workflow("standardWF",learner="rpartXse",pre="knnImp"),
    EstimationTask("mse",method=CV())
    )
```

Solutions to Exercise 1 (cont.)

- Estimate the MSE of a regression tree for forecasting alga *a1* using 10-fold Cross validation.

```
summary(res.a1)


##
## == Summary of a  Cross Validation Performance Estimation Experiment ==
##
## Task for estimating  mse  using
##  1 x 10 - Fold Cross Validation
##   Run with seed =  1234
##
## * Predictive Tasks ::  algaA1
## * Workflows  ::  standardWF
##
## -> Task:  algaA1
##   *Workflow: standardWF
##              mse
## avg      321.10
## std      200.70
## med      302.53
## iqr      302.49
## min       96.22
## max      637.87
## invalid    0.00
```

Go back

Solutions to Exercise 2

- Repeat the previous exercise this time trying some variants of random forests. Check what are the characteristics of the best performing variant.

```r
library(randomForest)
resrf.a1 <- performanceEstimation(
    PredTask(a1 ~ .,algae[,1:12],"algaA1"),
    workflowVariants("standardWF",
                     learner="randomForest",
                     learner.pars=list(ntree=c(500,750,1000)),
                     pre="knnImp"),
    EstimationTask("mse",method=CV())
    )
```

Solutions to Exercise 2 (cont.)

```
summary(resrf.a1)

##
## == Summary of a  Cross Validation Performance Estimation Experiment ==
##
## Task for estimating  mse  using
##  1 x 10 - Fold Cross Validation
##   Run with seed =  1234
##
## * Predictive Tasks ::  algaA1
## * Workflows  ::  randomForest.v1, randomForest.v2, randomForest.v3
##
## -> Task:  algaA1
##   *Workflow: randomForest.v1
##              mse
## avg     255.79
## std     167.89
## med     200.92
## iqr     178.99
## min      73.26
## max     640.69
## invalid   0.00
##
##   *Workflow: randomForest.v2
##              mse
## avg     256.09
## std     166.75
## med     203.92
## iqr     172.09
## min      74.05
```

Solutions to Exercise 2 (cont.)

- Repeat the previous exercise this time trying some variants of random forests. Check what are the characteristics of the best performing variant.

```
topPerformer(resrf.a1,"mse","algaA1")

## Workflow Object:
##  Workflow ID       ::  randomForest.v1
##  Workflow Function ::  standardWF
##       Parameter values:
##   learner.pars  ->  ntree=500
##   learner  ->  randomForest
```

Go back

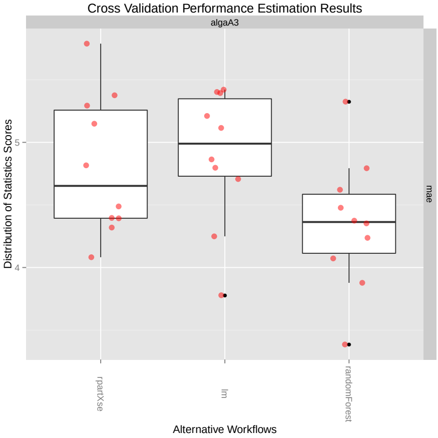
Solutions to Exercise 3

- Compare the results in terms of mean absolute error of the default variants of a regression tree, a linear regression model and a random forest, in the task of predicting alga a3. Use 2 repetitions of a 5-fold Cross Validation experiment. Plot the results

```
res.a3 <- performanceEstimation(
    PredTask(a3 ~ ., algae[,c(1:11,14)], "algaA3"),
    workflowVariants("standardWF",
                     learner=c("rpartXse","lm","randomForest"),
                     pre="knnImp"),
    EstimationTask("mae",method=CV(nReps=2,nFolds=5))
    )
```

Solutions to Exercise 3 (cont.)

```
plot(res.a3)
```



Go back

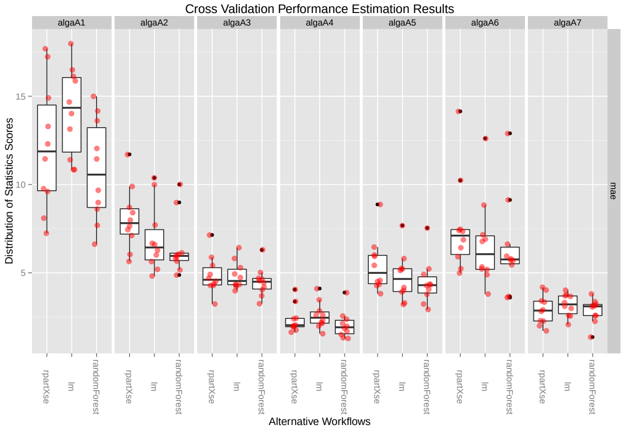
Solutions to Exercise 4

- Carry out an experiment designed to select what are the best models for each of the seven harmful algae. Use 10-fold Cross Validation. For illustrative purposes consider only the default variants of regression trees, linear regression and random forests.

```
tgts <- 12:18
tasks <- c()
for(t in tgts)
    tasks <- c(tasks,
               PredTask(as.formula(paste(colnames(algae)[t],'~ .')),
                        algae[,c(1:11,t)],
                        paste0("algaA",t-11),
                        copy=TRUE))
res.algae <- performanceEstimation(
    tasks,
    workflowVariants(learner=c("rpartXse","lm","randomForest"),
                     pre="knnImp"),
    EstimationTask("mae",method=CV())
    )
```

Solutions to Exercise 4 (cont.)

```
plot(res.algae)
```



Solutions to Exercise 4 (cont.)

```
topPerformers(res.algae)


## $algaA1
##           Workflow Estimate
## mae randomForest   10.785
##
## $algaA2
##           Workflow Estimate
## mae randomForest    6.461
##
## $algaA3
##           Workflow Estimate
## mae randomForest    4.486
##
## $algaA4
##           Workflow Estimate
## mae randomForest    2.059
##
## $algaA5
##           Workflow Estimate
## mae randomForest    4.466
##
## $algaA6
##           Workflow Estimate
## mae randomForest    6.453
##
## $algaA7
##           Workflow Estimate
## mae randomForest    2.855
```

Hands on Statistical Significance

Using the *algae* data set from package **DMwR2** answer the following questions

1. For the 7 different algae, choose a reasonable set of SVM variants and estimate their MSE error. solution
2. Check if these alternatives are significantly better than the SVM with the default parameter settings solution
3. Present the results of the previous question visually solution

Solutions to Exercise 1

- Check which workflow achieved the best score and carry out a paired comparison of the other alternatives against this workflow

```r
library(performanceEstimation)
library(e1071)
data(algae,package="DMwR2")
tgts <- 12:18
tasks <- c()
for(t in tgts)
    tasks <- c(tasks,
               PredTask(as.formula(paste(colnames(algae)[t],'~ .')),
                        algae[,c(1:11,t)],
                        paste0("algaA",t-11),
                        copy=TRUE))
res.algae <- performanceEstimation(
    tasks,
    c(Workflow(learner="svm",pre="knnImp",wfID="defaultSVM"),
      workflowVariants(learner="svm",
                       learner.pars=list(cost=c(1,3,5,10,15),gamma=c(0.01,0.05),
                                         epsilon=c(0.01,0.05)),
                       pre="knnImp")
      ),
    EstimationTask("mse",method=CV())
    )
```

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Solutions to Exercise 2

```
pcomp <- pairedComparisons(res.algae, baseline="defaultSVM")
pcomp$mse$F.test


## $chi
## [1] 42.07792
##
## $FF
## [1] 2.578249
##
## $critVal
## [1] 1.205512
##
## $rejNull
## [1] TRUE
```

Solutions to Exercise 2

```
pcomp$mse$BonferroniDunn.test


## $critDif
## [1] 10.02729
##
## $baseline
## [1] "defaultSVM"
##
## $rkDifs
##    svm.v1    svm.v2    svm.v3    svm.v4    svm.v5    svm.v6    svm.v7
## 12.142857 10.142857  8.571429  7.571429  6.428571  3.000000  2.571429
##    svm.v8    svm.v9   svm.v10   svm.v11   svm.v12   svm.v13   svm.v14
##  5.428571  9.000000 12.000000 10.571429  8.000000  6.857143  6.571429
##   svm.v15   svm.v16   svm.v17   svm.v18   svm.v19   svm.v20
##  5.142857  2.571429  2.428571  3.857143  8.285714  9.857143
##
## $signifDifs
##  svm.v1  svm.v2  svm.v3  svm.v4  svm.v5  svm.v6  svm.v7  svm.v8  svm.v9
##    TRUE    TRUE   FALSE   FALSE   FALSE   FALSE   FALSE   FALSE   FALSE
## svm.v10 svm.v11 svm.v12 svm.v13 svm.v14 svm.v15 svm.v16 svm.v17 svm.v18
##    TRUE    TRUE   FALSE   FALSE   FALSE   FALSE   FALSE   FALSE   FALSE
## svm.v19 svm.v20
##   FALSE   FALSE
```

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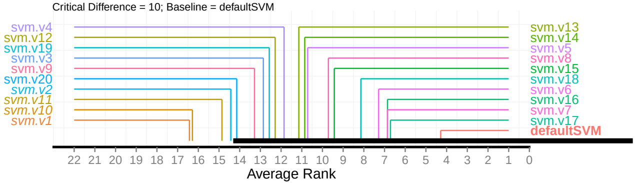
Solutions to Exercise 3

- Decide on a p-value and check which differences are statistically significant

```
CDdiagram.BD( pcomp )
```



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