Performance Estimation

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KNOYDA, Know Your Data!

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Evaluation Methodologies and Comparison of Models

Performance Estimation

The setting

- Predictive task: unknown function $Y = f(\mathbf{x})$ that maps the values of a set of predictors into a target variable value (can be a classification or a regression problem)
- A (training) data set $\{< \mathbf{x}_i, y_i >\}_{i=1}^N$, with known values of this mapping
- Performance evaluation criterion(a) - metric(s) of predictive performance (e.g. error rate or mean squared error)
- How to obtain a **reliable estimates** of the predictive performance of any solutions we consider to solve the task using the available data set?

Reliability of Estimates

Resubstitution estimates

- Given that we have a data set one possible way to obtain an estimate of the performance of a model is to evaluate it on this data set
- This leads to what is known as a **resubstitution estimate** of the prediction error
- These estimates are unreliable and should not be used as they tend to be over-optimistic!

Reliability of Estimates

Resubstitution estimates (2)

- Why are they unreliable?
  - Models are obtained with the goal of optimizing the selected prediction error statistic on the given data set
  - In this context it is expected that they get good scores!
  - The given data set is just a sample of the unknown distribution of the problem being tackled
  - What we would like is to have the performance of the model on this distribution
  - As this is usually impossible the best we can do is to evaluate the model on **new samples** of this distribution

Goal of Performance Estimation

Main Goal of Performance Estimation

Obtain a **reliable estimate** of the expected prediction error of a model on the unknown data distribution

- In order to be reliable it should be based on evaluation on unseen cases - *a test set*

Goal of Performance Estimation (2)

- Ideally we want to repeat the testing several times
- This way we can collect a series of scores and provide as our estimate the average of these scores, together with the standard error of this estimate
- In summary:
  - calculate the sample mean prediction error on the repetitions as an estimate of the true population mean prediction error
  - complement this sample mean with the standard error of this estimate

Goal of Performance Estimation (3)

- The golden rule of Performance Estimation:

The data used for evaluating (or comparing) any models cannot be seen during model development.

Goal of Performance Estimation (4)

- An experimental methodology should:
  - Allow obtaining several prediction error scores of a model, $E_1, E_2, \cdots, E_k$
  - Such that we can calculate a sample mean prediction error

$$\overline{E} = \frac{1}{k}\sum_{i=1}^{k} E_i$$

  - And also the respective standard error of this estimate

$$SE(\overline{E}) = \frac{s_E}{\sqrt{k}}$$

  where s_E is the sample standard deviation of E measured as $\sqrt{\frac{1}{k-1}\sum_{i=1}^{k}(E_i - \overline{E})^2}$

The Holdout Method and Random Subsampling

- The holdout method consists on **randomly dividing the available data sample in two sub-sets** - one used for training the model; and the other for testing/evaluating it
  - A frequently used proportion is 70% for training and 30% for testing

The Holdout Method (2)

- If we have a small data sample there is the danger of either having a too small test set (unreliable estimates as a consequence), or removing too much data from the training set (worse model than what could be obtained with the available data)
- We only get one prediction error score - no average score nor standard error
- If we have a very large data sample this is actually the preferred evaluation method

Random Subsampling

- The Random Subsampling method is a variation of holdout method and it simply consists of repeating the holdout process several times by randomly selecting the train and test partitions
- Has the same problems as the holdout with the exception that we already get several scores and thus can calculate means and standard errors
- If the available data sample is too large the repetitions may be too demanding in computation terms

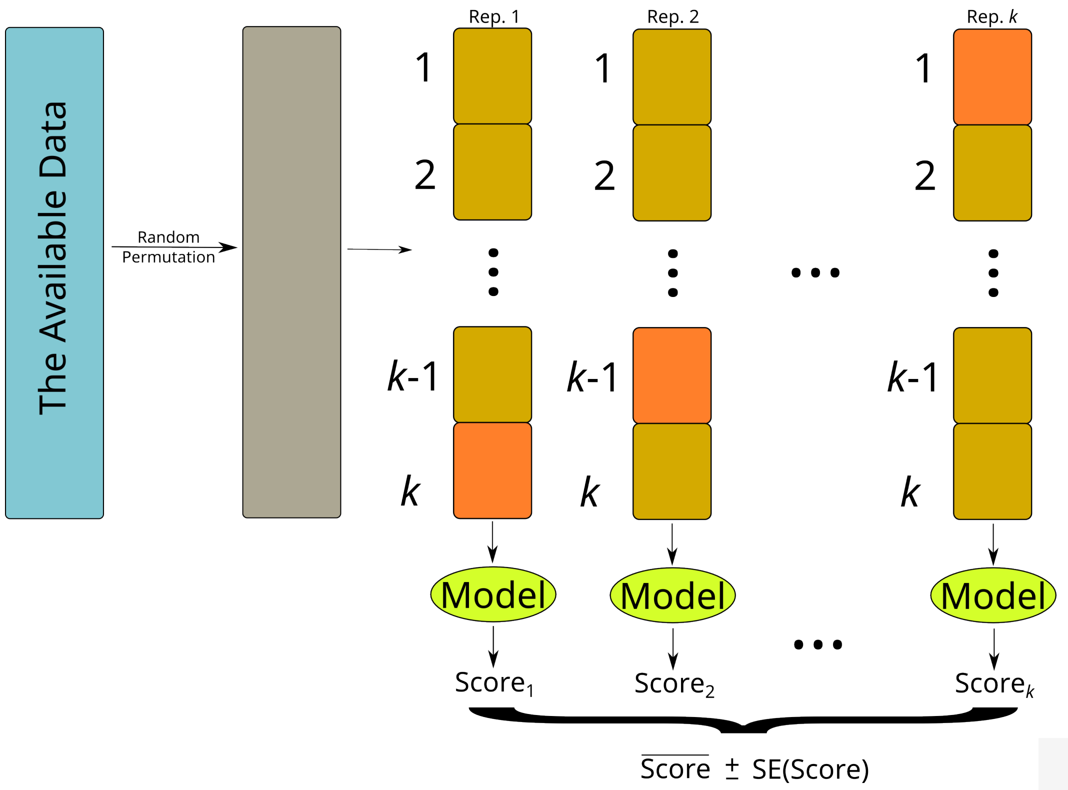
The Holdout method in R

```
library(DMwR2)
set.seed(1234)
data(Boston,package='MASS')
## random selection of the holdout
trPerc <- 0.7
sp <- sample(1:nrow(Boston),as.integer(trPerc*nrow(Boston)))
## division in two samples
tr <- Boston[sp,]
ts <- Boston[-sp,]
## obtaining the model and respective predictions on the test set
m <- rpartXse(medv ~.,tr)
p <- predict(m,ts)
## evaluation
mean((ts$medv-p)^2)

## [1] 22.1313
```


The k-fold Cross Validation Method

- The idea of k-fold Cross Validation (CV) is similar to random subsampling
- It essentially consists of *k* repetitions of training on part of the data and then test on the remaining
- The diference lies on the way the partitions are obtained

The k-fold Cross Validation Method (cont.)



Leave One Out Cross Validation Method (LOOCV)

- Similar idea to k-fold Cross Validation (CV) but in this case on each iteration a single case is left out of the training set
- This means it is essentially equivalent to *n*-fold CV, where *n* is the size of the available data set

The Bootstrap Method

- Train a model on a random sample of size *n* with replacement from the original data set (of size *n*)
  - Sampling with replacement means that after a case is randomly drawn from the data set, it is "put back on the sampling bag"
  - This means that several cases will appear more than once on the training data
  - On average only 63.2% of all cases will be on the training set
- Test the model on the cases that were not used on the training set
- Repeat this process many times (typically around 200)
- The average of the scores on these repetitions is known as the ϵ_0 bootstrap estimate
- The .632 bootstrap estimate is obtained by $.368 \times \epsilon_r + .632 \times \epsilon_0$, where ϵ_r is the resubstitution estimate

Bootstrap in R

```
data(Boston,package='MASS')
nreps <- 200
scores <- vector("numeric",length=nreps)
n <- nrow(Boston)
set.seed(1234)
for(i in 1:nreps) {
   # random sample with replacement
   sp <- sample(n,n,replace=TRUE)
   # data splitting
   tr <- Boston[sp,]
   ts <- Boston[-sp,]
   # model learning and prediction
   m <- lm(medv ~.,tr)
   p <- predict(m,ts)
   # evaluation
   scores[i] <- mean((ts$medv-p)^2)
}
# calculating means and standard errors
summary(scores)

##    Min. 1st Qu.  Median    Mean 3rd Qu.    Max.
##   16.37   21.70   24.20   24.56   26.47   48.82
```

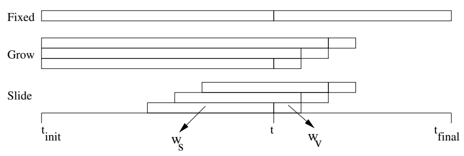
Evaluation with Time Series Data

- Most common evaluation methods revolve around resampling
  - Simulating the reality.
    - Obtain an evaluation estimate for unseen data.
- Resampling randomly permutes the order of the rows in the data sets
- Time series data are Special!
  - The order of the rows has a meaning - cannot be changed!

Correct Evalution of Time Series Models

- General Guidelines
  - Do not “forget” the time tags of the observations.
  - Do not evaluate a model on past data.
- A possible method
  - Divide the existing data in two time windows
    - Past data (observations till a time t).
    - “Future” data (observations after t).
  - Use one of these three learn-test alternatives
    - Fixed learning window.
    - Growing window.
    - Sliding window.

Learn-Test Strategies



Fixed Window

A single model is obtained with the available “training” data, and applied to all test period.

Growing Window

Every w_v test cases a new model is obtained using all data available till then.

Sliding Window

Every w_v test cases a new model is obtained using the previous w_s observations of the time series.

Dealing with model selection

- Most modelling techniques involve some form of parameters that usually need to be tunned.
- The following describes an evaluation methodology considering this issue:

	y_1 • • • y_s	• • • y_t	• • • y_n
Stage 1	Data used for obtaining the model alternatives	Model tunning and selection period	
Stage 2	Data used for obtaining the selected model alternative / variant		Final Evaluation Period

Some Metrics for Evaluating Predictive Performance

Absolute Measures

- Mean Squared Error (MSE)

$$MSE = \frac{1}{n}\sum_{i=1}^{n}(\hat{x}_i - x_i)^2$$

- Mean Absolute Deviation (MAD)

$$MAD = \frac{1}{n}\sum_{i=1}^{n}|\hat{x}_i - x_i|$$

Relative Measures

- Theil Coefficient

$$U = \frac{\sqrt{\sum_{i=1}^{n}(\hat{x}_i - x_i)^2}}{\sqrt{\sum_{i=1}^{n}(x_i - x_{i-1})^2}}$$

- Mean Absolute Percentage Error (MAPE)

$$MAPE = \frac{1}{n}\sum_{i=1}^{n}\left|\frac{(\hat{x}_i - x_i)}{x_i}\right|$$

The Metrics in R

```
set.seed(1234)
library(xts)
someSeries <- xts(rnorm(1000),seq.Date(from=Sys.Date(), length.out=1000,
                                        by ="1 day"))
somePreds <- xts(rnorm(1000),seq.Date(from=Sys.Date(), length.out=1000,
                                       by ="1 day"))
(mse <- mean((someSeries-somePreds)^2))

## [1] 1.846431

(mad <- mean(abs(someSeries-somePreds)))

## [1] 1.070021

(U <- sqrt(sum(((someSeries-somePreds)^2)[-1])) /
     sqrt(sum(((someSeries-lag(someSeries,1))^2)[-1])))

## [1] 0.9771318

(mape <- mean(abs((someSeries-somePreds)/someSeries)))

## [1] 4.551463
```

The Goal of an Experimental Comparison with Time Series Data

- Given a set of observations of a time series X.
- Given a set of alternative modelling approaches M.
- Obtain estimates of the predictive performance of each m_i for this time series.

More specifically,
given a forecasting period size, w_{test},
and a predictive performance statistic, Err,
we want to obtain a reliable estimate of the value of Err
for each m_i.

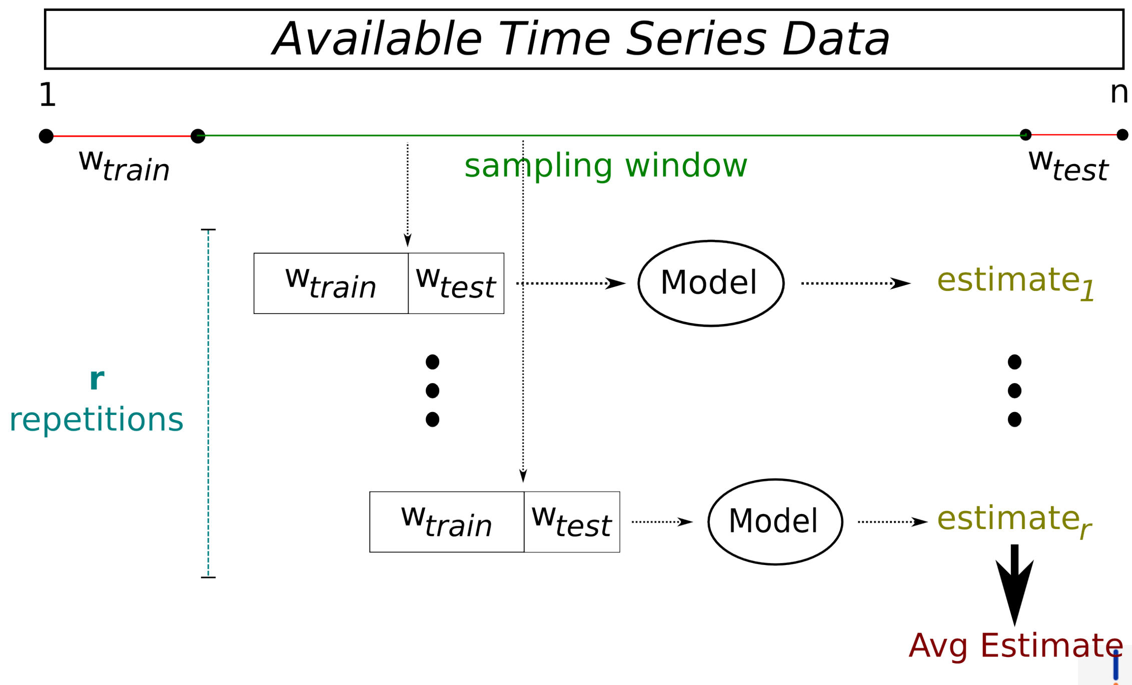
Using Monte Carlo Simulations for Obtaining Reliable Estimates of *Err*

- A possible approach would be to use our proposed method of Model Selection.
- This would give us one estimate of Err.
- More reliability is achievable if more repetitions of the process are carried out.

Monte Carlo Estimates for Time Series Forecasting

Given: a time series, a training window size, w_{train}, a testing window size, w_{test}, and a number of repetitions, r,
- randomly generate r points in the interval $]w_{train}..(n - w_{test})[$,
- for each point proceed according to our Model Selection strategy.

Using Monte Carlo Simulations for Obtaining Reliable Estimates of *Err* - 2



The Infra-Structure of package **performanceEstimation**

- The package **performanceEstimation** provides a set of functions that can be used to carry out comparative experiments of different models on different predictive tasks
- This infra-structure can be applied to any model/task/evaluation metric
- Installation:
  - Official release (from CRAN repositories):

```r
install.packages("performanceEstimation")
```

  - Development release (from Github):

```r
library(devtools)  # You need to install this package before!
install_github("ltorgo/performanceEstimation",ref="develop")
```

The Infra-Structure of package **performanceEstimation**

- The main function of the package is `performanceEstimation()`
  - It has 3 arguments:
    1. The predictive tasks to use in the comparison
    2. The models to be compared
    3. The estimation task to be carried out
- The function implements a wide range of experimental methodologies including all we have discussed

A Simple Example

- Suppose we want to estimate the mean squared error of regression trees in a certain regression task using cross validation

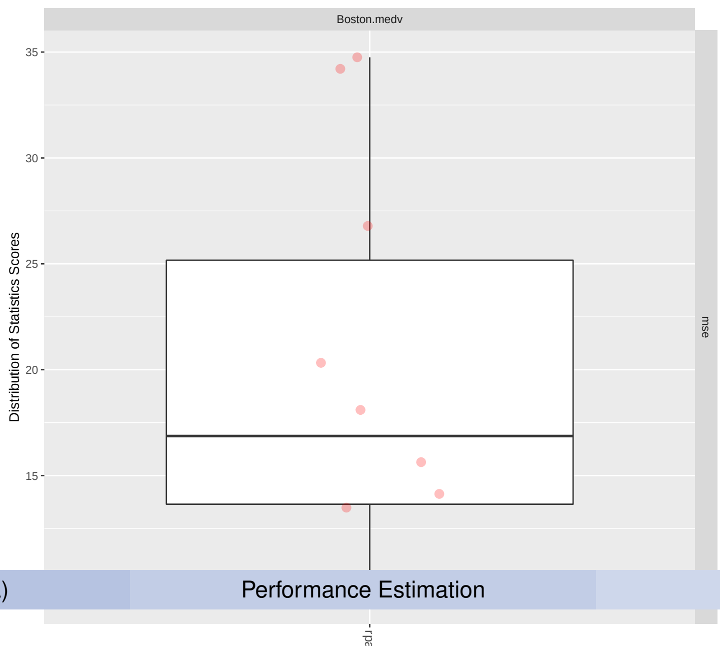
```
library(performanceEstimation)
library(DMwR2)
data(Boston,package='MASS')
res <- performanceEstimation(
    PredTask(medv ~ .,Boston),
    Workflow("standardWF",learner="rpartXse"),
    EstimationTask(metrics="mse",method=CV(nReps=1,nFolds=10)))
```

A Simple Example (2)

```
summary(res)

##
## == 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 ::  Boston.medv
## * Workflows  ::  rpartXse
##
## -> Task:  Boston.medv
##   *Workflow: rpartXse
##                 mse
## avg      19.610531
## std       9.375305
## med      16.867969
## iqr      11.523275
## min       9.266761
## max      34.752888
## invalid  0.000000
```


A Simple Example (3)

```
plot(res)

## Registered S3 methods overwritten by 'ggplot2':
##  method         from
##  [.quosures     rlang
##  c.quosures     rlang
##  print.quosures rlang
```



Predictive Tasks

- Objects of class **PredTask** describing a predictive task
  - Classification
  - Regression
  - Time series forecasting
- Created with the constructor with the same name

```
data(iris)
PredTask(Species ~ ., iris)

## Prediction Task Object:
##   Task Name          :: iris.Species
##   Task Type          :: classification
##   Target Feature     :: Species
##   Formula            :: Species ~ .
##   Task Data Source   :: iris

PredTask(Species  ~ ., iris,"IrisDS",copy=TRUE)

## Prediction Task Object:
##   Task Name          :: IrisDS
##   Task Type          :: classification
##   Target Feature     :: Species
##   Formula            :: Species ~ .
##   Task Data Source   :: internal  150x5 data frame.
```


Workflows

- Objects of class **Workflow** describing an approach to a predictive task
  - Standard Workflows
    - Function `standardWF` for classification and regression
    - Function `timeseriesWF` for time series forecasting
  - User-defined Workflows

Standard Workflows for Classification and Regression Tasks

```
library(e1071)
Workflow("standardWF",learner="svm",learner.pars=list(cost=10,gamma=0.1))

## Workflow Object:
##  Workflow ID       ::  svm
##  Workflow Function ::  standardWF
##       Parameter values:
##   learner  -> svm
##   learner.pars  -> cost=10 gamma=0.1
```

"standardWF" can be omitted ...

```
Workflow(learner="svm",learner.pars=list(cost=5))

## Workflow Object:
##  Workflow ID       ::  svm
##  Workflow Function ::  standardWF
##       Parameter values:
##   learner  -> svm
##   learner.pars  -> cost=5
```


The Infra-Structure of package performanceEstimation   Workflows and Workflow Variants

Standard Workflows for Classification and Regression Tasks (cont.)

- Main parameters of the constructor:
  - Learning stage
    - `learner` - which function is used to obtain the model for the training data
    - `learner.pars` - list with the parameter settings to pass to the learner
  - Prediction stage
    - `predictor` - function used to obtain the predictions (defaults to `predict()`)
    - `predictor.pars` - list with the parameter settings to pass to the predictor

Standard Workflows for Classification and Regression Tasks (cont.)

- Main parameters of the constructor (cont.):
  - Data pre-processing
    - `pre` - vector with function names to be applied to the training and test sets before learning
    - `pre.pars` - list with the parameter settings to pass to the functions
  - Predictions post-processing
    - `post` - vector with function names to be applied to the predictions
    - `post.pars` - list with the parameter settings to pass to the functions

Standard Workflows for Classification and Regression Tasks (cont.)

```
data(algae,package="DMwR2")
res <- performanceEstimation(
    PredTask(a1 ~ .,algae[,1:12],"A1"),
    Workflow(learner="lm",pre="centralImp",post="onlyPos"),
    EstimationTask("mse",method=CV())       # defaults to 1x10-fold CV
                             )

##
##
## ##### PERFORMANCE ESTIMATION USING  CROSS VALIDATION  #####
##
## ** PREDICTIVE TASK :: A1
##
## ++ MODEL/WORKFLOW :: lm
## Task for estimating  mse  using
##  1 x 10 - Fold Cross Validation
##   Run with seed =  1234
## Iteration :**********
```

Evaluating Variants of Workflows

Function `workflowVariants()`

Sometimes you want to evaluate different parameter variants of the same workflow - that is the goal of function `workflowVariants()`. It produces a vector of **Workflow** objects without having to specify all of them.

```
library(e1071)
data(Boston,package="MASS")
res2 <- performanceEstimation(
    PredTask(medv ~ .,Boston),
    workflowVariants(learner="svm",
                     learner.pars=list(cost=1:5,gamma=c(0.1,0.01))),
    EstimationTask(metrics="mse",method=CV()))
```


Evaluating Variants of Workflows (cont.)

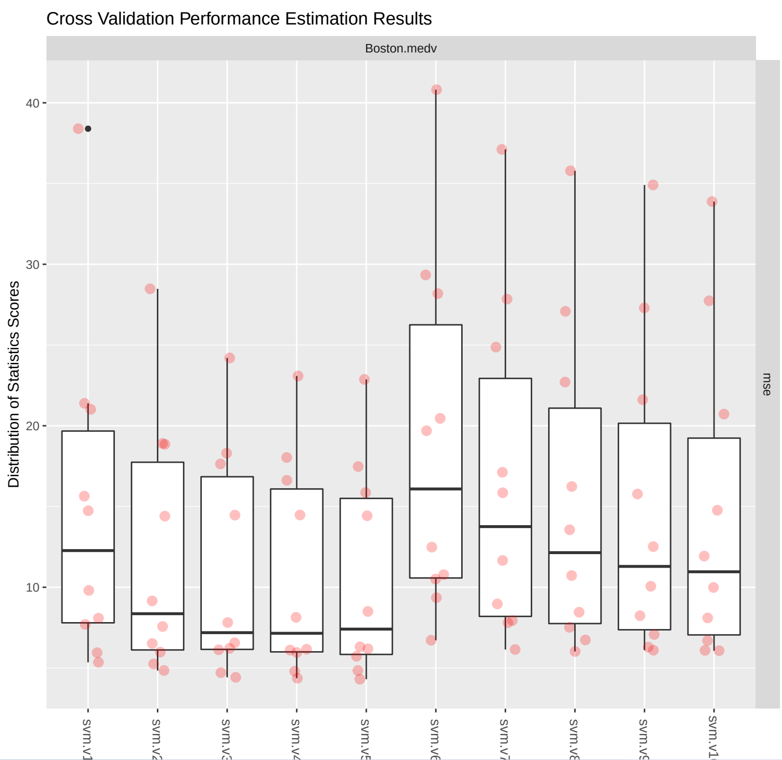
```
summary(res2)

##
## == 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 ::  Boston.medv
## * Workflows  ::  svm.v1, svm.v2, svm.v3, svm.v4, svm.v5, svm.v6, svm.v7, svm.v8, svm.v9, svm.v10
##
## -> Task:  Boston.medv
##   *Workflow: svm.v1
##                mse
## avg     14.80685
## std     10.15295
## med     12.27015
## iqr     11.87737
## min      5.35198
## max     38.39681
## invalid  0.00000
##
##   *Workflow: svm.v2
##                 mse
## avg     11.995178
## std      7.908371
## med      8.359433
## iqr     11.626306
## min      4.842848
## invalid  0.000000
##
```

Exploring the Results

```
getWorkflow("svm.v1",res2)

## Workflow Object:
##  Workflow ID       ::  svm.v1
##  Workflow Function ::  standardWF
##       Parameter values:
##   learner.pars  -> cost=1 gamma=0.1
##   learner  -> svm

topPerformers(res2)

## $Boston.medv
##      Workflow Estimate
## mse    svm.v5    10.65
```


Visualizing the Results

```
plot(res2)
```



Estimation Tasks

- Objects of class **EstimationTask** describing the estimation task
  - Main parameters of the constructor
    - **metrics** - vector with names of performance metrics
    - **method** - object of class **EstimationMethod** describing the method used to obtain the estimates

```
EstimationTask(metrics=c("F","rec","prec"),method=Bootstrap(nReps=100))

## Task for estimating  F,rec,prec  using
## 100  repetitions of  e0  Bootstrap experiment
##   Run with seed =  1234
```


The Infra-Structure of package performanceEstimation Estimation Tasks

Performance Metrics

- Many classification and regression metrics are available
  - Check the help page of functions `classificationMetrics` and `regressionMetrics`
- User can provide a function that implements any other metric she/he wishes to use
  - Parameters **evaluator** and **evaluator.pars** of the `EstimationTask` constructor

Comparing Different Algorithms on the Same Task

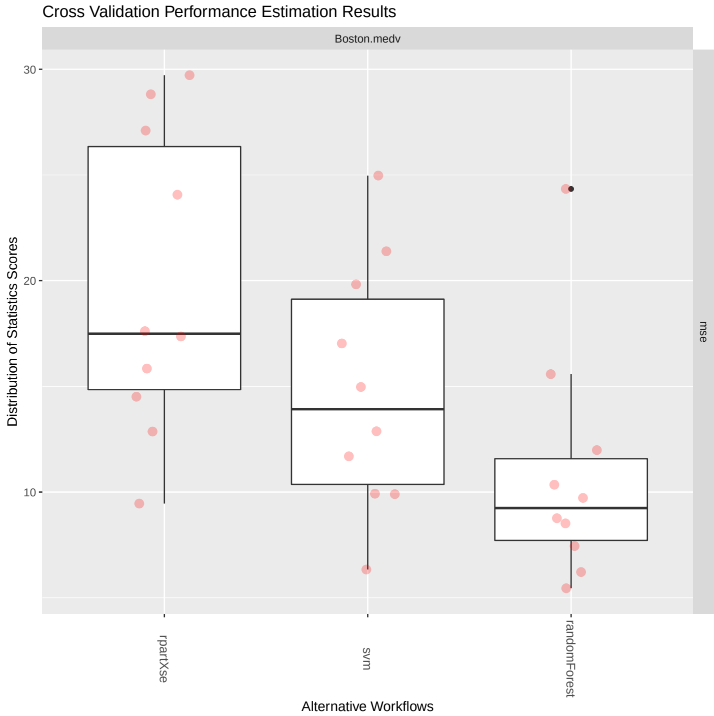
```r
library(randomForest)
library(e1071)
res3 <- performanceEstimation(
    PredTask(medv ~ ., Boston),
    workflowVariants("standardWF",
             learner=c("rpartXse","svm","randomForest")),
    EstimationTask(metrics="mse",method=CV(nReps=2,nFolds=5)))
```


Some auxiliary functions

```r
rankWorkflows(res3,3)

## $Boston.medv
## $Boston.medv$mse
##       Workflow Estimate
## 1 randomForest 10.83722
## 2          svm 14.89183
## 3     rpartXse 19.73468
```

The Results

```
plot(res3)
```

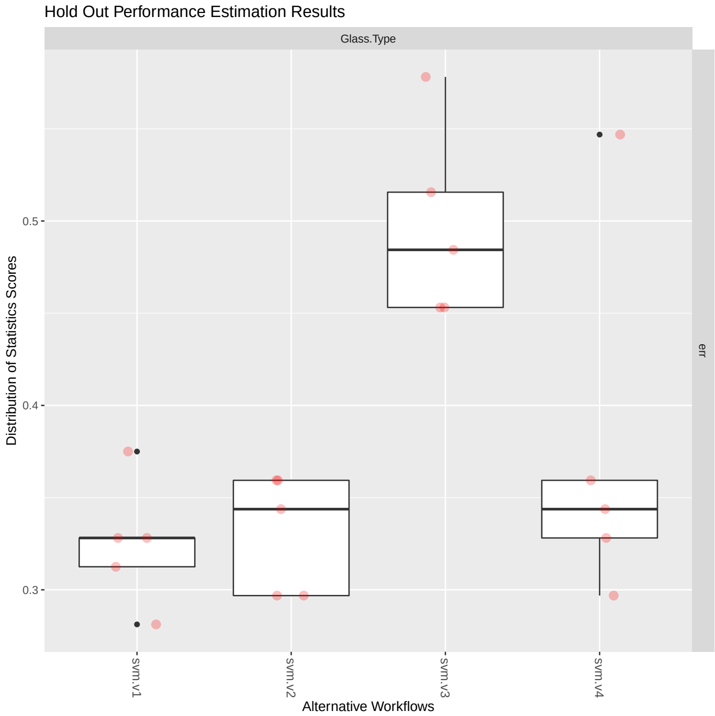


An example using Holdout and a classification task

```
data(Glass,package='mlbench')
res4 <- performanceEstimation(
    PredTask(Type ~ ., Glass),
    workflowVariants(learner="svm",   # You may omit "standardWF" !
                     learner.pars=list(cost=c(1,10),
                                       gamma=c(0.1,0.01))),
    EstimationTask(metrics="err",method=Holdout(nReps=5,hldSz=0.3)))
```

The Results

```
plot(res4)
```

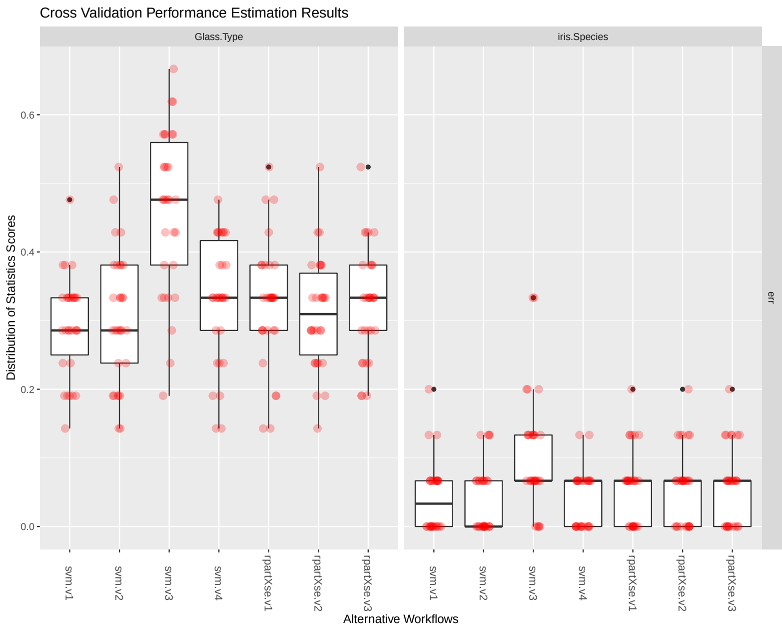


An example involving more than one task

```
data(Glass,package='mlbench')
data(iris)
res5 <- performanceEstimation(
    c(PredTask(Type ~ ., Glass),PredTask(Species ~.,iris)),
    c(workflowVariants(learner="svm",
                       learner.pars=list(cost=c(1,10),
                                         gamma=c(0.1,0.01))),
      workflowVariants(learner="rpartXse",
                       learner.pars=list(se=c(0,0.5,1)),
                       predictor.pars=list(type="class"))),
    EstimationTask(metrics="err",method=CV(nReps=3)))
```

The Results

```r
plot(res5)
```



The Results (2)

```r
topPerformers(res5)

## $Glass.Type
##      Workflow Estimate
## err    svm.v1    0.294
##
## $iris.Species
##      Workflow Estimate
## err    svm.v2     0.04

topPerformer(res5,"err","Glass.Type")

## Workflow Object:
##  Workflow ID        ::  svm.v1
##  Workflow Function ::  standardWF
##       Parameter values:
##   learner.pars  -> cost=1 gamma=0.1
##   learner  -> svm
```

An example involving time series

First getting the data and building an illustrative data set

```
library(quantmod)
library(lubridate)
getSymbols("GOOGL",from=Sys.Date() - years(5))

## [1] "GOOGL"

gg <- Delt(Cl(GOOGL))
library(DMwR2)
library(TTR)
dat <- createEmbedDS(gg, emb=7)
dat <- data.frame(cbind(lag(gg,-1),
                        dat,
                        MA10=SMA(gg,10),
                        RSI=RSI(gg),
                        BB=BBands(gg)$pctB))
colnames(dat)[1] <- "FutureT"
dat <- na.omit(dat)
```


An example involving time series - 2

Now comparing models

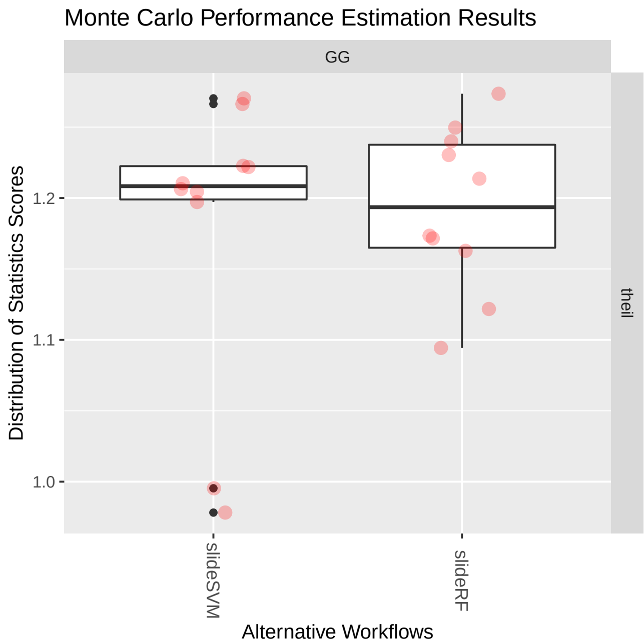
```
library(e1071)
library(randomForest)
tsExp <- performanceEstimation(
    PredTask(FutureT ~ .,dat,'GG'),
    c(Workflow('timeseriesWF',wfID="slideSVM",
               type="slide",relearn.step=90,
               learner='svm',learner.pars=list(cost=10,gamma=0.01)),
      Workflow('timeseriesWF',wfID="slideRF",
               type="slide",relearn.step=90,
               learner='randomForest',learner.pars=list(ntrees=500))
      ),
    EstimationTask(metrics="theil",
                   method=MonteCarlo(nReps=10,szTrain=0.5,szTest=0.25)))
```

Checking the results

```
summary( tsExp )

##
## == Summary of a  Monte Carlo Performance Estimation Experiment ==
##
## Task for estimating  theil  using
## 10  repetitions Monte Carlo Simulation using:
##   seed =  1234
##   train size =  0.5 x NROW(DataSet)
##   test size =  0.25 x NROW(DataSet)
##
## * Predictive Tasks ::  GG
## * Workflows  ::  slideSVM, slideRF
##
## -> Task:  GG
##   *Workflow: slideSVM
##                theil
## avg     1.17730919
## std     0.10350654
## med     1.20835823
## iqr     0.02347964
## min     0.97822580
## max     1.27029812
## invalid 0.00000000
##
##   *Workflow: slideRF
##                theil
## avg     1.19310303
## std     0.05801541
## med     1.19355379
## min     1.09432688
## max     1.27353411
## invalid 0.00000000
```


Checking the results - 2

```
plot( tsExp )
```



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