

An Infra-Structure for Performance Estimation and Experimental Comparison on Predictive Models

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December 28, 2013

Abstract

This document describes an infra-structure provided by the R package **performanceEstimation** that allows to estimate the predictive performance of different approaches (workflows) to predictive tasks. The infra-structure is generic in the sense that it can be used to estimate the values of any performance metrics, for any workflow on different predictive tasks, namely, classification, regression and time series tasks. The package also includes several standard workflows that allow users to easily set up their experiments limiting the amount of work and information they need to provide. The overall goal of the infra-structure provided by our package is to facilitate the task of estimating the predictive performance of different modeling approaches to predictive tasks in the R environment.

1 Introduction

The goal of this document is to describe the infra-structure that is available in package **performanceEstimation** to estimate the performance of different approaches to predictive tasks. The main goal of this package is to provide a general infra-structure that can be used to estimate the performance using several predictive performance metrics of any modelling approach to different predictive tasks, with a minimal effort from the user. The package provides this type of facilities for classification, regression and time series tasks. There is no limitation on the type of approaches to these tasks for which you can estimate the performance - the user just needs to provide a workflow function (following some interface rules) that implements the approach for which the predictive performance is to be estimated. The package includes some standard workflow functions that implement the standard learn+test+evaluate approach that most users will be interested in. This means that if you just want to estimate the performance of some variants of a method already implemented in R (e.g. an SVM), on some particular tasks, you will be able to use these standard workflow functions and thus your input will be limited to the minimum. The package also provides a series of predictive performance metrics for different tasks. Still, you

are not limited to these metrics and can use any metric as long as it exists in R or you provide a function calculating it.

This infra-structure implements different methods for estimating the predictive performance. Namely, you can select among: (i) cross validation, (ii) holdout and random subsampling, (iii) leave one out cross validation, (iv) (ϵ_0 and .631) bootstrap and also (v) Monte-Carlo experiments for time series forecasting tasks. For each of these tasks different options are implemented (e.g. use of stratified sampling).

Most of the times experimental methodologies for performance estimation are iterative processes that repeat the modelling task several times using different data samples with the goal of improving the accuracy of the estimates. The estimates are the result of aggregating the scores obtained on each of the repetitions. For each of these repetitions different training and testing samples are generated and the process being evaluated is "asked" to: (i) obtain the predictive model using the training data, and then (ii) use this model to obtain predictions for the respective test sample, which in turn (iii) can be used to calculate the scores of the performance metrics being estimated. This means that there is a workflow that starts with a predictive task for which training and testing samples are given, and that it should produce as result the scores of the performance metrics being estimated. There are far too many possible approaches and sub-steps for the implementation of this workflow. To ensure full generality of the infra-structure, we ask the user to provide a function that implements this workflow for each of the predictive approaches he/she wishes to compare and/or evaluate. This function can be parametrizable in the sense that there may be variants of the workflow that the user wishes to evaluate and/or compare. Still, the goal of this workflow implementation functions is very clear: (i) receive as input a predictive task for which training and test samples are given, as well as any eventual workflow specific parameters; and (ii) produce as result a set of scores for the evaluation metrics being estimated. These scores should be obtained by applying some modelling technique to the training sample and then use the resulting to model to obtain predictions for the test sample. These predictions should then be used to obtain the scores of the predictive metrics for which the user is interested in obtaining reliable estimates.

The infra-structure we describe here provides means for the user to indicate: (i) a set of predictive tasks with the respective data sets; (ii) a set of workflows and respective variants; and (iii) an experimental methodology. The infra-structure then takes care of all the process of experimentally estimating the predictive performance of the different approaches on the tasks, producing as result an object that can be explored in different ways to obtain the results of the estimation process. The infra-structure also provides several utility functions to explore these results objects, for instance to obtain summaries of the estimation process both in textual format as well as visually. Moreover, it also provides functions that carry out statistical significance tests based on the outcome of the experiments.

Finally, the infra-structure provides utility functions implementing frequently used workflows for common modelling techniques, as well as functions that facilitate the automatic generation of variants of workflows by specifying sets of parameters that the user wishes to consider in the comparisons.

2 A Simple Illustrative Example

Let us assume we are interested in estimating the predictive performance of several variants of an SVM on the **Iris** classification problem. More specifically, we want to obtain a reliable estimate of the error rate of these variants using 10-fold cross validation. The following code illustrates how these estimates could be obtained with our proposed infra-structure.

```
library(performanceEstimation) # Loading our infra-structure
library(e1071)                 # A package containing SVMs

data(iris)                     # The data set we are going to use

res <- performanceEstimation(
  PredTask(Species ~ .,iris),
  workflowVariants('standardWF',
    learner='svm',
    learner.pars=list(cost=c(1,5,10),gamma=c(0.1,0.001))
  ),
  CvSettings(nReps=1,nFolds=10))
```

This simple example illustrates several key concepts of our infra-structure. First of all, we have the main function - `performanceEstimation()`, which is used to carry out the estimation process. It has 3 arguments: (i) a vector of predictive tasks (in the example a single one); (ii) a vector of workflows; and (iii) the estimation settings.

Predictive tasks are S4 objects of class **PredTask**. This class, also defined in our package, describes a predictive task by: (i) a formula; (ii) the source data set (an R data frame); and (iii) an optional name of the task (a string).

Workflows are S4 objects of class **Workflow**, which are also defined within the package. These objects include two pieces of information: (i) the name of the function (a string) implementing the workflow; and (ii) the list of parameters to this function. The function will be called from within `performanceEstimation()` with a formula in the first argument, a training sample (a data frame) on the second argument, a test sample (another data frame) on the third, and then all the parameters the user specifies in the list of parameters used when creating the **Workflow** object. This means that the object

```
Workflow('svmTrial',pars=list(cost=10,gamma=0.5)),
```

if used in a call to `performanceEstimation`, will generate calls of the type `svmTrial(someFormula, someTrainingSample, someTestSample, cost=10, gamma=0.5)`. In the illustrative example above we are using the function `workflowVariants()` from our package to automatically generate a vector of **Workflow** objects. This function can be used to generate different variants of a workflow function using all combinations of some parameters of the workflow. In the code above the workflow function is `standardWF` which is another auxiliary function we provide. This function implements a typical workflow for different modelling techniques that are indicated through its parameter `learner`. Above we are using it to generate variants of calls to the `svm()` function, which is an implementation of an SVM available in package `e1071` [MDH⁺12]. Later we will provide more details on the `standardWF` function. For now we can think of the call to the `workflowVariants()` function as generating the following vector:

```

c(Workflow('standardWF',
  pars=list(learner='svm',
    learner.pars=list(cost=1,gamma=0.1))
),
Workflow('standardWF',
  pars=list(learner='svm',
    learner.pars=list(cost=5,gamma=0.1))
),
...
...
)

```

The workflow implemented through function `standardWF()` by default calculates the error rate of the used modelling techniques if handling classification tasks, though we will see later that we can specify other metrics.

Finally, the third parameter of the function `performanceEstimation()` specifies the estimation settings to use in the process. It is an S4 object of class **EstimationSettings** that in effect is an union that includes among others the S4 class **CvSettings**. Objects of this latter class include information on the number of repetitions of the cross validation process (in our example 1 single repetition, which is the default), the number of folds (10 above, which is also the default), the random number generator seed and a logical indicating whether stratified samples should be used (defaulting to `FALSE`, i.e. no stratification).

The result of the call to `performanceEstimation()` is an S4 object of the class **ComparisonResults**. These objects typically are not directly explored by the end-user so we omit their details here¹. There are several utility functions that allow the users to explore the results of the experimental comparisons. Here are a few illustrative examples:

```

summary(res)

##
## == Summary of a Cross Validation Performance Estimation Experiment ==
## 1 x 10 - Fold Cross Validation run with seed = 1234
##
## * Predictive Tasks :: iris
## * Workflows :: svm.v1, svm.v2, svm.v3, svm.v4, svm.v5, svm.v6
##
## * Summary of Experiment Results:
##
## -> Dataset: iris
##
## *Workflow: svm.v1
##      err
## avg      0.04667
## std      0.05488
## min      0.00000
## max      0.13333
## invalid 0.00000
##
## *Workflow: svm.v2
##      err
## avg      0.04000

```

¹Interested readers may have a look at the corresponding help page - `class?ComparisonResults`.

```

## std      0.04661
## min      0.00000
## max      0.13333
## invalid  0.00000
##
## *Workflow: svm.v3
##          err
## avg      0.04000
## std      0.04661
## min      0.00000
## max      0.13333
## invalid  0.00000
##
## *Workflow: svm.v4
##          err
## avg      0.6867
## std      0.2014
## min      0.3333
## max      0.9333
## invalid  0.0000
##
## *Workflow: svm.v5
##          err
## avg      0.15333
## std      0.11780
## min      0.06667
## max      0.46667
## invalid  0.00000
##
## *Workflow: svm.v6
##          err
## avg      0.10667
## std      0.06441
## min      0.00000
## max      0.20000
## invalid  0.00000

```

The generic function `summary` allows us to obtain the estimated scores for each compared approach on each predictive task. For each performance metric (in this case only the error rate), the function shows the estimated average performance, the standard error of this estimate as well as minimum and maximum scores on the different iterations of the experimental comparison. Moreover, information is also given on eventual failures on some of the iterations.

The best scores for each predictive task and metric can be obtained as follows:

```

topPerformers(res)

## $iris
##      Workflow Estimate
## err   svm.v2      0.04

```

The generic function `plot` can be used to obtain a graphical display of the distribution of performance metrics across the different iterations of the estimation process using box-plots, as show in Figure 1.

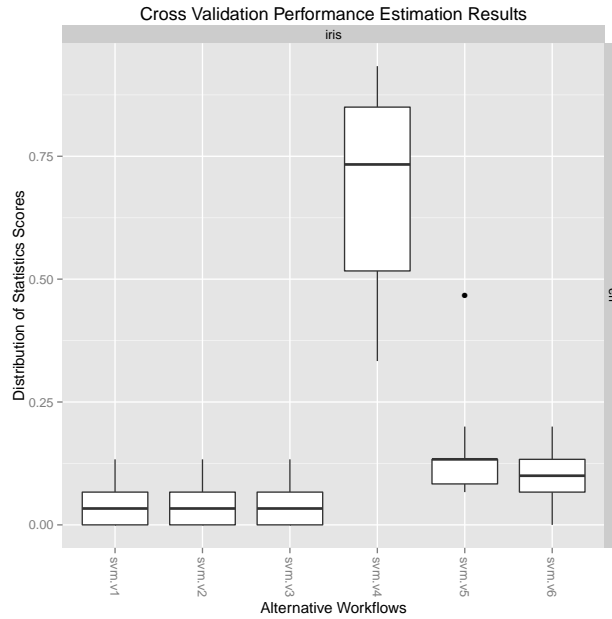


Figure 1: The distribution of the error rate on the 10 folds.

```
plot(res)
```

You might have observed that the infra-structure uses some IDs to describe each workflow variant (e.g. `svm.v1`). The user can check the parameter configuration corresponding to some ID as follows:

```
getWorkflow('svm.v1',res)

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

3 Predictive Tasks

Predictive tasks are data analysis problems where we want to obtain a model of an unknown function $Y = f(X_1, X_2, \dots, X_p)$ that relates a target variable Y with a set of p predictors X_1, X_2, \dots, X_p . The model is usually obtained using a sample of n observations of the mapping of the unknown function, $D = \{(\mathbf{x}_i, Y_i)\}_{i=1}^n$, where \mathbf{x}_i is a vector with the p predictors values and Y_i the respective target variable value. These data sets in R are usually stored in data frames, and formula objects are used to specify the form of the functional

dependency that we are trying to model, i.e. which is the target variable and the predictors.

Objects of class **PredTask** encapsulate the information of a predictive task, i.e. the functional form and the data required for solving it. For convenience they also allow the user to assign a name to each task. These S4 objects can be created using the constructor function `PredTask()`, as seen in the following example:

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

## Prediction Task Object:
## Task Name :: irisClassificationTask
## Formula   :: Species ~ .
## Task Data ::
## 'data.frame': 150 obs. of  5 variables:
## $ Species      : Factor w/ 3 levels "setosa","versicolor",...: 1 1 1 1 1 1 1 1 1 1 ...
## $ Sepal.Length: num  5.1 4.9 4.7 4.6 5 5.4 4.6 5 4.4 4.9 ...
## $ Sepal.Width : num  3.5 3 3.2 3.1 3.6 3.9 3.4 3.4 2.9 3.1 ...
## $ Petal.Length: num  1.4 1.4 1.3 1.5 1.4 1.7 1.4 1.5 1.4 1.5 ...
## $ Petal.Width : num  0.2 0.2 0.2 0.2 0.2 0.4 0.3 0.2 0.2 0.1 ...
```

We should remark that the objects of this class only store the data required for the specified task, as it should be clear from this other simple example:

```
data(iris)
PredTask(Species ~ Petal.Length + Sepal.Length,iris,'ShortIrisTask')

## Prediction Task Object:
## Task Name :: ShortIrisTask
## Formula   :: Species ~ Petal.Length + Sepal.Length
## Task Data ::
## 'data.frame': 150 obs. of  3 variables:
## $ Species      : Factor w/ 3 levels "setosa","versicolor",...: 1 1 1 1 1 1 1 1 1 1 ...
## $ Petal.Length: num  1.4 1.4 1.3 1.5 1.4 1.7 1.4 1.5 1.4 1.5 ...
## $ Sepal.Length: num  5.1 4.9 4.7 4.6 5 5.4 4.6 5 4.4 4.9 ...
```

So, although we have supplied the full data frame to the constructor function, as the task only uses 3 of the columns, the resulting **PredTask** object only includes the information on the columns required for this task.

4 Workflows

Estimation methodologies work most of the times by re-sampling the available data set D in order to create different train and test samples from D (an exception being a single repetition of hold-out). The goal is to estimate the predictive performance of a proposed workflow to solve the task, by using these different samples to increase our confidence on the estimates. This workflow consists on the process of obtaining a model from a given training sample and then use it to obtain predictions for the given test set. This process can include several steps, e.g. specific data pre-processing steps, and may use any modelling approach, eventually developed by the user.

4.1 User-defined Workflows

With the goal of ensuring that the proposed infra-structure is able to cope with all these possible usage scenarios, we ask the user to take care of the writing of a function implementing each workflow being compared/evaluated. These user-defined workflow functions should be written assuming that the first three parameters are: (i) the formula defining the predictive task; (ii) the provided training sample; and (iii) the test sample where to evaluate the obtained model. The functions may eventually accept other arguments with specific parameters of the workflow. The following is a general sketch of a user-defined workflow function:

```
myWorkflow <- function(form,train,test,...,
                      .outPreds=TRUE, .outModel=TRUE) {
  require(mySpecialPackage,quietly=T)
  ## carry out some data pre-processing
  myTrain <- mySpecificPreProcessingSteps(train)
  ## now obtain the model
  myModel <- myModelingTechnique(form,myTrain,...)
  ## obtain the predictions
  preds <- predict(myModel,test)
  ## obtain the evaluation metric scores
  scores <- mySpecialEvaluationMetrics(responseValues(form,test),preds)
  ## finally produce the workflow output object
  res <- WFoutput(scores)
  if (.outPreds)
    workflowPredictions(res) <- list(responseValues(form,test),
                                     preds,
                                     rownames(test))
  if (.outModel) workflowInformation(res) <- list(model=myModel)
  res
}
```

Not all workflows will require all these steps, though some may even require more. This is clearly something that is up to the user. The only strict requirements for these functions are: (i) the first 3 parameters of the workflow function should be the formula, train and test data frames; and (ii) the result of the function should be an object of the S4 class **WFoutput**.

Objects of class **WFoutput** contain the result of applying the workflow to a train+test partition. They are created using the constructor function **WFoutput()** that takes as argument a named vector with the scores of the metrics being estimated. These objects may optionally contain information on the true and predicted values for the target variable in the provided test set, as well as any other information the creator of the workflow function deems important to return. These two optional pieces of information are typically "attached" to the object using the replacement functions **workflowPredictions()** and **workflowInformation()**, respectively. The **workflowPredictions()** function takes as value a list with at least two components. The first component is a vector with the true values of the target variable in the test set. The second component are the corresponding predictions made by the workflow. Finally, you may optionally provide a vector with the names of the rows in the test set. Regarding the **workflowInformation()** function it accepts as value also a list

but whose content is completely free and left to the creator of the workflow function. Both these two functions can also be used to obtain the respective content from **WFoutput** objects, as we will see later in some of the illustrative examples.

The sketch shown above also illustrates the use of the function `responseValues()` that can be used to obtain the values of the target variable given a formula and a data frame.

Users should write one such workflow function for each process they want to evaluate/compare. As mentioned before these functions may accept further parameters on top of the 3 mandatory parameters. These extra parameters will typically be parameters of the modelling technique being used within the workflow but it is up to the user to control this. As we have seen in Section 2 we provide the function `workflowVariants()` to facilitate the specification of different variants of any workflow function by trying all combinations of several of its specific parameters. For instance, if the modelling function in the above example workflow (function `myModelingTechnique()`) had an integer parameter `x` and a Boolean parameter `y`, we could generate several **Workflow** objects to be evaluated/compared using the `performanceEstimation()` function, as follows:

```
workflowVariants('myWorkflow',x=c(0,3,5,7),y=c(T,F))
```

This would generate 8 variants of the same workflow with all combinations of the specified values for the 2 parameters. This means that any parameter of the `workflowVariants()` function that has more than one element is assumed to be a source for generation of variants. There may be situations where this is not intended, because a particular argument of the workflow function is supposed to be a vector. In these cases the user needs to “tell” the `workflowVariants()` function that it should not generate variants from the values of that parameter. Suppose that on the above example the parameter `x` takes as values a vector, and thus your meaning in the above statement is that you only have two variants of the workflow (the different values of the parameter `y`). You could get that effect by calling the `workflowVariants()` function as follows:

```
workflowVariants('myWorkflow',x=c(0,3,5,7),y=c(T,F),as.is=c('x'))
```

While the previous call would generate 8 variants, this one only generates 2.

Let us see a concrete example of a user supplied workflow function. Imagine we want to evaluate a kind of ensemble model formed by a regression tree and a multiple linear regression model on an algae blooms data set [Tor10]. Moreover, let us suppose we are interested in using the correlation between the predictions and true values as evaluation metric. We could start by writing the following workflow function that implements our modelling approach:

```
RLensemble <- function(f,tr,ts,weightRT=0.5,step=FALSE,...) {
  require(DMwR,quietly=F)
  noNAsTR <- knnImputation(tr)
  noNAsTS <- knnImputation(ts)
  r <- rpartXse(f,tr,...)
  l <- lm(f,noNAsTR)
  if (step) l <- step(l,trace=0)
```

```

pr <- predict(r,ts)
pl <- predict(l,noNAsTS)
ps <- weightRT*pr+(1-weightRT)*pl
WfOutput(c(correlation=cor(responseValues(f,ts),ps)))
}

```

This workflow starts by building two modified samples of the training and testing sets, with the NA values being filled in using a nearest neighbour strategy (see the help page of the function `knnImputation()` of package **DMwR** [Tor10] for more details). These versions are to be used by the `lm()` function that is unable to cope with cases with missing values. After obtaining the two models and their predictions the function calculates a weighted average of both predictions before obtaining and returning the respective correlation score.

To evaluate different variants of this workflow we could run the following experiment:

```

data(algae,package='DMwR')
expRes <- performanceEstimation(
  PredTask(a1 ~ .,algae[,1:12],'algal'),
  workflowVariants('RLensemble',
    se=c(0,1),step=c(T,F),weightRT=c(0.4,0.5,0.6)),
  BootSettings(nReps=100,type='e0'))

```

In this experimental comparison we have used 100 repetitions of a ϵ_0 bootstrap estimation procedure as estimation methodology (further details on this and other methodologies will be given later), to compare 12 variants of our workflow.

4.2 Generic Workflows

Writing workflow functions may be tedious on large comparisons, particularly when few details change among them. Moreover, the most frequent use of our infra-structure will probably be to compare existing modelling techniques (or variants of them) on one or more problems. This means that the most frequently used workflows will essentially build a model using some existing algorithm, obtain its predictions and then calculate some standard prediction error metrics. To facilitate this type of tasks, we also provide generic workflow functions that carry out this type of process for any modelling technique. The idea is to save the user from having to write these functions provided his/her workflow fits this generic schema.

4.2.1 Classification and Regression Tasks

Function `standardWF()` implements a typical workflow for both classification and regression tasks. Apart from a formula, a training set data frame and a test set data frame, this function has the following parameters that help the user to specify is intended workflow:

learner - the name of a R function that obtains a model from the training data. This function will be called with a formula in the first argument and the training set data frame in the second.

learner.pars - a list specifying any extra parameter settings that should be added to the formula and training set, at the time the learner function is called (defaults to `NULL`).

predictor - the name of a R function that is able to obtain the predictions of the model obtained with **learner**. This function will be called with the object resulting from the **learner** call on the first argument and the test set data frame in the second (it defaults to function `predict()`).

predictor.pars - a list specifying any extra parameter settings that should be added to the model and test set, at the time the predictor function is called (defaults to `NULL`).

evaluator - the name of a R function that is able to calculate the evaluation metrics you want to estimate based on the predictions of the model and the true values of the target variable on the given test set (it will default to `classificationMetrics()` function if it is a classification task, and to `regressionMetrics()` if a regression task - check the respective help pages to see what are the default metrics that are calculated for each). This function will be called with the values of the target variable in the test set on the first argument and with the result of the call to the predictor function on the second.

evaluator.pars - a list specifying any extra parameter settings that should be added to the true values and predictions, at the time the evaluator function is called (defaults to `NULL`). A typical usage here would be to use the parameter **stats** of functions `classificationMetrics()` and `regressionMetrics()` to specify the metrics you want to calculate, provided you are using these functions as evaluators.

Below you find an example of one of the most frequent type of comparisons users carry out - checking which is the “best” model for a given predictive task. Let us restrict the search to a small set of models for illustrative purposes and let us play with the well-known Boston housing regression task:

```
data(Boston,package='MASS')
library(DMwR)
library(e1071)
library(randomForest)
bostonRes <- performanceEstimation(
  PredTask(medv ~ .,Boston),
  workflowVariants('standardWF',
    learner=c('rpartXse','svm','randomForest')),
  CvSettings(nReps=1,nFolds=10)
)
```

Notice that on this simple example we have used all modelling tools with their default parameter settings which is not necessarily a good idea when we are looking for the best performance. Still, the goal of this illustration is to show you how simple this type of experiments can be if you are using a standard workflow setting. In case you want to use the modelling tools with other parameter

settings then you should separate them in different `workflowVariants()` calls, as shown in the following example:

```
data(Boston, package='MASS')
library(DMwR)
library(e1071)
library(randomForest)
bostonRes <- performanceEstimation(
  PredTask(medv ~ ., Boston),
  c(workflowVariants('standardWF', learner='rpartXse',
    learner.pars=list(se=c(0,1))),
    workflowVariants('standardWF', learner='svm',
    learner.pars=list(cost=c(1,5), gamma=c(0.01,0.1))),
    workflowVariants('standardWF', learner='randomForest',
    learner.pars=list(ntree=c(500,1000)))),
  CvSettings(nReps=1, nFolds=10)
)
```

Notice that this code involves estimating the mean squared error on the Boston Housing task for 8 different models through 10-fold cross validation.

4.2.2 Time Series Tasks

Our infra-structure also includes another generic workflow function that is specific for predictive tasks with time-dependent data (e.g. time series forecasting problems). This workflow function implements two different approaches to the problem of training a model with a set of time-dependent data and then use it to obtain predictions for a test set in the future. These two approaches contrast with the standard approach of learning a model with the available training sample and then use it to obtain predictions for all test period. This standard approach could be applied using the previously described `standardWF()` function. However, there are alternatives to this procedure, two of the most common being the sliding and growing window approaches, which are implemented in another workflow function developed specifically for time series tasks.

Predictive tasks for time-dependent data are different from standard classification and regression tasks because they require that the test samples have time stamps that are more recent than training samples. In this context, experimental methodologies handling these tasks typically do not shuffle the observations to maintain the time ordering in the original data. The most common setup is that we have a L time steps training window containing observations in the period $[t_1, t_L]$ and a F time steps test window typically containing the observations in the time window $[t_{L+1}, t_{L+F}]$.

The idea of the sliding window method is that if we want a prediction for time point t_k belonging to the test interval $[t_{L+1}, t_{L+F}]$ then we can assume that all data from t_{L+1} till t_{k-1} is already past, and thus usable by the model. In this context, it may be wise to use this new data in the interval $[t_{L+1}, t_{k-1}]$ to update the original model obtained using only the initial training period data. This is particularly advisable if we suspect that the conditions may have changed since the training period has ended. Model updating using the sliding window method is carried out by using the data in the L last time steps, i.e. every new model is always obtained using the last L data observations, as if

the training window was slid forward in time. Our `timeseriesWF()` function implements this idea for both time series with a numeric target variable and a nominal target variable. This function has a parameter (`type`) that if set to “slide” will use a sliding window approach. As with the `standardWF()` function, this `timeseriesWF()` function also accepts parameters specifying the learner, predictor, evaluator and their respective parameters. Moreover, this function also includes an extra parameter, named `relearn.step`, which allows the user to establish the frequency of model updating. By default this is every new test sample, i.e. 1, but the user may set a less frequent model-updating policy by using higher values of this parameter.

The idea of the growing window approach is very similar. The only difference is on the data used when updating the models. Whilst sliding window uses the data occurring in the last L time steps, growing window keeps increasing the original training window with the newly available data points, i.e. the models are obtained with increasingly larger training samples. By setting the parameter `type` to “grow” you get the `timeseriesWF()` function to use this method.

5 Estimation Methodologies

There are different ways of providing reliable estimates of the predictive performance of a workflow. Our infra-structure implements some of the most common estimation methods. In this section we briefly describe them and provide short illustrative examples of their use.

5.1 Cross Validation

k -Fold cross validation (CV) is one of the most common methods to estimate the predictive performance of a model. By including an S4 object of class `CvSettings` in the third argument of function `performanceEstimation()` we can carry out experiments of this type.

The function `CvSettings()` can be used as a constructor of objects of class `CvSettings`. It accepts the following parameters:

nReps - the number of repetitions of the k -fold CV experiment (default is 1)

nFolds - the number of k folds to use (default is 10)

seed - the random number generator seed to use (default is 1234)

strat - whether to use stratified samples (default is `FALSE`)

dataSplits - a list containing user-supplied data splits for each of the folds and repetitions (check the help page of the class for further details). This parameter defaults to `NULL`, i.e. no user-supplied splits, they are decided internally by the infra-structure.

Bellow you can find a small illustration using the Breast Cancer data set available in package `mlbench`. On this example we compare some variants of an SVM using a 3×10 -fold cross validation process with stratified sampling because one of the two classes has a considerably lower frequency.

```

data(BreastCancer,package='mlbench')
library(e1071)
library(DMwR)
bc <- knnImputation(BreastCancer[, -1])
bcExp <- performanceEstimation(
  PredTask(Class ~ ., bc, 'BreastCancer'),
  workflowVariants('standardWF',
    learner='svm',
    learner.pars=list(cost=c(1,5), gamma=c(0.01,0.1)),
    evaluator.pars=list(stats=c("F", "prec", "rec"),
                          posClass="malignant")
  ),
  CvSettings(nReps=3, nFolds=10, strat=TRUE))

```

Please note the use of the `evaluator.pars` parameter of the `standardWF()` function. We have used it to indicate several settings to be used in the call to the evaluation function, which by default is `classificationMetrics` in the case of classification problems when using our standard workflow. In this case we are specifying some of the available classification metrics and indicating which of the two classes of the problem is to be considered the positive class².

5.2 Bootstrapping

Bootstrapping or bootstrap resampling is another well-known experimental methodology that is implemented in our infra-structure. Namely, we implement two of the most common methods of obtaining bootstrap estimates: ϵ_0 and .632 bootstrap. By including an S4 object of class **BootSettings** in the third argument of function `performanceEstimation()` we can carry out experiments of this type.

Function `BootSettings()` can be used as a constructor of objects of class **BootSettings**. It accepts the following arguments:

type - a string with the type of bootstrap estimates: either "e0" for ϵ_0 bootstrap, or ".632" for .632 bootstrap (default is "e0")

nReps - the number of repetitions of the bootstrap experiment (default is 200)

seed - the random number generator seed to use (default is 1234)

dataSplits - a list containing user-supplied data splits for each of the repetitions (check the help page of the class for further details). This parameter defaults to `NULL`, i.e. no user-supplied splits, they are decided internally by the infra-structure.

Bellow you can find a small illustration using the Servo data set available in package **mlbench**. On this example we compare some variants of an artificial neural network using 100 repetitions of a bootstrap experiment.

²The F-measure, Recall and Precision metrics are calculated for two-class problems with respect to one of the classes, usually named the "positive" class.

```

data(Servo,package='mlbench')
library(nnet)
nnExp <- performanceEstimation(
  PredTask(Class ~ .,Servo),
  workflowVariants('standardWF',
    learner='nnet',
    learner.pars=list(trace=F,linout=T,
      size=c(3,5),decay=c(0.01,0.1))
  ),
  BootSettings(nReps=100))

```

5.3 Holdout and Random Subsampling

The Holdout is another frequently used experimental methodology, particularly for large data sets. To carry out this type of experiments in our infra-structure we can include an S4 object of class **HldSettings** in the third argument of function `performanceEstimation()`.

Function `HldSettings()` can be used as a constructor of objects of class **HldSettings**. It accepts the following arguments:

nReps - the number of repetitions of the Holdout experiment (default is 1)

hldSz - the percentage of cases (a number between 0 and 1) to leave as holdout (test set) (default is 0.3)

seed - the random number generator seed to use (default is 1234)

strat - whether to use stratified samples (default is FALSE)

dataSplits - a list containing user-supplied data splits for each of the repetitions (check the help page of the class for further details). This parameter defaults to NULL, i.e. no user-supplied splits, they are decided internally by the infra-structure.

Please note that for the usual meaning of Holdout the number of repetitions should be 1 (the default), while larger values of this parameter correspond to what is usually known as random subsampling.

The following is a small illustrative example of the use of the random subsampling with the LetterRecognition classification task from package **mlbench**.

```

data(LetterRecognition,package='mlbench')
ltrExp <- performanceEstimation(
  PredTask(lettr ~ .,LetterRecognition),
  workflowVariants('standardWF',
    learner='rpartXse',
    learner.pars=list(se=c(0,1)),
    predictor.pars=list(type='class')
  ),
  HldSettings(nReps=3,hldSz=0.3))

```

Please note the use of the `predictor.pars` parameter of our `standardWF()` function to be able to cope with the fact that the `predict` method for classification trees requires the use of `type="class"` to get actual predicted class labels instead of class probabilities.

5.4 Leave One Out Cross Validation

Leave one out cross validation is a type of cross validation method that is mostly used for small data sets. You can think of leave one out cross validation as a k -fold cross validation with k equal to the size of the available data set. To carry out this type of experiments in our infra-structure we can include an S4 object of class **LoocvSettings** in the third argument of function `performanceEstimation()`.

Function `LoocvSettings()` can be used as a constructor of objects of class **LoocvSettings**. It accepts the following arguments:

seed - the random number generator seed to use (default is 1234)

verbose - whether the execution of the experiments should provide a verbose form of output (default is `FALSE`)

The following is a small illustrative example of the use of the Holdout with the LetterRecognition classification task from package **mlbench**.

```
data(iris)
library(e1071)
irisExp <- performanceEstimation(
  PredTask(Species ~ ., iris),
  workflowVariants('standardWF',
    learner='svm',
    learner.pars=list(cost=c(1,10))
  ),
  LoocvSettings())
```

5.5 Monte Carlo Experiments

Monte Carlo experiments are similar to random subsampling (or repeated Holdout) in the sense that they consist of repeating a learning + testing cycle several times using different data samples. The main difference lies on the way the samples are obtained. In Monte Carlo experiments the original order of the observations is respected and train and test splits are obtained such that the testing samples appear “after” the training samples, thus being the methodology of choice when you are comparing time series forecasting models. The idea of Monte Carlo experiments is the following: (i) given a data set spanning from time t_1 till time t_N , (ii) given a training set time interval size L and a test set time interval size F , such that $T + F < N$, (iii) Monte Carlo experiments generate R random time points from the interval $[t_{1+T}, t_{N-F}]$, and then (iv) for each of these R time points they generate a training set with data in the interval $[t_{R-T+1}, t_R]$ and a test set with data in the interval $[t_{R+1}, t_{R+F}]$. Using this process R train+test cycles are carried out using the user-supplied workflow

function, and the experiment estimates result from the average of the R scores as usual.

To carry out this type of experiments in our infra-structure we can include an S4 object of class **McSettings** in the third argument of function `performanceEstimation()`.

The function `McSettings()` can be used as a constructor of objects of class **McSettings**. It accepts the following arguments:

nReps - the number of repetitions of the Monte Carlo experiment (default is 10)

szTrain - the percentage (a number between 0 and 1) or the actual number of cases to use in the training samples (default is 0.25)

szTest - the percentage (a number between 0 and 1) or the actual number of cases to use in the test samples (default is 0.25)

seed - the random number generator seed to use (default is 1234)

dataSplits - a list containing user-supplied data splits for each of the repetitions (check the help page of the class for further details). This parameter defaults to NULL, i.e. no user-supplied splits, they are decided internally by the infra-structure.

The following is a small illustrative example using the quotes of the SP500 index. This example compares two random forests with 500 regression trees, one applied in a standard way, and the other using a sliding window with a relearn step of 5 days. The experiment uses 10 repetitions of a train+test cycle using 50% of the available data for training and 25% for testing.

```
library(quantmod)
library(randomForest)
getSymbols('^GSPC',from='2008-01-01',to='2012-12-31')
data.model <- specifyModel(
  Next(100*Delt(Ad(GSPC))) ~ Delt(Ad(GSPC),k=1:10)+Delt(Vo(GSPC),k=1:3))
data <- modelData(data.model)
colnames(data)[1] <- 'PercVarClose'
spExp <- performanceEstimation(
  PredTask(PercVarClose ~ .,data,'SP500_2012'),
  c(Workflow('standardWF',wfID="standRF",
    learner='randomForest',learner.pars=list(ntree=500)),
    Workflow('timeseriesWF',efID,"slideRF",
    learner='randomForest',
    learner.pars=list(ntree=500,relearn.step=5))
  ),
  McSettings(10,0.5,0.25))
```

Note that in the above example we have not tried any variants of the two workflows that are applied to the task. This means that we have used directly the `Workflow` constructor to create our workflow. Note also the use of the `wfID` parameter of this constructor to allow you to give a particular workflow ID to some approach.

6 Statistical Significance of Differences

The estimation methodologies that we have presented in the previous section allow the user to obtain estimates of the mean predictive performance of different workflows or variants of these workflows, on different predictive tasks. We have seen that by applying the `summary` method to the objects resulting from the estimation experiments we can obtain the average performance for each candidate workflow on each task. These numbers are estimates of the expected mean performance of the workflows on the respective tasks. Being estimates, the obvious next question is to check whether the observed differences in performance between the workflows are statistically significant. More formally, we want to know that confidence level of rejecting the null hypothesis that the difference between the estimated averages is zero.

That is the goal of the function `pairedComparisons()`. This function carries out a series of pairwise comparisons between a selected baseline workflow and a set of alternatives. The goal of each of these paired comparisons is to check the confidence we have in rejecting the null hypothesis that the difference between the mean performance of the baseline workflow and that of the alternatives is zero. These paired comparisons are carried out for all predictive tasks included in the estimation process.

Our experimental infra-structure ensures that all compared workflows are run on exactly the same train+test partitions on all repetitions and for all predictive tasks. In this context, we can focus on pairwise statistical significance tests. Given that we cannot ensure that the different iterations are statistically independent (for instance there may be some overlap between the training samples)³, we use the Wilcoxon signed rank test to assess the statistical significance of the differences between every pair of compared workflows. Let us see a concrete example:

```
library(DMwR)
data(LetterRecognition, package='mlbench')
ltrExp <- performanceEstimation(
  PredTask(lettr ~ ., LetterRecognition),
  workflowVariants('standardWF',
    learner='rpartXse',
    learner.pars=list(se=c(0,1)),
    predictor.pars=list(type='class')
  ),
  HldSettings(3,0.3))
```

Using the `topPerformers()` function we can find out the best scoring variant of this comparison of `rpartXse`-based workflows,

```
topPerformers(ltrExp)

## $LetterRecognition
##      Workflow Estimate
## err rpartXse.v1      0.143
```

³That independence can only be ensured for a single repetition of Holdout.

Now we can proceed to check whether the advantage of this variant over the others is statistically significant,

```
pairedComparisons(ltrExp, 'rpartXse.v1')

## , , err, LetterRecognition
##
##           AvgScore  SdScore           Diff p.value
## rpartXse.v1   0.1434 0.005453           NA      NA
## rpartXse.v2   0.1486 0.011612 -0.005222    0.25
```

The function `pairedComparisons()` receives as first argument the object resulting from the comparative experiments. The second argument is the baseline workflow against which you want to compare the others to. The output of this function is array with four dimensions. The first dimension contains the different workflows involved on each paired comparison, with the baseline in the first row (and with the columns “Diff” and “p.value” set to NA). The second dimension includes the information provided for each workflow, namely: i) the average estimated score for the metric; ii) the respective standard error of this estimate; iii) the difference between the score of the baseline and the score of each alternative; and iv) the confidence level (p-value) for rejecting the null hypothesis that the difference is zero. The third dimension of the array are the metrics involved in the estimation experiment (in the above example it is a single one - the error rate), whilst the fourth dimension is the predictive tasks (again the above example only includes a single task).

In the above example the p-value for the single paired comparison that is carried out by the function is too high (0.25) and thus we can not reject the hypothesis that the difference between the error rate of two alternative workflows is zero in this particular predictive task.

7 Larger Examples

The main advantage of the infra-structure we are proposing is to automate large scale performance estimation experiments. It is on these very large setups that the use of the infra-structure spares more time to the user. However, in these contexts the objects resulting from the estimation process are very large and some of the tools we have shown before for exploring the results may produce over-cluttered output. In effect, if you have an experiment involving dozens of predictive tasks and eventually hundreds of workflow variants being compared on several evaluation metrics, doing a plot of the resulting object is simply not possible as the graph will be unreadable. This section illustrates some of these cases and presents some solutions to overcome the difficulties they bring.

Extremely large experiments may take days or weeks to complete, depending on the available hardware. In this context, it may not be wise to run the experiments on a single call to the `performanceEstimation()` function because if something goes wrong in the middle you may loose lots of work/time. Using the random number generation seeds that are available in all experimental settings objects we can split the experiments in several calls and still ensure that the same data folds are used in all estimation experiments. Moreover, we will

see that when all experiments are finished we will be able to merge the objects of each call into a single object as if we had issued a single call. Let us see an example.

```
library(DMwR)
library(e1071)
library(randomForest)

data(algae)
DSs <- sapply(names(algae)[12:18],
  function(x,names.attrs) {
    f <- as.formula(paste(x,"~ ."))
    PredTask(f,algae[,c(names.attrs,x)],x)
  },
  names(algae)[1:11])

WFs <- list()
WFs$svm <- list(learner.pars=list(cost=c(10,150,300),
  gamma=c(0.01,0.001),epsilon=c(0.1,0.05)))
WFs$randomForest <- list(learner.pars=list(mtry=c(5,7),
  ntree=c(500,750,1500)))

for(d in seq_along(DSs)) {
  for(w in names(WFs)) {
    resObj <- paste(names(DSs)[d],w,'Res',sep='')
    assign(resObj,
      performanceEstimation(
        DSs[d],
        c(
          do.call('workflowVariants',
            c(list('standardWF',
              learner=w,
              evaluator.pars=list(stats=c('mse','mae'))),
              WFs[[w]]))
        ),
        CvSettings(3,10,1234))
    )

    save(list=resObj,file=paste(names(DSs)[d],w,'Rdata',sep='.'))
  }
}
```

The above code compares 12 SVM variants with 6 random forest variants, on 7 algae blooms regression tasks, using 3×10 -fold cross validation. Although this is not a very large experimental comparison it still includes applying 18 different workflow variants on 7 different prediction tasks, 30 times, i.e. 3780 train+test cycles. Instead of running all these experiments on a single call to the function `performanceEstimation()` (which would obviously still be possible), we have made different calls for each workflow type (SVM, random forest and MARS) and for each predictive task. This means that each call will run all variants of a certain workflow on a certain predictive task. The result of each of these calls will be assigned to an object with a name composed of the task name and workflow learner (the `resObj` variable). In the end each of these objects

is saved on a file with a similar name, for future loading and results analysis. For instance, in the end there will be a file with name “a1.svm.Rdata” which contains an object of class **ComparisonResults** named **a1svmRes**. This object contains the MSE and MAE estimated scores of the SVM variants on the task of predicting the target variable “a1” (one of the eight algae in this data set).

Later on, after the above experiment has finished you can load the saved objects back into R and moreover, join them into a single object, as shown below:

```
nD <- paste('a',1:7,sep='')
nL <- c('svm','randomForest')
res <- NULL
for(d in nD) {
  resD <- NULL
  for(l in nL) {
    load(paste(d,l,'Rdata',sep='.'))
    x <- get(paste(d,l,'Res',sep=''))
    resD <- if (is.null(resD)) x else mergeEstimationRes(resD,x,by='workflows')
  }
  res <- if (is.null(res)) resD else mergeEstimationRes(res,resD,by='tasks')
}
save(res,file='allResultsAlgae.Rdata')
```

The `mergeEstimationRes()` function when applied to objects of class **ComparisonResults** allows merging of these objects across different dimensions. Namely, such objects have the individual scores of all experiments spread across 4 dimensions: the iterations, the metrics, the workflows and the tasks. The argument `by` of the `mergeEstimationRes()` function allows you to specify how to merge the given objects. The most common situations are: (i) merging the results of different workflows over the same data sets - you should use “`by='workflows'`”, or (ii) merging the results of the same workflows across different tasks - you should use “`by='tasks'`”.

The following code can be used to check that the merging was OK, and also to illustrate a few other utility functions whose purpose should be obvious:

```
res
##
## == Cross Validation Performance Estimation Experiment ==
##
## 3 x 10 - Fold Cross Validation run with seed = 1234
## 18 workflows
## tested on 7 predictive tasks

taskNames(res)
## [1] "a1" "a2" "a3" "a4" "a5" "a6" "a7"

workflowNames(res)
## [1] "svm.v1" "svm.v2" "svm.v3" "svm.v4"
## [5] "svm.v5" "svm.v6" "svm.v7" "svm.v8"
## [9] "svm.v9" "svm.v10" "svm.v11" "svm.v12"
## [13] "randomForest.v1" "randomForest.v2" "randomForest.v3" "randomForest.v4"
## [17] "randomForest.v5" "randomForest.v6"

metricNames(res)
## [1] "mse" "mae"
```

With such large objects the most we can do is obtaining the best scores or rankings of the workflows:

```
topPerformers(res)

## $a1
##           Workflow Estimate
## mse randomForest.v5  233.379
## mae randomForest.v1   10.29
##
## $a2
##           Workflow Estimate
## mse randomForest.v5  102.505
## mae          svm.v1    6.088
##
## $a3
##           Workflow Estimate
## mse randomForest.v5   48.309
## mae          svm.v4    4.135
##
## $a4
##           Workflow Estimate
## mse randomForest.v1   13.701
## mae          svm.v10    1.724
##
## $a5
##           Workflow Estimate
## mse randomForest.v5   46.665
## mae          svm.v10    4.223
##
## $a6
##           Workflow Estimate
## mse   svm.v12  114.123
## mae   svm.v12   5.859
##
## $a7
##           Workflow Estimate
## mse   svm.v2   27.723
## mae   svm.v4    2.501
```

```
rankWorkflows(res)

## $a1
## $a1$mse
##           Workflow Estimate
## 1 randomForest.v5   233.4
## 2 randomForest.v1   233.7
## 3 randomForest.v3   235.0
## 4 randomForest.v2   236.4
## 5 randomForest.v4   238.1
##
## $a1$mae
##           Workflow Estimate
```

```

## 1 randomForest.v1    10.29
## 2 randomForest.v5    10.31
## 3 randomForest.v2    10.34
## 4 randomForest.v3    10.34
## 5 randomForest.v6    10.37
##
##
## $a2
## $a2$mse
##      Workflow Estimate
## 1 randomForest.v5    102.5
## 2 randomForest.v1    103.5
## 3 randomForest.v3    103.8
## 4 randomForest.v6    104.2
## 5 randomForest.v2    104.8
##
## $a2$mae
##      Workflow Estimate
## 1   svm.v1      6.088
## 2   svm.v7      6.155
## 3   svm.v10     6.204
## 4   svm.v4      6.226
## 5   svm.v5      6.248
##
##
## $a3
## $a3$mse
##      Workflow Estimate
## 1 randomForest.v5    48.31
## 2 randomForest.v3    48.37
## 3 randomForest.v1    48.40
## 4 randomForest.v2    49.06
## 5 randomForest.v6    49.17
##
## $a3$mae
##      Workflow Estimate
## 1   svm.v4      4.135
## 2   svm.v10     4.155
## 3   svm.v7      4.224
## 4   svm.v1      4.248
## 5   svm.v5      4.269
##
##
## $a4
## $a4$mse
##      Workflow Estimate
## 1 randomForest.v1    13.70
## 2 randomForest.v3    13.85
## 3 randomForest.v5    13.87
## 4 randomForest.v4    13.99
## 5 randomForest.v6    14.05
##
## $a4$mae

```

```

##           Workflow Estimate
## 1      svm.v10      1.724
## 2      svm.v4       1.726
## 3      svm.v7       1.769
## 4 randomForest.v3   1.783
## 5 randomForest.v1   1.788
##
##
## $a5
## $a5$mse
##           Workflow Estimate
## 1 randomForest.v5   46.66
## 2 randomForest.v3   46.72
## 3 randomForest.v1   46.89
## 4 randomForest.v6   47.79
## 5 randomForest.v4   47.89
##
## $a5$mae
##           Workflow Estimate
## 1  svm.v10      4.223
## 2   svm.v4      4.252
## 3   svm.v1      4.292
## 4   svm.v7      4.305
## 5  svm.v11      4.335
##
##
## $a6
## $a6$mse
##           Workflow Estimate
## 1      svm.v12   114.1
## 2      svm.v6   115.9
## 3      svm.v5   122.5
## 4      svm.v11  122.9
## 5 randomForest.v3 131.7
##
## $a6$mae
##           Workflow Estimate
## 1  svm.v12      5.859
## 2  svm.v6       5.913
## 3  svm.v1       5.950
## 4  svm.v7       5.959
## 5  svm.v11      5.978
##
##
## $a7
## $a7$mse
##           Workflow Estimate
## 1      svm.v2      27.72
## 2      svm.v8      27.86
## 3 randomForest.v3  28.26
## 4 randomForest.v5  28.36
## 5      svm.v1      28.50
##

```



```
## $a7$mae
## Workflow Estimate
## 1 svm.v4 2.501
## 2 svm.v10 2.506
## 3 svm.v1 2.513
## 4 svm.v7 2.515
## 5 svm.v11 2.530
```

Notice that both `topPerformers()` and `rankWorkflows()` assume that the evaluation metrics are to be minimized, i.e. they assume the lower the better the scores. Still, both functions have a parameter named `maxs` that accepts a vector with as many Boolean values as there are evaluation metrics being estimated, which you may use to indicate that some particular metric is to be maximized and not minimized (the default). So for instance, if you had an experiment where the 1st and 3rd metrics are to be minimized, whilst the second is to be maximized, you could call these functions as `rankWorkflows(resObj,maxs=c(F,T,F))`.

In order to obtain further results from these large objects one usually proceeds by analyzing parts of the object, for instance focusing on a particular task or metric, or even a subset of the workflows. To facilitate this we can use the generic function `subset()` that can also be applied to objects of class **ComparisonResults**. An example of its use is given below, which results in a graph of the performance of the different workflows in the predictive task “a1”, in terms of “MSE”, which is show in Figure 2.

```
plot(subset(res,tasks='a1',statistics='mae'))
```

As before we are using the generic function `plot()` but this time applied to a subset of the original object with all results. This subset is obtained using the generic function `subset()` that accepts several parameters to specify the subset we are interested on. In this case we are using the parameters `tasks` and `statistics` to indicate that we want to analyze only the results concerning the task “a1” and the metric “mae”. Other possibility is the parameter `workflows` for indicating a subset of the workflows. Both `workflows`, `tasks` and `statistics` accept as values a character string containing a regular expression that will be used internally with the R function `grep()` over the vector of names of the respective objects (names of the workflows, names of the tasks and names of the metrics, respectively). For instance, if you want to constrain the previous graph even further to the workflows whose name ends in “4” (absurd example of course!), you could use the following:

```
plot(subset(res,tasks='a1',workflows='4$'))
```

If you are more familiar with the syntax of “wildcards” you may use the R function `glob2rx()` to convert to regular expressions, as show in the following example:

```
summary(subset(res,tasks='a1',workflows=glob2rx('*svm*'),statistics='mse'))
##
## == Summary of a Cross Validation Performance Estimation Experiment ==
```

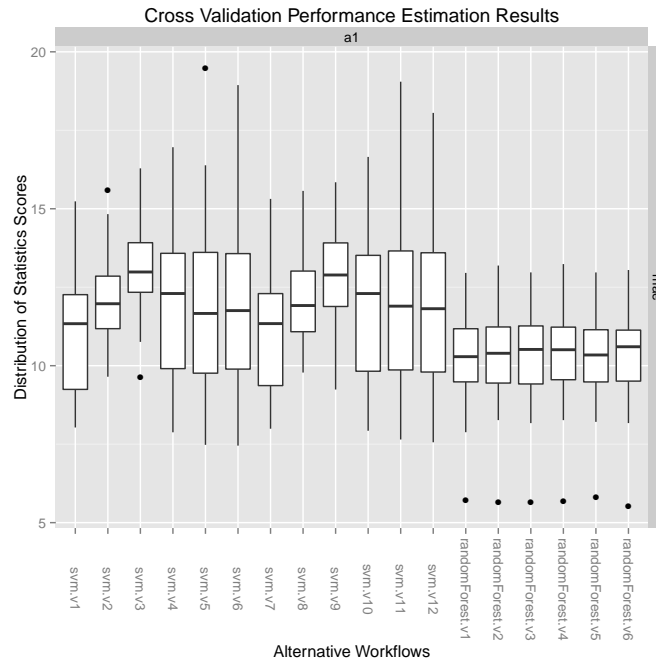


Figure 2: The MAE results for the task “a1”.

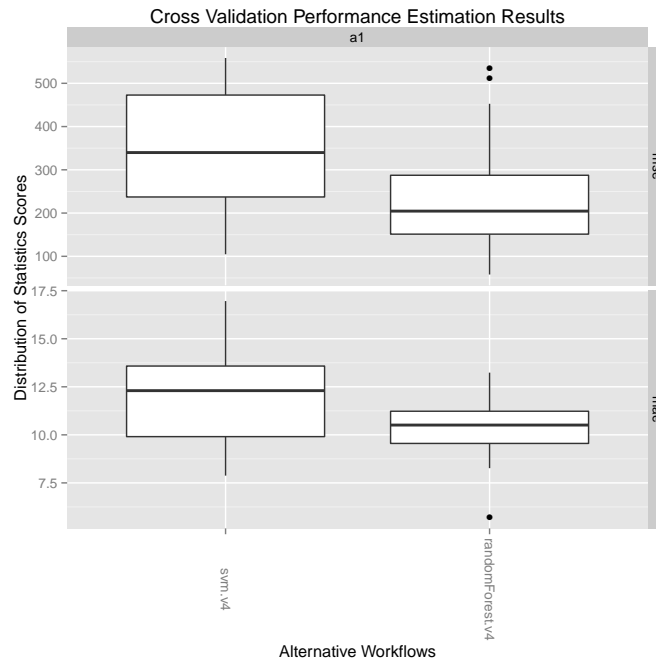


Figure 3: Illustration of the use of regular expressions in sub-setting the results objects.

```

## 3 x 10 - Fold Cross Validation run with seed = 1234
##
## * Predictive Tasks :: a1
## * Workflows :: svm.v1, svm.v2, svm.v3, svm.v4, svm.v5, svm.v6, svm.v7, svm.v8, svm.v9, svm.v10,
##
## * Summary of Experiment Results:
##
## -> Dataset: a1
##
## *Workflow: svm.v1
##      mse
## avg    278.6
## std    106.5
## min    121.2
## max    503.3
## invalid 0.0
##
## *Workflow: svm.v2
##      mse
## avg    278.7
## std    107.3
## min    126.0
## max    603.8
## invalid 0.0
##
## *Workflow: svm.v3
##      mse
## avg    309.6
## std    114.8
## min    145.1
## max    659.3
## invalid 0.0
##
## *Workflow: svm.v4
##      mse
## avg    340.0
## std    138.7
## min    104.7
## max    558.5
## invalid 0.0
##
## *Workflow: svm.v5
##      mse
## avg    348.08
## std    213.27
## min     97.36
## max   1001.13
## invalid 0.00
##
## *Workflow: svm.v6
##      mse
## avg    362.3
## std    256.9

```

```

## min      106.5
## max      1268.0
## invalid   0.0
##
## *Workflow: svm.v7
##          mse
## avg      277.5
## std      104.7
## min      124.2
## max      496.0
## invalid   0.0
##
## *Workflow: svm.v8
##          mse
## avg      279.2
## std      106.9
## min      129.5
## max      609.4
## invalid   0.0
##
## *Workflow: svm.v9
##          mse
## avg      305.7
## std      114.0
## min      145.9
## max      651.8
## invalid   0.0
##
## *Workflow: svm.v10
##          mse
## avg      340.31
## std      139.09
## min      97.38
## max      562.07
## invalid   0.00
##
## *Workflow: svm.v11
##          mse
## avg      351.0
## std      211.0
## min      105.8
## max      1082.0
## invalid   0.0
##
## *Workflow: svm.v12
##          mse
## avg      350.5
## std      223.2
## min      115.5
## max      1129.8
## invalid   0.0

```

The following are some illustrations of the use of other available utility functions.

Obtaining the scores on all iterations and metrics of a workflow on a particular task:

```
getIterationsResults(res, 'svm.v6', 'a3')
```

```
##           mse    mae
## [1,]  35.167  3.738
## [2,]  85.866  5.720
## [3,]  24.207  3.062
## [4,]  58.519  4.421
## [5,] 161.427  6.916
## [6,]  43.422  3.818
## [7,]  77.363  5.972
## [8,]  13.756  2.989
## [9,]  31.301  3.522
## [10,] 31.060  4.421
## [11,] 98.894  7.058
## [12,] 34.912  3.984
## [13,] 28.457  3.358
## [14,] 51.942  4.479
## [15,] 120.784  5.356
## [16,] 18.346  3.115
## [17,] 67.551  5.057
## [18,] 78.109  4.645
## [19,] 37.893  3.866
## [20,] 23.811  3.021
## [21,] 12.475  2.573
## [22,] 32.153  3.327
## [23,]  8.395  2.284
## [24,] 72.897  5.643
## [25,] 35.598  3.699
## [26,] 73.571  5.157
## [27,] 116.683  5.329
## [28,] 68.635  4.154
## [29,] 49.770  4.765
## [30,] 57.290  4.611
```

Getting the summary of the results of a particular workflow on a predictive task :

```
estimationSummary(res, 'svm.v3', 'a7')
```

```
##           mse    mae
## avg       28.632  3.060
## std       25.950  1.062
## min        4.234  1.462
## max      110.198  6.196
## invalid    0.000  0.000
```

Finally, the `metricsSummary()` function allows you to apply any summary

function (defaulting to `mean()`) to the iterations estimates. The following calculates the median of the results of the SVMs on the task “a1”,

```
metricsSummary(subset(res,workflows=glob2rx('*svm*'),tasks='a1'),
               summary='median')

## $a1
##      svm.v1 svm.v2 svm.v3 svm.v4 svm.v5 svm.v6 svm.v7 svm.v8 svm.v9 svm.v10 svm.v11
## mse 261.78 253.78 293.82  339.9 285.49 286.73 267.68 255.11 282.80  342.4  287.8
## mae  11.34  11.97  12.99   12.3  11.66  11.76  11.34  11.92  12.89   12.3   11.9
##      svm.v12
## mse  285.40
## mae   11.82
```

References

- [MDH⁺12] David Meyer, Evgenia Dimitriadou, Kurt Hornik, Andreas Weingessel, and Friedrich Leisch. *e1071: Misc Functions of the Department of Statistics (e1071), TU Wien*, 2012. R package version 1.6-1.
- [Tor10] Luis Torgo. *Data Mining with R: learning with case studies*. Chapman & Hall/CRC Press, 2010.