Variable Selection Using The caret Package

Max Kuhn max.kuhn@pfizer.com

December 7, 2009

1 Models with Built-In Feature Selection

Many models that can be accessed using caret's train function produce prediction equations that do not necessarily use all the predictors. These models are thought to have built—in feature selection and include rpart, gbm, ada, glmboost, gamboost, blackboost, ctree, sparseLDA, sddaLDA, sddaQDA glmnet, lasso, lars, spls, earth, fda, bagEarth, bagFDA, pam and others. Many of the functions have an ancillary method called predictors that returns a vector indicating which predictors were used in the final model.

In many cases, using these models with built—in feature selection will be more efficient than algorithms where the search routine for the right predictors is external to the model (see Section 2). Built—in feature selection typically couples the predictor search algorithm with the parameter estimation and are usually optimize with a single objective function (e.g. error rates or likelihood).

2 Feature Selection Using Search Algorithms

2.1 Searching the Feature Space

Many feature selection routines used a "wrapper" approach to find appropriate variables such that an algorithm that searches the feature space repeatedly fits the model with different predictor sets. The best predictor set is determined by some measure of performance (i.e. R^2 , classification accuracy, etc). Examples of search functions are genetic algorithms, simulated annealing and forward/backward/stepwise selection methods. In theory, each of these search routines could converge to an optimal set of predictors.

An example of one search routine is backwards selection (a.k.a. recursive feature elimination).

2.1.1 Backwards Selection

First, the algorithm fits the model to all predictors. Each predictor is ranked using it's importance to the model. Let S be a sequence of ordered numbers which are candidate values for the number of predictors to retain $(S_1 > S_2, ...)$. At each iteration of feature selection, the S_i top raked predictors are retained, the model is refit and performance is assessed. The value of S_i with the best performance is determined and the top S_i predictors are used to fit the final model. Algorithm 1 has a more complete definition.

The algorithm has an optional step (line 1.8) where the predictor rankings are recomputed on the model on the reduced feature set. Svetnik *el al* (2004) showed that, for random forest models, there was a decrease in performance when the rankings were re—computed at every step. However, in other cases when the initial rankings are not good (e.g. linear models with highly collinear predictors), re—calculation can slightly improve performance.

Algorithm 1: Recursive feature elimination

- 1.1 Tune/train the model on the training set using all predictors
- 1.2 Calculate model performance
- 1.3 Calculate variable importance or rankings
- 1.4 for Each subset size S_i , $i = 1 \dots S$ do
- 1.5 Keep the S_i most important variables
- 1.6 Tune/train the model on the training set using S_i predictors
- 1.7 Calculate model performance
- 1.8 Optional Recalculate the rankings for each predictor
- 1.9 end
- 1.10 Calculate the performance profile over the S_i
- 1.11 Determine the appropriate number of predictors
- 1.12 Determine the final ranks of each predictor
- 1.13 Fit the final model based on the optimal S_i

One potential issue over—fitting to the predictor set such that the wrapper procedure could focus on nuances of the training data that are not found in future samples (i.e. over—fitting to predictors and samples).

For example, suppose a very large number of uninformative predictors were collected and one such predictor randomly correlated with the outcome. The RFE algorithm would give a good rank to this variable and the prediction error (on the same data set) would be lowered. It would take a different test/validation to find out that this predictor was uninformative. The was referred to as

"selection bias" by Ambroise and McLachlan (2002).

In the current RFE algorithm, the training data is being used for at least three purposes: predictor selection, model fitting and performance evaluation. Unless the number of samples is large, especially in relation to the number of variables, one static training set may not be able to fulfill these needs.

2.2 Resampling and External Validation

Since feature selection is part of the model building process, resampling methods (e.g. cross-validation, the bootstrap) should factor in the variability caused by feature selection when calculating performance. For example, the RFE procedure in Algorithm 1 can estimate the model performance on line 1.6, which during the selection process. Ambroise and McLachlan (2002) and Svetnik *el al* (2004) showed that improper use of resampling to measure performance will result in models that perform poorly on new samples.

To get performance estimates that incorporate the variation due to feature selection, it is suggested that the steps in Algorithm 1 be encapsulated inside an outer layer of resampling (e.g. 10–fold cross–validation). Algorithm 2 shows a version of the algorithm that uses resampling.

While this will provide better estimates of performance, it is more computationally burdensome. For users with access to machines with multiple processors, the first For loop in Algorithm 2 (line 2.1) can be easily parallelized. Another complication to using resampling is that multiple lists of the "best" predictors are generated at each iteration. At first this may seem like a disadvantage, but it does provide a more probabilistic assessment of predictor importance than a ranking based on a single fixed data set. At the end of the algorithm, a consensus ranking can be used to determine the best predictors to retain.

Algorithm 2: Recursive feature elimination incorporating resampling

```
2.1 for Each Resampling Iteration do
        Partition data into training and test/hold-back set via resampling
 2.2
        Tune/train the model on the training set using all predictors
 2.3
        Predict the held-back samples
 2.4
        Calculate variable importance or rankings
 2.5
        for Each subset size S_i, i = 1 ... S do
 2.6
           Keep the S_i most important variables
 2.7
           Tune/train the model on the training set using S_i predictors
 2.8
           Predict the held-back samples
 2.9
           [Optional] Recalculate the rankings for each predictor
2.10
        end
2.11
2.12 end
2.13 Calculate the performance profile over the S_i using the held-back samples
2.14 Determine the appropriate number of predictors
2.15 Estimate the final list of predictors to keep in the final model
2.16 Fit the final model based on the optimal S_i using the original training set
```

3 Recursive Feature Elimination via caret

In caret, Algorithm 1 is implemented by the function rfeIter. The resampling-based Algorithm 2 is in the rfe function. Given the potential selection bias issues, this document focuses on rfe. There are several arguments:

- x, a matrix or data frame of predictor variables
- y, a vector (numeric or factor) of outcomes
- sizes, a integer vector for the specific subset sizes that should be tested (which need not to include ncol(x))
- rfeControl, a list of options that can be used to specify the model and the methods for prediction, ranking etc.

For a specific model, a set of functions must be specified in rfeControl\$functions. Section 3.2 below has descriptions of these sub-functions. There are a number of pre-defined sets of functions for several models, including: linear regression (in the object lmFuncs), random forests (rfFuncs), naive Bayes (nbFuncs), bagged trees (treebagFuncs) and functions that can be used with caret's train function (caretFuncs). The latter is useful if the model has tuning parameters that must be determined at each iteration.

3.1 An Example

To test the algorithm, the "Friedman 1" benchmark (Friedman, 1991) was used. There are five informative variables generated by the equation

$$y = 10\sin(\pi x_1 x_2) + 20(x_3 - 0.5)^2 + 10x_4 + 5x_5 + N(0, \sigma^2)$$

In the simulation used here:

```
> n <- 100
> p <- 40
> sigma <- 1
> set.seed(1)
> sim <- mlbench.friedman1(n, sd = sigma)
> x <- cbind(sim$x, matrix(rnorm(n * p), nrow = n))
> y <- sim$y
> colnames(x) <- paste("var", 1:ncol(x), sep = "")</pre>
```

Of the 50 predictors, there are 45 pure noise variables: 5 are uniform on [0, 1] and 40 are random univariate standard normals. The predictors are centered and scaled:

```
> normalization <- preProcess(x)
> x <- predict(normalization, x)
> x <- as.data.frame(x)
> subsets <- c(1:5, 10, 15, 20, 25)</pre>
```

The simulation will fit models with subset sizes of 25, 20, 15, 10, 5, 4, 3, 2, 1.

As previously mentioned, to fit linear models, the lmFuncs set of functions can be used. To do this, a control object is created with the rfeControl function. We also specify that 10-fold cross-validation should be used in line 2.1 of Algorithm 2. The number of folds can be changed via the number argument to rfeControl (defaults to 10). The verbose option prevents copious amounts of output from being produced and the returnResamp argument specifies that the 10 performance estimates should be saved only for the optimal subset size.

```
> set.seed(10)
> ctrl <- rfeControl(functions = lmFuncs, method = "cv", verbose = FALSE,
+ returnResamp = "final")
> lmProfile <- rfe(x, y, sizes = subsets, rfeControl = ctrl)
> lmProfile
```

Recursive feature selection

Outer resamping method was 10 iterations of cross-validation.

Resampling performance over subset size:

```
Variables RMSE Rsquared RMSESD RsquaredSD Selected
        1 3.473
                  0.5285 0.4706
                                     0.1219
        2 3.134
                  0.6161 0.5937
                                     0.1757
        3 2.954
                  0.6770 0.9152
                                     0.2242
        4 3.055
                  0.6520 0.9889
                                     0.2359
        5 3.229
                  0.6188 0.8714
                                     0.1966
       10 3.493
                  0.5549 0.9811
                                     0.2098
       15 3.754
                  0.5010 1.1806
                                     0.2243
       20 3.893
                  0.4725 1.0039
                                     0.2026
       25 4.306
                  0.4009 0.9284
                                     0.1870
       50 4.306
                  0.4009 0.9284
                                     0.1870
```

```
The top 3 variables (out of 3): var4, var5, var2
```

The output shows that the best subset size was estimated to be 3 predictors. This set includes informative variables but did not include them all. The predictors function can be used to get a

text string of variable names that were picked in the final model. The lmProfile is a list of class "rfe" that contains an object fit that is the final linear model with the remaining terms. The model can be used to get predictions for future or test samples.

```
> predictors(lmProfile)
[1] "var4" "var5" "var2"
```

> lmProfile\$fit

Call:

```
lm(formula = y ~ ., data = tmp)
```

Coefficients:

(Intercept)	var4	var5	var2
14.613	2.625	1.967	1.648

> lmProfile\$resample

	RMSE	Rsquared	Variables
[1,]	3.640221	0.5471438	3
[2,]	2.270739	0.7953448	3
[3,]	2.425445	0.6704767	3
[4,]	3.195171	0.8108668	3
[5,]	4.994849	0.2072672	3
[6,]	2.184304	0.7963478	3
[7,]	2.602312	0.8716050	3
[8,]	1.968237	0.9170471	3
[9,]	2.714145	0.7397995	3
[10,]	3.548103	0.4141139	3

There are also several plot methods to visualize the results. plot(lmProfile) produces the performance profile across different subset sizes, as shown in Figure 1. Also the resampling results are stored in the sub-object lmProfile\$resample and can be used with several lattice functions. Univariate lattice functions (densityplot, histogram) can be used to plot the resampling distribution while bivariate functions (xyplot, stripplot) can be used to plot the distributions for different subset sizes. In the latter case, the option returnResamp = "all" in rfeControl can be used to save all the resampling results. See Figure 4 for two examples.





Figure 1: Performance profiles for recursive feature elimination using linear models. These images were generated by plot(lmProfile) and plot(lmProfile, metric = "Rsquared").

3.2 Helper Functions

To use feature elimination for an arbitrary model, a set of functions must be passed to rfe for each of the steps in Algorithm 2. This section defines those functions and uses the existing random forest functions as an illustrative example.

3.2.1 The summary Function

The summary function takes the observed and predicted values and computes one or more performance metrics (see line 2.13). The input is a data frame with columns obs and pred. The output should be a named vector of numeric variables. Note that the metric argument of the rfe function should reference one of the names of the output of summary.

3.2.2 The fit Function

This function builds the model based on the current data set (lines line 2.3, 2.8 and 2.16). The arguments for the function must be:

- x: the current training set of predictor data with the appropriate subset of variables
- y: the current outcome data (either a numeric or factor vector)
- first: a single logical value for whether the current predictor set has all possible variables (e.g. line 2.3)
- last: similar to first, but TRUE when the last model is fit with the final subset size and predictors. (line 2.16)
- ...: optional arguments to pass to the fit function in the call to rfe

The function should return a model object that can be used to generate predictions. For random forest, the fit function is simple:

> rfFuncs\$fit

```
function (x, y, first, last, ...)
{
    library(randomForest)
    randomForest(x, y, importance = first, ...)
}
<environment: namespace:caret>
```

For feature selection without re—ranking at each iteration, the random forest variable importances only need to be computed on the first iterations when all of the predictors are in the model. This can be accomplished using importance = first.

3.2.3 The pred Function

This function returns a vector of predictions (numeric or factors) from the current model (lines 2.4 and 2.9). The input arguments must be

- object: the model generated by the fit function
- x: the current set of predictor set for the held-back samples

For random forests, the function is a simple wrapper for the predict function:

> rfFuncs\$pred

```
function (object, x)
{
    predict(object, x)
}
<environment: namespace:caret>
```

For classification, it is probably a good idea to ensure that the resulting factor variables of predictions has the same levels as the input data.

3.2.4 The rank Function

This function is used to return the predictors in the order of the most important to the least important (lines 2.5 and 2.10). Inputs are:

- object: the model generated by the fit function
- x: the current set of predictor set for the training samples
- y: the current training outcomes

The function should return a data frame with a column called vars that has the current variable names. The first row should be the most important predictor etc. Other columns can be included in the output and will be returned in the final rfe object.

For random forests, the function below uses caret's varImp function to extract the random forest importances and orders them. For classification, randomForest will produce a column of importances for each class. In this case, the default ranking function orders the predictors by the averages importance across the classes.

> rfFuncs\$rank

3.2.5 The selectSize Function

This function determines the optimal number of predictors based on the resampling output (line 2.14). Inputs for the function are:

- x: a matrix with columns for the performance metrics and the number of variables, called Variables
- metric: a character string of the performance measure to optimize (e.g. RMSE, Accuracy)
- maximize: a single logical for whether the metric should be maximized

This function should return an integer corresponding to the optimal subset size.

caret comes with two examples functions for this purpose: pickSizeBest and pickSizeTolerance. The former simply selects the subset size that has the best value. The latter takes into account the whole profile and tries to pick a subset size that is small without sacrificing too much performance. For example, suppose we have computed the RMSE over a series of variables sizes:

```
> example <- data.frame(RMSE = c(3.215, 2.819, 2.414, 2.144, 2.014, 1.997, 2.025, 1.987, 1.971, 2.055, 1.935, 1.999, 2.047, 2.002, 1.895, 2.018), Variables = 1:16) > example
```

	RMSE	Variables
1	3.215	1
2	2.819	2
3	2.414	3
4	2.144	4
5	2.014	5
6	1.997	6
7	2.025	7
8	1.987	8
9	1.971	9
10	2.055	10
11	1.935	11
12	1.999	12
13	2.047	13
14	2.002	14
15	1.895	15
16	2.018	16

These are depicted in Figure 2. The solid circle identifies the subset size with the absolute smallest RMSE. However, there are many smaller subsets that produce approximately the same performance but with fewer predictors. In this case, we might be able to accept a slightly larger error for less predictors.

The pickSizeTolerance determines the absolute best value then the percent difference of the other points to this value. In the case of RMSE, this would be

$$RMSE_{tol} = 100 \times \frac{RMSE - RMSE_{opt}}{RMSE_{opt}}$$

where $RMSE_{opt}$ is the absolute best error rate. These "tolerance" values are plotted in the bottom panel of Figure 2. The solid triangle is the smallest subset size that is within 10% of the optimal value.

This approach can produce good results for many of the tree based models, such as random forest, where there is a plateau of good performance for larger subset sizes. For trees, this is usually because unimportant variables are infrequently used in splits and do not significantly affect performance.

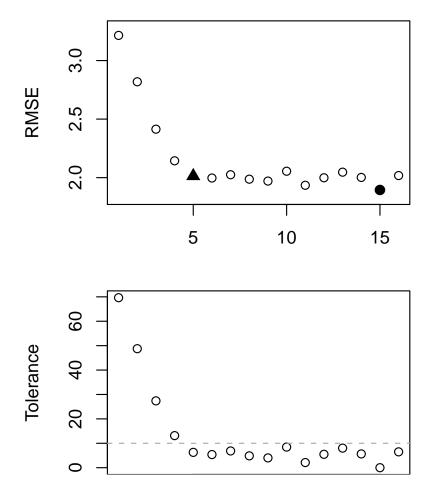


Figure 2: An example of where a smaller subset sizes is not necessarily the best choice. The solid circle in the top panel indicates the subset size with the absolute smallest RMSE. If the percent differences from the smallest RMSE are calculated (lower panel), the user may want to accept a pre–specified drop in performance as long as the drop is within some limit of the optimal.

3.2.6 The selectVar Function

After the optimal subset size is determined, this function will be used to calculate the best rankings for each variable across all the resampling iterations (line 2.15). Inputs for the function are:

- y: a list of variables importance for each resampling iteration and each subset size (generated by the user-defined rank function). In the example, each each of the cross-validation groups the output of the rank function is saved for each of the 10 subset sizes (including the original subset). If the rankings are not recomputed at each iteration, the values will be the same within each cross-validation iteration.
- size: the integer returned by the selectSize function

This function should return a character string of predictor names (of length size) in the order of most important to least important

For random forests, only the first importance calculation (line 2.5) is used since these are the rankings on the full set of predictors. These importances are averaged and the top predictors are returned.

> rfFuncs\$selectVar

```
function (y, size)
{
   imp <- lapply(y, function(x) x[[1]])
   imp <- do.call("rbind", imp)
   finalImp <- aggregate(imp$Overall, list(var = imp$var), mean,
        na.rm = TRUE)
   finalImp <- finalImp[order(finalImp$x, decreasing = TRUE),
        ]
   as.character(finalImp$var[1:size])
}
<environment: namespace:caret>
```

Note that if the predictor rankings are recomputed at each iteration (line 2.10) the user will need to write their own selection function to use the other ranks.

3.2.7 The Example

For random forest, we fit the same series of model sizes as the linear model. The option to save all the resampling results across subset sizes was changed for this model and are used to show the lattice plot function capabilities in Figure 4.

```
> ctrl$functions <- rfFuncs
> ctrl$returnResamp <- "all"
> set.seed(10)
> rfProfile <- rfe(x, y, sizes = subsets, rfeControl = ctrl)
> print(rfProfile)
```

Recursive feature selection

Outer resamping method was 10 iterations of cross-validation.

Resampling performance over subset size:

```
Variables RMSE Rsquared RMSESD RsquaredSD Selected
       1 3.768
                 0.4025 0.3996
                                   0.1628
       2 3.107
                 0.6291 0.5292
                                   0.1538
       3 2.879
                0.7014 0.5282
                                   0.1741
       4 2.875
                0.7333 0.4653
                                   0.1346
       5 3.104 0.7002 0.3718
                                   0.1514
                                   0.1317
      10 3.148
                0.7123 0.3036
      15 3.309
               0.6828 0.3918
                                   0.1161
      20 3.421
                0.6435 0.3255
                                   0.1375
      25 3.573
                0.6199 0.3633
                                   0.1471
      50 3.555
                0.6297 0.4062
                                   0.1155
```

The top 4 variables (out of 4): var4, var5, var2, var1





Figure 3: Performance profiles for random forest.

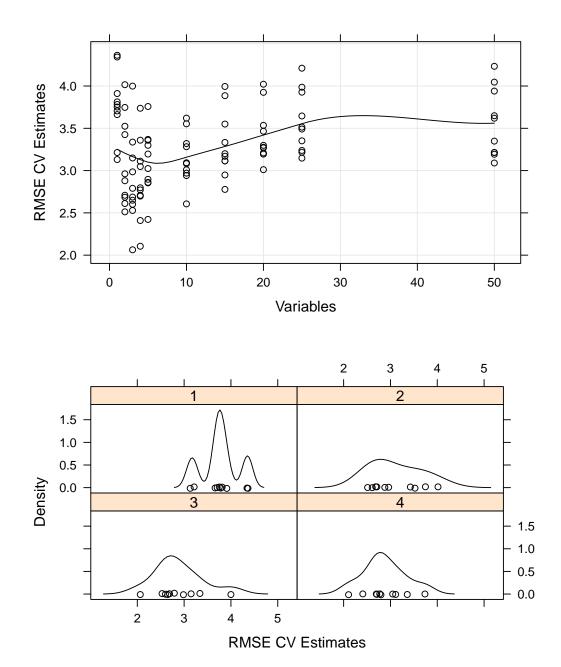


Figure 4: Resampling RMSE estimates for random forests across different subset sizes. These plots were generated using xyplot(rfProfile) and densityplot(rfProfile, subset = Variables < 5)

4 Feature Selection Using Univariate Filters

Another approach to feature selection is to pre–screen the predictors using simple univariate statistical methods then only use those that pass some criterion in the subsequent model steps. Similar to recursive selection, cross-validation of the subsequent models will be biased as the remaining predictors have already been evaluate on the data set. Proper performance estimates via resampling should include the feature selection step.

As an example, it has been suggested for classification models, that predictors can be filtered by conducting some sort of k-sample test (where k is the number of classes) to see if the mean of the predictor is different between the classes. Wilcoxon tests, t-tests and ANOVA models are sometimes used. Predictors that have statistically significant differences between the classes are then used for modeling.

The caret function sbf (for selection by filter) can be used to cross-validate such feature selection schemes. Similar to rfe, functions can be passed into sbf for the computational components: univariate filtering, model fitting, prediction and performance summaries (details are given below).

The function is applied to the entire training set and also to different resampled versions of the data set. From this, generalizable estimates of performance can be computed that properly take into account the feature selection step. Also, the results of the predictor filters can be tracked over resamples to understand the uncertainty in the filtering.

4.1 Basic Syntax

Similar to the rfe function, the syntax for sbf is:

```
sbf(predictors, outcome, sbfControl = sbfControl(), ...)
## or
sbf(formula, data, sbfControl = sbfControl(), ...)
```

In this case, the details are specificed using the sbfControl function. Here, the argument functions dictates what the different components should do. This argument should have elements called filter, fit, pred and summary.

4.1.1 The filter Function

This function takes as inputs the predictors and the outcome in objects called x and y, respectively. The output should be a named logical vector where the names correspond to the column names of x. Columns with values of TRUE will be used in the subsequent model.

There are two built—in functions called anovaFilter and gamFilter. anovaFilter treats the outcome as the independent variable and the predictor as the outcome. In this way, the null

hypothesis is that the mean predictor values are equal across the different classes. For regression, gamFilter fits a smoothing spline in the predictor to the outcome using a generalized additive model and tests to see if there is any functional relationship between the two.

4.1.2 The fit Function

The component is very similar to the function described in Section 3.2.2. For sbf, there are no first or last arguments. The function should have arguments x, y and The data within x have been filtered using the filter function described above. The output of the fit function should be a fitted model.

With some data sets, no predictors will survive the filter. In these cases, a model with predictors cannot be computed, but the lack of viable predictors should not be ignored in the final results. To account for this issue, caret contains a model function called nullModel that fits a simple model that is independent of any of the predictors. For problems where the outcome is numeric, the function predicts every sample using the simple mean o the training set outcomes. For classification, the model predicts all samples using the most prevalent class in the training data.

This function can be used in the fit component function to "error-trap" cases where no predictors are selected. For example, there are several built—in functions for some models. The object rfSBF is a set of functions that may be useful for fitting random forest models with filtering. The fit function here uses nullModel to check for cases with no predictors:

> rfSBF\$fit

```
function (x, y, ...)
{
    if (ncol(x) > 0) {
        library(randomForest)
        randomForest(x, y, ...)
    }
    else nullModel(y = y)
}
<environment: namespace:caret>
```

4.1.3 The summary and pred Functions

The summary function is used to calculate model performance on held-out samples. The pred function is used to predict new samples using the current predictor set. The arguments and outputs for these two functions are identical to the previously discussed summary and pred functions in Sections 3.2.1 and 3.2.3, respectively.

4.2 The Example

Returning to the example from (Friedman, 1991), we can fit another random forest model with the predictors pre-filtered using the generalized additive model approach described in Section 4.1.1.

```
> set.seed(10)
> rfWithFilter <- sbf(x, y, sbfControl = sbfControl(functions = rfSBF,</pre>
      method = "cv", verbose = FALSE))
> print(rfWithFilter)
Selection By Filter
Outer resamping method was 10 iterations of cross-validation.
Resampling performance:
  RMSE Rsquared RMSESD RsquaredSD
         0.2799 0.4713
 4.133
                           0.1818
Using the training set, 7 variables were selected:
   var1, var2, var3, var21, var23...
During resampling, the top 5 selected variables (out of a possible 14):
   var1 (100%), var3 (100%), var42 (100%), var2 (90%), var23 (60%)
On average, 6.4 variables were selected (min = 5, max = 9)
```

In this case, the training set indicated that 7 should be used in the random forest model, but the resampling results indicate that there is some variation in this number. Some of the informative predictors are used, but a few others are erroneous retained.

Similar to rfe, there are methods for predictors, densityplot, histogram and varImp.

5 Session Information

- R version 2.10.0 RC (2009-10-18 r50160), x86_64-apple-darwin9.8.0
- Locale: en_US.UTF-8/en_US.UTF-8/C/C/en_US.UTF-8/en_US.UTF-8
- Base packages: base, datasets, graphics, grDevices, grid, methods, splines, stats, tools, utils

- Other packages: akima 0.5-3, caret 4.31, class 7.3-1, e1071 1.5-20, ellipse 0.3-5, gam 1.0.1, gbm 1.6-3, Hmisc 3.7-0, ipred 0.8-8, kernlab 0.9-9, klaR 0.6-0, lattice 0.17-26, MASS 7.3-3, mlbench 1.1-6, nnet 7.3-1, pls 2.1-0, plyr 0.1.9, proxy 0.4-4, randomForest 4.5-33, reshape 0.8.3, rpart 3.1-45, survival 2.35-7
- Loaded via a namespace (and not attached): cluster 1.12.1

6 References

- Ambroise, C. and McLachlan, J. H. (2002) "Selection bias in gene extraction on the basis of microarray gene-expression data," *Proceedings of the National Academy of Science*, 99, 6562–6566
- Friedman, J. H. (1991) "Multivariate adaptive regression splines (with discussion)," Annals of Statistics, 19, 1–141
- Svetnik, V., Liaw, A., Tong, C amd Wang, T. (2004) "Application of Breiman's random forest to modeling structure-activity relationships of pharmaceutical molecules," *Multiple Classier Systems, Fifth International Workshop*, 3077, 334–343