

Variable Selection

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Variable Selection

For many models, predictive performance is degraded as the number of uninformative predictors increases.

Simpler model requires less computational resources.

Model is more interpretable with fewer predictors.

Classes of variable selection techniques

Intrinsic methods

Examples: tree based models, regularization based methods, such as the lasso

Pros: no external feature selection tool is required

Cons: These approaches are specific to a model being used.

Filter methods

Evaluate the relevance of predictors using some statistic (e.g., information gain, odds-ratio, χ^2 statistics, correlation). Only keep predictors that pass some threshold criterion.

Typically, each feature is viewed as independent of the others, effectively ignoring interactions between features.

Pros: computationally efficient

Cons: redundant predictors may be selected; hard to detect interaction and nonlinear effects; a selection of predictors that meets a filtering may not be a set that improves predictive performance.

Wrapper methods

Deterministic wrapper feature selection methods either start with no features or with all features included in the model and iteratively refine the set of chosen features according to some model quality measures.

- forward-selection; backward-selection (*recursive feature elimination* or RFE)

Stochastic wrapper feature selection procedures

- genetic algorithms (GA); simulated annealing (SA).

Wrappers have the potential advantage of searching a wider variety of predictor subsets than filters.

- computationally demanding—need to fit a potentially time consuming model multiple times.

Summary: The different types of feature selection methods have their own pros and cons.

- It is important to remember that the globally best subset is often difficult to find.

The Effect of Irrelevant Features

The effect depends on:

- the type of model;
- the nature of the predictors;
- the ratio of the size of the training set to the number of predictors.

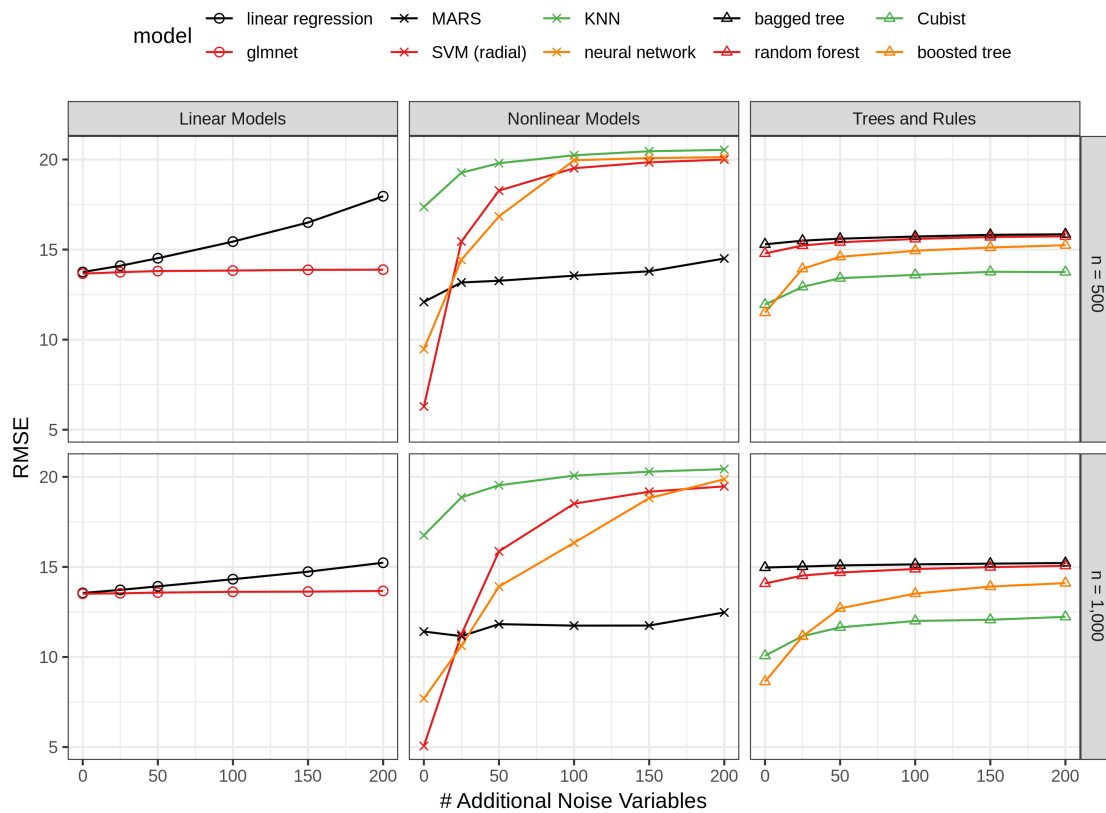
Let us take a look at a simulation in Chapter 10.3 of **Feature Engineering and Selection** by *Max Kuhn and Kjell Johnson* (<https://bookdown.org/max/FES/feature-selection-simulation.html>).

- The code for the simulation is here: https://github.com/topepo/FES_Selection_Simulation
- The simulation setting is taken from Sapp, Laan, and Canny (2014) .

$$y = x_1 + \sin(x_2) + \log(|x_3|) + x_4^2 + x_5x_6 + I(x_7x_8x_9 < 0) + I(x_{10} > 0) + x_{11}I(x_{11} > 0) + \sqrt{|x_{12}|} + \cos(x_{13}) + 2x_{14} + |x_{15}| + I(x_{16} < -1) + x_{17}I(x_{17} < -1) - 2x_{18} - x_{19}x_{20} + \epsilon \quad (1)$$

- input variables $x_j \sim N(0, 1)$; the error $\epsilon \sim N(0, 3^2)$;
- between 10 and 200 extra columns of input variables with no connection to the outcome were added;
- the training size $n = 500$ or $n = 1,000$.

The focus of simulation is to look at the relative impact of irrelevant predictors and not at absolute performance.



Overfitting When Selecting Input Variables

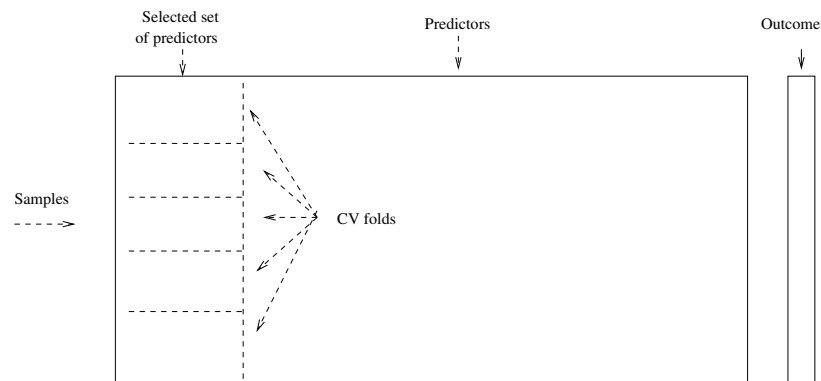
Often it is possible to find a subset of input variables that has good predictive performance on the training set

- but has *poor performance* when used on a **test set**.

Feature selection needs to be part of the cross-validation (or more generally resampling) **process**.

Wrong approach

The **most common mistake** is to only conduct cross-validation inside of the variable selection procedure.



Algorithm:

1. Rank the predictors using the training set;
2. **For** each subset size, S_i
 - 2.1 **For** each split into training/validation set
 - Fit model with S_i most important variables on the training set.
 - Predict the validation set.
 - 2.2 Calculate the model performance with S_i variables
3. Determine the appropriate number of predictors (i.e., the S_i with best performance)
4. Fit the final model based on the optimal S_i

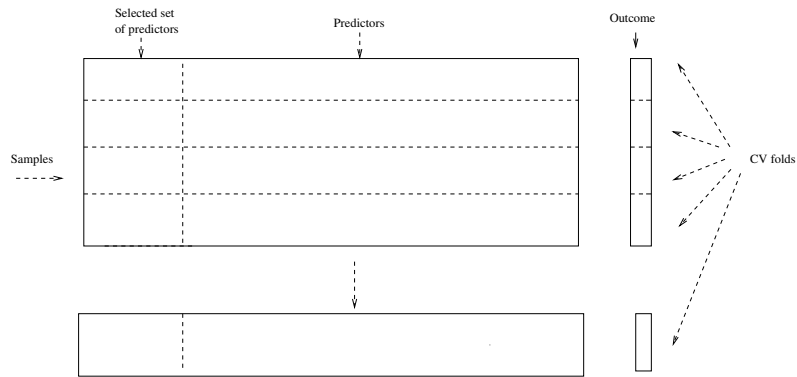
Two key problems with the above procedure:

- The feature selection is performed outside cross-validation. CV cannot effectively measure the impact of the selection process.
- The same data are being used to measure performance of the model and to select the input variables. This is the same issue that arises when fitting a model to the training set and then using the same training set to measure performance. There is an obvious bias in measuring the performance of the model if it can closely fit the training data. We need out-of-sample data to accurately determine how well the model is doing. If the variable selection process results in overfitting, there are no data remaining that could possibly inform us of the problem.

Correct approach

We must include variable selection as a component of the modeling process.

- In the same way that we are choosing other tuning parameters for the model.



Algorithm:

1. For each fold of cross-validation, $1 \dots k$
 1. Split data into training/validation set
 2. Rank the predictors using the training set
 3. **For** each subset size, S_i
 - Fit model with S_i most important variables on the training set.
 - Predict the validation set.
2. Calculate the model performance with S_i variables
3. Determine the appropriate number of variables
4. Fit the final model based on the optimal number of variables using the original training set

In the above procedure, the number of variables to select is treated as a tuning parameter.

- feature selection is done within cross-validation;
- different set of input variables may be selected on each one of the cross-validation folds;
- computational cost increases.

Large data sets tend to greatly reduce the risk of overfitting to the predictors during variable selection. Using separate data splits for variable ranking/filtering, modeling, and evaluation can be both efficient and effective.

Example: Amyotrophic Lateral Sclerosis

We are going to explore the following two variable selection procedures

- Boruta package: stochastic wrapper procedure that uses random forest to compute variable importance measures
- Recursive Feature Elimination: a classical deterministic wrapper method

The data is from this paper:

- Model-Based and Model-Free Techniques for Amyotrophic Lateral Sclerosis Diagnostic Prediction and Patient Clustering. by Tang, M., Gao, C, Goutman, SA, Kalinin, A, Mukherjee, B, Guan, Y, and Dinov, ID.

Amyotrophic Lateral Sclerosis (ALS) is a rare but devastating disease. The data are from a large clinical trial including big, multi-source and heterogeneous datasets. The clinical data shows that the rate of ALS progression varies significantly among patients. Majority of the patients die within 3 to 5 years after ALS onset, however, a few are able survive for over 10 years. This heterogeneity of disease course hinders demonstration of its biological mechanism and development of effective treatment.

We need to develop reliable predictive models of ALS progression to understand the pathophysiology of the disease.

The dataset contains 2,223 observations and 131 numeric variables. We select `ALSFRS_slope` as our outcome variable, as it captures the patients' clinical decline over a year.

```
ALS.train<-read.csv("ALS_TrainingData_2223.csv")
summary(ALS.train)
```

```
##      ID      Age_mean  Albumin_max  Albumin_median  Albumin_min  Albumin_range
## Min.   :    1  Min.   :18.0  Min.   :37.0  Min.   :34.5  Min.   :24.0  Min.   :0.0000
## 1st Qu.: 614  1st Qu.:47.0  1st Qu.:45.0  1st Qu.:42.0  1st Qu.:39.0  1st Qu.:0.0090
## Median :1213  Median :55.0  Median :47.0  Median :44.0  Median :41.0  Median :0.0121
## Mean   :1215  Mean   :54.6  Mean   :47.0  Mean   :44.0  Mean   :40.8  Mean   :0.0138
## 3rd Qu.:1816  3rd Qu.:63.0  3rd Qu.:49.0  3rd Qu.:46.0  3rd Qu.:43.0  3rd Qu.:0.0159
## Max.   :2424  Max.   :81.0  Max.   :70.3  Max.   :51.1  Max.   :49.0  Max.   :0.2439
## ALSFRS_slope ALSFRS_Total_max ALSFRS_Total_median ALSFRS_Total_min ALSFRS_Total_range
## Min.   :-4.35  Min.   :11.0  Min.   : 2.5  Min.   : 0.0  Min.   :0.0000
## 1st Qu.: -1.09  1st Qu.:29.0  1st Qu.:23.0  1st Qu.:14.0  1st Qu.:0.0140
## Median : -0.62  Median :33.0  Median :28.0  Median :20.0  Median :0.0233
## Mean   : -0.73  Mean   :31.7  Mean   :27.1  Mean   :19.9  Mean   :0.0260
## 3rd Qu.: -0.28  3rd Qu.:36.0  3rd Qu.:32.0  3rd Qu.:27.0  3rd Qu.:0.0348
## Max.   : 1.21  Max.   :40.0  Max.   :40.0  Max.   :40.0  Max.   :0.1176
## ALT.SGPT._max ALT.SGPT._median ALT.SGPT._min  ALT.SGPT._range AST.SGOT._max AST.SGOT._median
## Min.   : 10  Min.   : 8  Min.   : 1.6  Min.   :0.003  Min.   : 11  Min.   : 9.0
## 1st Qu.: 32  1st Qu.: 22  1st Qu.: 15.0  1st Qu.:0.030  1st Qu.: 30  1st Qu.: 22.0
## Median : 45  Median : 30  Median : 21.0  Median :0.048  Median : 38  Median : 27.0
## Mean   : 54  Mean   : 33  Mean   : 23.0  Mean   :0.071  Mean   : 43  Mean   : 29.1
## 3rd Qu.: 65  3rd Qu.: 40  3rd Qu.: 28.0  3rd Qu.:0.078  3rd Qu.: 48  3rd Qu.: 34.0
## Max.   :944  Max.   :193  Max.   :109.0  Max.   :2.383  Max.   :911  Max.   :100.0
## AST.SGOT._min AST.SGOT._range Bicarbonate_max Bicarbonate_median Bicarbonate_min
## Min.   : 1.0  Min.   :0.000  Min.   :20.0  Min.   :19.5  Min.   : 2.5
## 1st Qu.:17.0  1st Qu.:0.024  1st Qu.:29.0  1st Qu.:26.0  1st Qu.:22.0
## Median :20.0  Median :0.035  Median :31.0  Median :27.0  Median :23.0
## Mean   :21.5  Mean   :0.049  Mean   :30.9  Mean   :27.0  Mean   :23.2
## 3rd Qu.:25.0  3rd Qu.:0.052  3rd Qu.:32.0  3rd Qu.:28.0  3rd Qu.:24.4
## Max.   :86.0  Max.   :1.917  Max.   :52.0  Max.   :39.5  Max.   :34.0
## Bicarbonate_range Blood.Urea.Nitrogen..BUN._max Blood.Urea.Nitrogen..BUN._median
## Min.   :0.0000  Min.   : 2.92  Min.   : 2.19
## 1st Qu.:0.0127  1st Qu.: 5.84  1st Qu.: 4.64
```

```

## Median :0.0149      Median : 6.94                      Median : 5.42
## Mean :0.0169      Mean : 7.35                      Mean : 5.56
## 3rd Qu.:0.0181      3rd Qu.: 8.21                      3rd Qu.: 6.35
## Max. :0.2143      Max. :25.19                      Max. :11.87
## Blood.Urea.Nitrogen..BUN._min Blood.Urea.Nitrogen..BUN._range bp_diastolic_max bp_diastolic_median
## Min. : 0.58      Min. :0.0000      Min. : 70      Min. : 56.0
## 1st Qu.: 3.29      1st Qu.:0.0041      1st Qu.: 88      1st Qu.: 78.0
## Median : 4.07      Median :0.0058      Median : 90      Median : 80.0
## Mean : 4.16      Mean :0.0071      Mean : 92      Mean : 81.1
## 3rd Qu.: 5.00      3rd Qu.:0.0084      3rd Qu.: 98      3rd Qu.: 85.0
## Max. :10.22      Max. :0.0695      Max. :140      Max. :110.0
## bp_diastolic_min bp_diastolic_range bp_systolic_max bp_systolic_median bp_systolic_min
## Min. : 20.0      Min. :0.000      Min. :100      Min. : 90      Min. : 72
## 1st Qu.: 65.0      1st Qu.:0.035      1st Qu.:138      1st Qu.:120      1st Qu.:108
## Median : 70.0      Median :0.043      Median :145      Median :130      Median :110
## Mean : 69.9      Mean :0.048      Mean :147      Mean :130      Mean :113
## 3rd Qu.: 75.0      3rd Qu.:0.054      3rd Qu.:157      3rd Qu.:136      3rd Qu.:120
## Max. :100.0      Max. :0.714      Max. :220      Max. :190      Max. :165
## bp_systolic_range Calcium_max Calcium_median Calcium_min Calcium_range Chloride_max
## Min. :0.000      Min. :2.17      Min. :2.05      Min. :0.244      Min. :0.00000      Min. : 96
## 1st Qu.:0.053      1st Qu.:2.40      1st Qu.:2.28      1st Qu.:2.171      1st Qu.:0.00037      1st Qu.:106
## Median :0.065      Median :2.47      Median :2.35      Median :2.230      Median :0.00047      Median :107
## Mean :0.071      Mean :2.47      Mean :2.35      Mean :2.223      Mean :0.00054      Mean :107
## 3rd Qu.:0.082      3rd Qu.:2.53      3rd Qu.:2.40      3rd Qu.:2.298      3rd Qu.:0.00059      3rd Qu.:109
## Max. :0.405      Max. :9.46      Max. :2.80      Max. :2.650      Max. :0.01290      Max. :119
## Chloride_median Chloride_min Chloride_range Creatinine_max Creatinine_median Creatinine_min
## Min. : 90      Min. : 76.0      Min. :0.0000      Min. : 22.0      Min. : 18.0      Min. : 0.0
## 1st Qu.:102      1st Qu.: 98.0      1st Qu.:0.0125      1st Qu.: 65.0      1st Qu.: 53.0      1st Qu.: 39.0
## Median :104      Median :100.0      Median :0.0159      Median : 79.6      Median : 62.0      Median : 53.0
## Mean :104      Mean : 99.3      Mean :0.0179      Mean : 78.8      Mean : 65.2      Mean : 52.0
## 3rd Qu.:105      3rd Qu.:101.0      3rd Qu.:0.0199      3rd Qu.: 88.4      3rd Qu.: 78.8      3rd Qu.: 61.9
## Max. :111      Max. :109.0      Max. :0.2143      Max. :248.0      Max. :176.8      Max. :168.0
## Creatinine_range Gender_mean Glucose_max Glucose_median Glucose_min Glucose_range
## Min. :0.000      Min. :1.00      Min. : 4.2      Min. : 3.50      Min. : 0.00      Min. :0.0000
## 1st Qu.:0.038      1st Qu.:1.00      1st Qu.: 5.8      1st Qu.: 4.91      1st Qu.: 4.05      1st Qu.:0.0031
## Median :0.049      Median :2.00      Median : 6.5      Median : 5.30      Median : 4.44      Median :0.0047
## Mean :0.058      Mean :1.64      Mean : 7.2      Mean : 5.49      Mean : 4.27      Mean :0.0063
## 3rd Qu.:0.070      3rd Qu.:2.00      3rd Qu.: 7.6      3rd Qu.: 5.70      3rd Qu.: 4.80      3rd Qu.:0.0074
## Max. :0.421      Max. :2.00      Max. :33.7      Max. :26.20      Max. :12.20      Max. :0.0975
## hands_max hands_median hands_min hands_range Hematocrit_max Hematocrit_median
## Min. :0.00      Min. :0.00      Min. :0.00      Min. :0.0000      Min. : 0.4      Min. : 0.4
## 1st Qu.:5.00      1st Qu.:3.00      1st Qu.:0.00      1st Qu.:0.0036      1st Qu.:42.3      1st Qu.:40.0
## Median :7.00      Median :5.50      Median :3.00      Median :0.0067      Median :45.2      Median :42.6
## Mean :6.18      Mean :4.91      Mean :3.05      Mean :0.0069      Mean :41.9      Mean :39.5
## 3rd Qu.:8.00      3rd Qu.:7.00      3rd Qu.:5.00      3rd Qu.:0.0095      3rd Qu.:47.7      3rd Qu.:45.0
## Max. :8.00      Max. :8.00      Max. :8.00      Max. :0.0429      Max. :81.0      Max. :56.0
## Hematocrit_min Hematocrit_range Hemoglobin_max Hemoglobin_median Hemoglobin_min Hemoglobin_range
## Min. : 0.3      Min. :0.0000      Min. :116      Min. :106      Min. : 6.2      Min. :0.000
## 1st Qu.:37.0      1st Qu.:0.0072      1st Qu.:144      1st Qu.:136      1st Qu.:128.0      1st Qu.:0.023
## Median :40.0      Median :0.0097      Median :152      Median :145      Median :136.0      Median :0.031
## Mean :37.0      Mean :0.0114      Mean :152      Mean :144      Mean :135.5      Mean :0.038
## 3rd Qu.:42.7      3rd Qu.:0.0136      3rd Qu.:160      3rd Qu.:152      3rd Qu.:145.0      3rd Qu.:0.042
## Max. :52.9      Max. :0.1857      Max. :280      Max. :182      Max. :180.0      Max. :0.562
## leg_max leg_median leg_min leg_range mouth_max mouth_median
## Min. :0.00      Min. :0.00      Min. :0.00      Min. :0.0000      Min. : 1.0      Min. : 0.0
## 1st Qu.:3.00      1st Qu.:2.50      1st Qu.:1.00      1st Qu.:0.0034      1st Qu.:10.0      1st Qu.: 8.0
## Median :5.00      Median :3.00      Median :2.00      Median :0.0054      Median :12.0      Median :11.0
## Mean :5.31      Mean :4.05      Mean :2.49      Mean :0.0062      Mean :10.7      Mean : 9.7
## 3rd Qu.:8.00      3rd Qu.:6.00      3rd Qu.:3.00      3rd Qu.:0.0087      3rd Qu.:12.0      3rd Qu.:12.0

```

```

## Max. :8.00 Max. :8.00 Max. :8.00 Max. :0.0420 Max. :12.0 Max. :12.0
## mouth_min mouth_range onset_delta_mean onset_site_mean Platelets_max Platelets_median
## Min. : 0.00 Min. :0.0000 Min. : -3119 Min. :1.0 Min. : 84 Min. : 73
## 1st Qu.: 5.00 1st Qu.:0.0018 1st Qu.: -887 1st Qu.:2.0 1st Qu.:239 1st Qu.:204
## Median : 9.00 Median :0.0053 Median : -572 Median :2.0 Median :275 Median :233
## Mean : 7.78 Mean :0.0066 Mean : -683 Mean :1.8 Mean :285 Mean :239
## 3rd Qu.:11.00 3rd Qu.:0.0103 3rd Qu.: -374 3rd Qu.:2.0 3rd Qu.:320 3rd Qu.:270
## Max. :12.00 Max. :0.0368 Max. : -16 Max. :3.0 Max. :866 Max. :526
## Platelets_min Potassium_max Potassium_median Potassium_min Potassium_range pulse_max
## Min. : 0 Min. : 3.4 Min. :3.00 Min. :2.40 Min. :0.0000 Min. : 53.0
## 1st Qu.:175 1st Qu.: 4.4 1st Qu.:4.00 1st Qu.:3.70 1st Qu.:0.0011 1st Qu.: 84.0
## Median :204 Median : 4.5 Median :4.20 Median :3.90 Median :0.0014 Median : 90.0
## Mean :208 Mean : 4.6 Mean :4.19 Mean :3.86 Mean :0.0017 Mean : 90.6
## 3rd Qu.:236 3rd Qu.: 4.8 3rd Qu.:4.30 3rd Qu.:4.00 3rd Qu.:0.0019 3rd Qu.: 96.0
## Max. :476 Max. :43.0 Max. :5.10 Max. :5.10 Max. :0.0987 Max. :144.0
## pulse_median pulse_min pulse_range respiratory_max respiratory_median respiratory_min
## Min. : 50 Min. : 18.0 Min. :0.005 Min. :2.00 Min. :0.00 Min. :0.00
## 1st Qu.: 72 1st Qu.: 60.0 1st Qu.:0.037 1st Qu.:4.00 1st Qu.:3.00 1st Qu.:2.00
## Median : 77 Median : 64.0 Median :0.049 Median :4.00 Median :4.00 Median :3.00
## Mean : 77 Mean : 65.4 Mean :0.054 Mean :3.91 Mean :3.59 Mean :2.79
## 3rd Qu.: 81 3rd Qu.: 70.0 3rd Qu.:0.062 3rd Qu.:4.00 3rd Qu.:4.00 3rd Qu.:4.00
## Max. :115 Max. :102.0 Max. :0.500 Max. :4.00 Max. :4.00 Max. :4.00
## respiratory_range Sodium_max Sodium_median Sodium_min Sodium_range SubjectID
## Min. :0.00000 Min. :134 Min. :128 Min. :112 Min. :0.0000 Min. : 533
## 1st Qu.:0.00000 1st Qu.:142 1st Qu.:139 1st Qu.:135 1st Qu.:0.0106 1st Qu.:240826
## Median :0.00183 Median :143 Median :140 Median :137 Median :0.0131 Median :496835
## Mean :0.00251 Mean :143 Mean :140 Mean :137 Mean :0.0150 Mean :498880
## 3rd Qu.:0.00365 3rd Qu.:145 3rd Qu.:141 3rd Qu.:138 3rd Qu.:0.0173 3rd Qu.:750300
## Max. :0.02542 Max. :169 Max. :146 Max. :145 Max. :0.1429 Max. :999482
## trunk_max trunk_median trunk_min trunk_range Urine.Ph_max Urine.Ph_median
## Min. :0.0 Min. :0.00 Min. :0.00 Min. :0.0000 Min. :5.00 Min. :5.00
## 1st Qu.:5.0 1st Qu.:3.00 1st Qu.:1.00 1st Qu.:0.0036 1st Qu.:6.00 1st Qu.:5.00
## Median :7.0 Median :5.00 Median :3.00 Median :0.0069 Median :7.00 Median :6.00
## Mean :6.2 Mean :4.89 Mean :2.96 Mean :0.0071 Mean :6.82 Mean :5.71
## 3rd Qu.:8.0 3rd Qu.:6.50 3rd Qu.:5.00 3rd Qu.:0.0096 3rd Qu.:7.00 3rd Qu.:6.00
## Max. :8.0 Max. :8.00 Max. :8.00 Max. :0.0420 Max. :9.00 Max. :9.00
## Urine.Ph_min
## Min. :5.00
## 1st Qu.:5.00
## Median :5.00
## Mean :5.18
## 3rd Qu.:5.00
## Max. :8.00

```

- diverse variables
- multiple features are highly correlated
- some of variables represent statistics like max, min and median values of the same clinical measurements

Boruta()

<https://mbq.github.io/Boruta/>

- reference: <https://cran.r-project.org/web/packages/Boruta/Boruta.pdf>
- vignette: <https://cran.r-project.org/web/packages/Boruta/vignettes/inahurry.pdf>
- detailed methodology: <https://www.jstatsoft.org/article/view/v036i11>

Overview of boruta algorithm:

- adds randomness to data by creating shuffled copies of all features (shadow features);
- train a random forest on the extended data set to compute feature importance;
- iteratively remove features that are less important than the best shadow features;
- stops when all features are confirmed or rejected or a specified limit of random forest runs is reached.

Note: This will take a few minutes to complete.

```
library(Boruta)
set.seed(43612)
als <- Boruta(ALSFRS_slope~.-ID, data=ALS.train, doTrace=0)
als
```

```
## Boruta performed 99 iterations in 2.04 mins.
## 28 attributes confirmed important: ALSFRS_Total_max, ALSFRS_Total_median,
## ALSFRS_Total_min, ALSFRS_Total_range, Creatinine_max and 23 more;
## 62 attributes confirmed unimportant: Age_mean, Albumin_max, Albumin_median, Albumin_min,
## Albumin_range and 57 more;
## 9 tentative attributes left: Hematocrit_median, Hematocrit_range, Hemoglobin_max,
## Hemoglobin_median, Hemoglobin_min and 4 more;
```

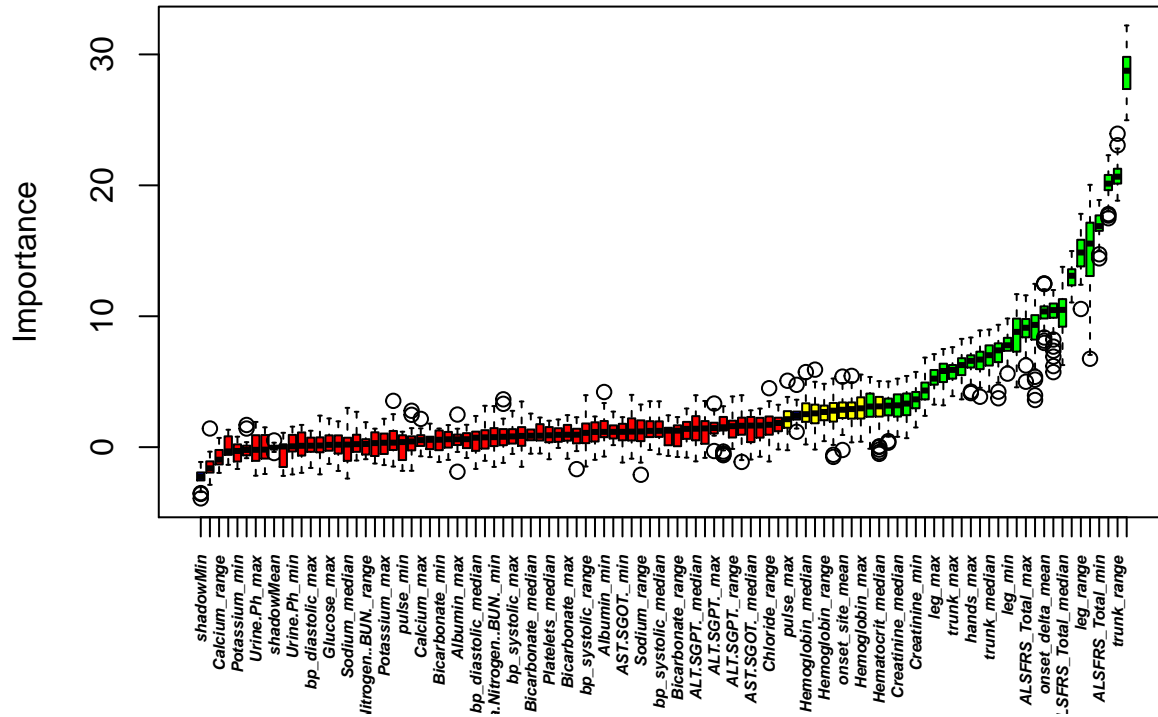
The importance scores for all features at every iteration are stored in the data frame `als$ImpHistory`.

```
als$ImpHistory[1:6, 1:10]
```

```
##      Age_mean Albumin_max Albumin_median Albumin_min Albumin_range ALSFRS_Total_max
## [1,]   0.4120     0.857         0.439       1.324         2.15           8.27
## [2,]   0.4091     0.436         1.250       1.167         2.90           7.66
## [3,]   0.1518     2.493         0.859       1.839         1.00           7.12
## [4,]   0.1460     0.257         2.468       2.547         1.91           8.62
## [5,]   1.8671     0.162         1.189       0.841         1.40           8.46
## [6,]  -0.0595     0.483         1.531      -0.239         1.63           8.34
##      ALSFRS_Total_median ALSFRS_Total_min ALSFRS_Total_range ALT.SGPT._max
## [1,]                6.27             15.0             25.2           1.500
## [2,]                8.26             16.6             26.0           2.924
## [3,]                6.82             15.4             26.3           1.804
## [4,]                8.24             16.7             25.5           1.039
## [5,]                8.70             16.3             26.3           1.304
## [6,]                8.00             16.8             25.2           0.887
```


A graph depicting the essential features.

```
plot(als, xlab="", xaxt="n")
lz<-lapply(1:ncol(als$ImpHistory), function(i)
als$ImpHistory[is.finite(als$ImpHistory[, i]), i])
names(lz)<-colnames(als$ImpHistory)
lb<-sort(sapply(lz, median))
axis(side=1, las=2, labels=names(lb), at=1:ncol(als$ImpHistory), cex.axis=0.5, font = 4)
```



Variables with green boxes are more important than the ones represented with red boxes, and we can see the range of importance scores within a single variable in the graph.

It may be desirable to get rid of tentative features.

- use only when a strict decision is highly desired.

```
final.als<-TentativeRoughFix(als)
final.als
```

```
## Boruta performed 99 iterations in 2.04 mins.
## Tentatives roughfixed over the last 99 iterations.
## 30 attributes confirmed important: ALSFRS_Total_max, ALSFRS_Total_median,
## ALSFRS_Total_min, ALSFRS_Total_range, Creatinine_max and 25 more;
## 69 attributes confirmed unimportant: Age_mean, Albumin_max, Albumin_median, Albumin_min,
## Albumin_range and 64 more;
```

```
final.als$finalDecision
```

##	Age_mean	Albumin_max	Albumin_median
##	Rejected	Rejected	Rejected
##	Albumin_min	Albumin_range	ALSFRS_Total_max
##	Rejected	Rejected	Confirmed
##	ALSFRS_Total_median	ALSFRS_Total_min	ALSFRS_Total_range
##	Confirmed	Confirmed	Confirmed
##	ALT.SGPT._max	ALT.SGPT._median	ALT.SGPT._min
##	Rejected	Rejected	Rejected
##	ALT.SGPT._range	AST.SGOT._max	AST.SGOT._median
##	Rejected	Rejected	Rejected
##	AST.SGOT._min	AST.SGOT._range	Bicarbonate_max
##	Rejected	Rejected	Rejected
##	Bicarbonate_median	Bicarbonate_min	Bicarbonate_range
##	Rejected	Rejected	Rejected
##	Blood.Urea.Nitrogen..BUN._max	Blood.Urea.Nitrogen..BUN._median	Blood.Urea.Nitrogen..BUN._min
##	Rejected	Rejected	Rejected
##	Blood.Urea.Nitrogen..BUN._range	bp_diastolic_max	bp_diastolic_median
##	Rejected	Rejected	Rejected
##	bp_diastolic_min	bp_diastolic_range	bp_systolic_max
##	Rejected	Rejected	Rejected
##	bp_systolic_median	bp_systolic_min	bp_systolic_range
##	Rejected	Rejected	Rejected
##	Calcium_max	Calcium_median	Calcium_min
##	Rejected	Rejected	Rejected
##	Calcium_range	Chloride_max	Chloride_median
##	Rejected	Rejected	Rejected
##	Chloride_min	Chloride_range	Creatinine_max
##	Rejected	Rejected	Confirmed
##	Creatinine_median	Creatinine_min	Creatinine_range
##	Confirmed	Confirmed	Rejected
##	Gender_mean	Glucose_max	Glucose_median
##	Rejected	Rejected	Rejected
##	Glucose_min	Glucose_range	hands_max
##	Rejected	Rejected	Confirmed
##	hands_median	hands_min	hands_range
##	Confirmed	Confirmed	Confirmed
##	Hematocrit_max	Hematocrit_median	Hematocrit_min
##	Confirmed	Rejected	Confirmed
##	Hematocrit_range	Hemoglobin_max	Hemoglobin_median
##	Rejected	Rejected	Rejected
##	Hemoglobin_min	Hemoglobin_range	leg_max
##	Confirmed	Rejected	Confirmed
##	leg_median	leg_min	leg_range
##	Confirmed	Confirmed	Confirmed
##	mouth_max	mouth_median	mouth_min
##	Confirmed	Confirmed	Confirmed
##	mouth_range	onset_delta_mean	onset_site_mean
##	Confirmed	Confirmed	Rejected
##	Platelets_max	Platelets_median	Platelets_min
##	Rejected	Rejected	Rejected
##	Potassium_max	Potassium_median	Potassium_min
##	Rejected	Rejected	Rejected

```
##          Potassium_range          pulse_max          pulse_median
##          Rejected          Confirmed          Rejected
##          pulse_min          pulse_range          respiratory_max
##          Rejected          Rejected          Rejected
##          respiratory_median          respiratory_min          respiratory_range
##          Rejected          Confirmed          Confirmed
##          Sodium_max          Sodium_median          Sodium_min
##          Rejected          Rejected          Rejected
##          Sodium_range          SubjectID          trunk_max
##          Rejected          Rejected          Confirmed
##          trunk_median          trunk_min          trunk_range
##          Confirmed          Confirmed          Confirmed
##          Urine.Ph_max          Urine.Ph_median          Urine.Ph_min
##          Rejected          Rejected          Rejected
## Levels: Tentative Confirmed Rejected
```

Report the Boruta “Confirmed” & “Tentative” features, removing the “Rejected” ones

```
print(final.als$finalDecision[final.als$finalDecision %in% c("Confirmed", "Tentative")])
```

```
##      ALSFRS_Total_max ALSFRS_Total_median ALSFRS_Total_min ALSFRS_Total_range Creatinine_max
##      Confirmed      Confirmed      Confirmed      Confirmed      Confirmed
##      Creatinine_median Creatinine_min      hands_max      hands_median      hands_min
##      Confirmed      Confirmed      Confirmed      Confirmed      Confirmed
##      hands_range      Hematocrit_max      Hematocrit_min      Hemoglobin_min      leg_max
##      Confirmed      Confirmed      Confirmed      Confirmed      Confirmed
##      leg_median      leg_min      leg_range      mouth_max      mouth_median
##      Confirmed      Confirmed      Confirmed      Confirmed      Confirmed
##      mouth_min      mouth_range      onset_delta_mean      pulse_max      respiratory_min
##      Confirmed      Confirmed      Confirmed      Confirmed      Confirmed
##      respiratory_range      trunk_max      trunk_median      trunk_min      trunk_range
##      Confirmed      Confirmed      Confirmed      Confirmed      Confirmed
## Levels: Tentative Confirmed Rejected
```

Recursive feature elimination (RFE)

Recursive feature elimination (RFE) is basically a backward selection.

- build a model on the entire set of variables
- compute an importance score for each variables
- remove the least important variable(s) from the model
- re-build a model and re-compute importance scores
- ...

The subset size is a tuning parameter for RFE

- the subset size that optimizes the loss is used to select the variables based on the importance rankings;
- the optimal subset is then used to train the final model.

RFE is frequently used with random forest models

- random forest tends not to exclude variables
- internal method for measuring variable importance

Measuring variable importance in suffers from multicollinearity. When there are highly correlated variables in a training set that are useful for predicting the outcome, then which variable is chosen for partitioning the samples is essentially a random selection.

- dilutes the importance scores
- it might be beneficial to filter out highly correlated features

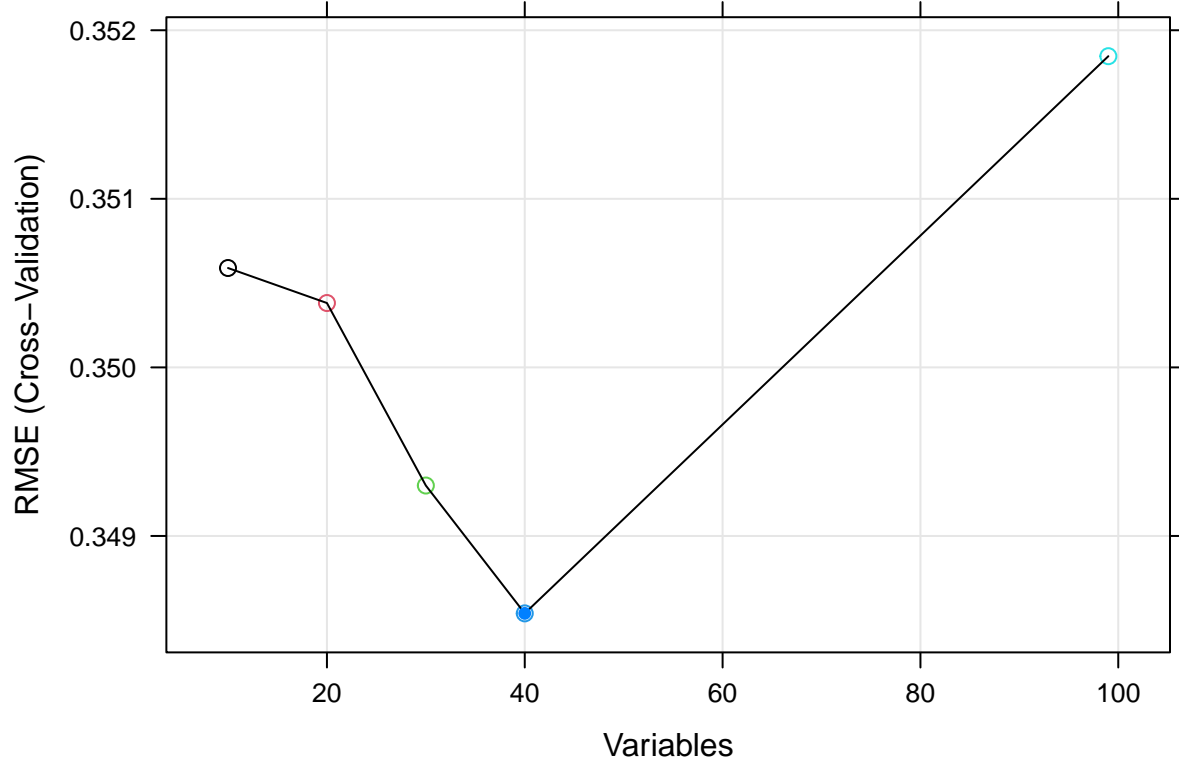
Note: This will take a few minutes to complete.

```
library(caret)
library(randomForest)
set.seed(43612)
control <- rfeControl(functions = rfFuncs, method = "cv", number=10)
rf.train <- rfe(ALS.train[, -c(1, 7)], ALS.train[, 7],
               sizes=c(10, 20, 30, 40), rfeControl=control)
rf.train

##
## Recursive feature selection
##
## Outer resampling method: Cross-Validated (10 fold)
##
## Resampling performance over subset size:
##
##  Variables  RMSE Rsquared  MAE RMSESD RsquaredSD  MAESD Selected
##      10 0.351   0.684 0.249 0.0364   0.0586 0.0201
##      20 0.350   0.685 0.248 0.0366   0.0559 0.0197
##      30 0.349   0.687 0.248 0.0343   0.0546 0.0194
##      40 0.349   0.689 0.248 0.0339   0.0524 0.0186      *
##      99 0.352   0.682 0.250 0.0343   0.0539 0.0176
##
## The top 5 variables (out of 40):
##  ALSFRS_Total_range, trunk_range, hands_range, mouth_range, ALSFRS_Total_min
```

- the `sizes=` option allows us to specify the number of variables we want to include in the model

```
plot(rf.train, type=c("g", "o"), cex=1, col=1:5)
```



Common variables chosen by the two techniques:

```
predRFE <- predictors(rf.train)
predBoruta <- getSelectedAttributes(final.als, withTentative = F)
intersect(predBoruta, predRFE)
```

```
## [1] "ALSFRS_Total_max"    "ALSFRS_Total_median" "ALSFRS_Total_min"    "ALSFRS_Total_range"
## [5] "Creatinine_max"      "Creatinine_median"   "Creatinine_min"      "hands_max"
## [9] "hands_median"        "hands_min"           "hands_range"         "Hematocrit_max"
## [13] "Hemoglobin_min"     "leg_max"             "leg_median"          "leg_min"
## [17] "leg_range"          "mouth_median"        "mouth_min"           "mouth_range"
## [21] "onset_delta_mean"   "respiratory_min"     "respiratory_range"   "trunk_max"
## [25] "trunk_median"       "trunk_min"           "trunk_range"
```

Example: Simulation Study

Let us also investigate the two procedures on a simulation benchmark where we know the true variable. We are going to use the “Friedman 1” benchmark (Friedman, 1991; Breiman, 1996). Inputs are 10 independent variables uniformly distributed on the interval $[0, 1]$, only 5 out of these 10 are actually related to the outputs. Outputs are created according to the formula

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

where $\epsilon \sim \mathcal{N}(0, \sigma^2)$.

We use the `mlbench` library to obtain the data.

```
library(mlbench)
n <- 100
p <- 40
sigma <- 1
set.seed(4125)
sim <- mlbench.friedman1(n, sd = sigma)
colnames(sim$x) <- c(paste("real", 1:5, sep = ""),
                    paste("bogus", 1:5, sep = ""))
bogus <- matrix(rnorm(n * p), nrow = n)
colnames(bogus) <- paste("bogus", 5+(1:ncol(bogus)), sep = "")
x <- cbind(sim$x, bogus)
y <- sim$y
```

We added 40 additional pure noise variables that are 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)
```

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

Note: This will take a few minutes to complete.

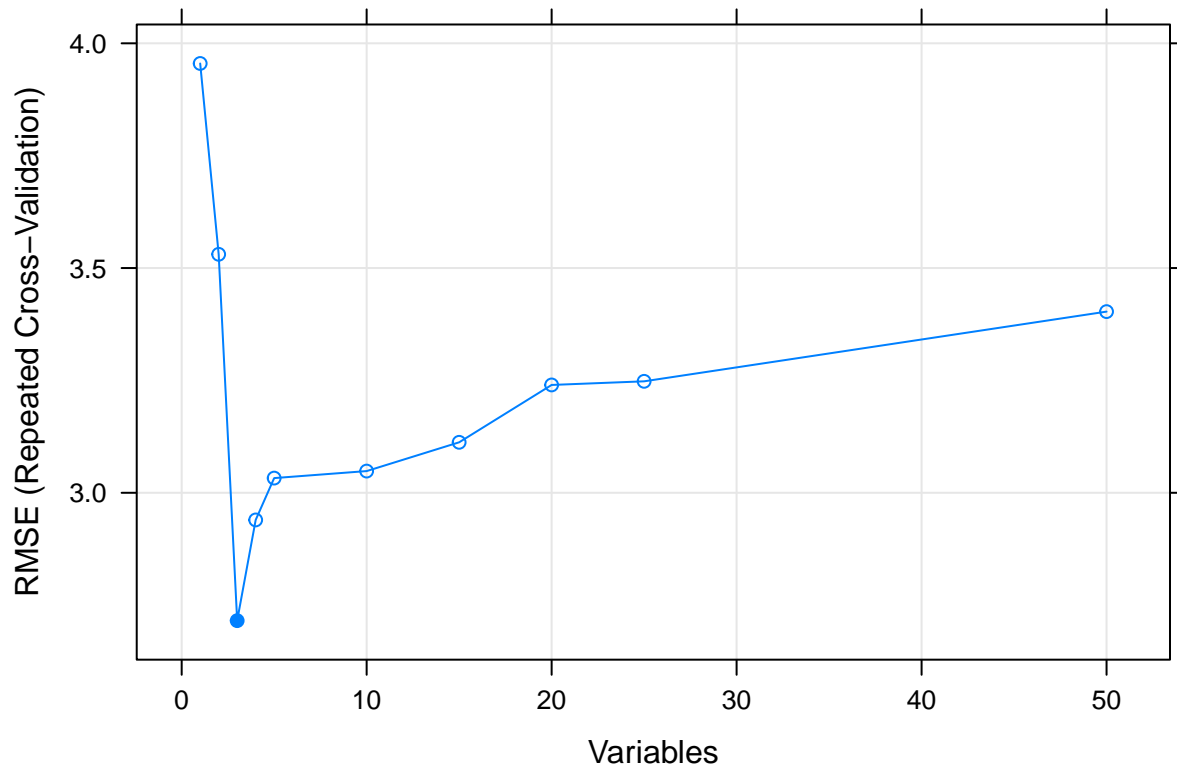
```
control <- rfeControl(functions = rfFuncs, method = "repeatedcv", number=10, repeats = 5)
rf.sim <- rfe(x, y, sizes=subsets, rfeControl=control)
rf.sim
```

```
##
## Recursive feature selection
##
## Outer resampling method: Cross-Validated (10 fold, repeated 5 times)
##
## Resampling performance over subset size:
##
## Variables RMSE Rsquared MAE RMSESD RsquaredSD MAESD Selected
##      1 3.96    0.409 3.15  0.690    0.224 0.653
##      2 3.53    0.519 2.89  0.535    0.177 0.505
##      3 2.72    0.743 2.22  0.434    0.116 0.368      *
##      4 2.94    0.721 2.41  0.484    0.156 0.448
##      5 3.03    0.724 2.50  0.485    0.140 0.432
##     10 3.05    0.738 2.52  0.470    0.142 0.409
##     15 3.11    0.722 2.55  0.471    0.146 0.389
```

```
##      20 3.24    0.715 2.65  0.496    0.142 0.392
##      25 3.25    0.714 2.66  0.470    0.137 0.376
##      50 3.40    0.707 2.79  0.478    0.134 0.384
```

```
##
## The top 3 variables (out of 3):
##   real4, real2, real1
```

```
plot(rf.sim, type = c("g", "o"))
```



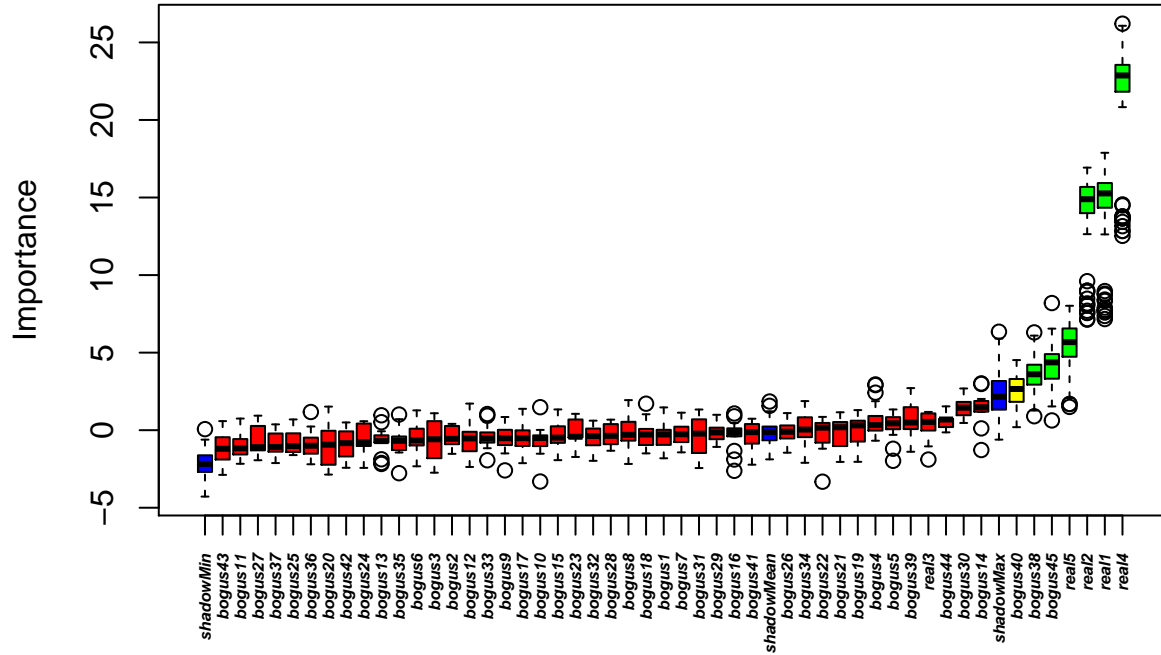
Note: This will take a few minutes to complete.

```
boruta.sim <- Boruta(x, y)
boruta.sim
```

```
## Boruta performed 99 iterations in 1.52 secs.
## 6 attributes confirmed important: bogus38, bogus45, real1, real2, real4 and 1 more;
## 43 attributes confirmed unimportant: bogus1, bogus10, bogus11, bogus12, bogus13 and 38
## more;
## 1 tentative attributes left: bogus40;
```

Result plot

```
plot(boruta.sim, xlab="", xaxt="n")
lz<-lapply(1:ncol(boruta.sim$ImpHistory), function(i)
boruta.sim$ImpHistory[is.finite(boruta.sim$ImpHistory[, i]), i])
names(lz)<-colnames(boruta.sim$ImpHistory)
lb<-sort(sapply(lz, median))
axis(side=1, las=2, labels=names(lb), at=1:ncol(boruta.sim$ImpHistory), cex.axis=0.5, font = 4)
```



Attribute statistics

```
attStats(boruta.sim)
```

##		meanImp	medianImp	minImp	maxImp	normHits	decision
##	real1	14.4168	15.2651	7.165	17.884	1.0000	Confirmed
##	real2	14.1189	14.8900	7.127	16.929	1.0000	Confirmed
##	real3	0.2871	0.5332	-1.892	1.176	0.0000	Rejected
##	real4	21.7585	22.8692	12.530	26.208	1.0000	Confirmed
##	real5	5.4911	5.6776	1.501	8.020	0.8990	Confirmed
##	bogus1	-0.4122	-0.2757	-1.812	1.468	0.0000	Rejected
##	bogus2	-0.4758	-0.5583	-1.525	0.408	0.0000	Rejected
##	bogus3	-0.6822	-0.5854	-2.740	1.093	0.0000	Rejected
##	bogus4	0.6139	0.3295	-0.679	2.950	0.0202	Rejected
##	bogus5	0.2790	0.4434	-1.974	1.337	0.0000	Rejected
##	bogus6	-0.5103	-0.6569	-2.328	1.277	0.0000	Rejected
##	bogus7	-0.1858	-0.2598	-1.428	1.128	0.0000	Rejected
##	bogus8	-0.1147	-0.2987	-2.176	1.938	0.0000	Rejected
##	bogus9	-0.5360	-0.5172	-2.591	0.850	0.0000	Rejected
##	bogus10	-0.6803	-0.5030	-3.309	1.482	0.0000	Rejected
##	bogus11	-1.0344	-1.1706	-2.166	0.751	0.0000	Rejected
##	bogus12	-0.5189	-0.5325	-2.371	1.715	0.0000	Rejected
##	bogus13	-0.6902	-0.7050	-2.178	0.962	0.0000	Rejected
##	bogus14	1.4234	1.4774	-1.279	3.015	0.0000	Rejected
##	bogus15	-0.3233	-0.4783	-1.932	1.338	0.0000	Rejected
##	bogus16	-0.3419	-0.1283	-2.620	1.076	0.0000	Rejected
##	bogus17	-0.5127	-0.5152	-2.126	1.377	0.0000	Rejected
##	bogus18	-0.2664	-0.2824	-1.496	1.708	0.0000	Rejected
##	bogus19	-0.0180	0.3102	-2.039	1.296	0.0000	Rejected
##	bogus20	-0.8763	-0.9344	-2.861	1.520	0.0000	Rejected
##	bogus21	-0.1871	0.1884	-2.046	1.154	0.0000	Rejected
##	bogus22	-0.2004	0.1631	-3.322	0.856	0.0000	Rejected
##	bogus23	-0.0901	-0.4230	-1.726	1.055	0.0000	Rejected
##	bogus24	-0.6113	-0.7626	-2.431	0.578	0.0000	Rejected


```
## bogus25 -0.7665 -1.0224 -1.605 0.693 0.0000 Rejected
## bogus26 -0.1394 -0.0987 -1.453 1.102 0.0000 Rejected
## bogus27 -0.6906 -1.0923 -1.938 0.936 0.0000 Rejected
## bogus28 -0.3204 -0.3632 -1.325 0.680 0.0000 Rejected
## bogus29 -0.0660 -0.1477 -1.078 0.993 0.0000 Rejected
## bogus30 1.4097 1.4494 0.467 2.689 0.0000 Rejected
## bogus31 -0.4300 -0.2220 -2.440 1.334 0.0000 Rejected
## bogus32 -0.4727 -0.3760 -1.975 0.614 0.0000 Rejected
## bogus33 -0.3896 -0.5270 -1.939 1.042 0.0000 Rejected
## bogus34 0.0572 0.0412 -2.102 1.876 0.0000 Rejected
## bogus35 -0.7085 -0.6838 -2.773 1.010 0.0000 Rejected
## bogus36 -0.8124 -1.0011 -2.196 1.172 0.0000 Rejected
## bogus37 -0.8787 -1.0829 -2.120 0.375 0.0000 Rejected
## bogus38 3.5504 3.6036 0.900 6.305 0.7778 Confirmed
## bogus39 0.6811 0.4962 -1.391 2.714 0.0303 Rejected
## bogus40 2.5564 2.6559 0.195 4.521 0.6162 Tentative
## bogus41 -0.3359 -0.1254 -2.225 0.738 0.0000 Rejected
## bogus42 -0.9072 -0.8360 -2.424 0.498 0.0000 Rejected
## bogus43 -1.0997 -1.1976 -2.881 0.585 0.0000 Rejected
## bogus44 0.5732 0.6881 -0.140 1.535 0.0000 Rejected
## bogus45 4.1863 4.3719 0.630 8.197 0.8182 Confirmed
```

Let us now try with a slightly large sample size $n = 200$. Everything else is the same.

Note: This will take a few minutes to complete.

```
n <- 200
p <- 40
sigma <- 1
set.seed(4125)
sim <- mlbench.friedman1(n, sd = sigma)
colnames(sim$x) <- c(paste("real", 1:5, sep = ""),
                    paste("bogus", 1:5, sep = ""))
bogus <- matrix(rnorm(n * p), nrow = n)
colnames(bogus) <- paste("bogus", 5+(1:ncol(bogus)), sep = "")
x <- cbind(sim$x, bogus)
y <- sim$y
normalization <- preProcess(x)
x <- predict(normalization, x)
x <- as.data.frame(x)
subsets <- c(1:5, 10, 15, 20, 25)

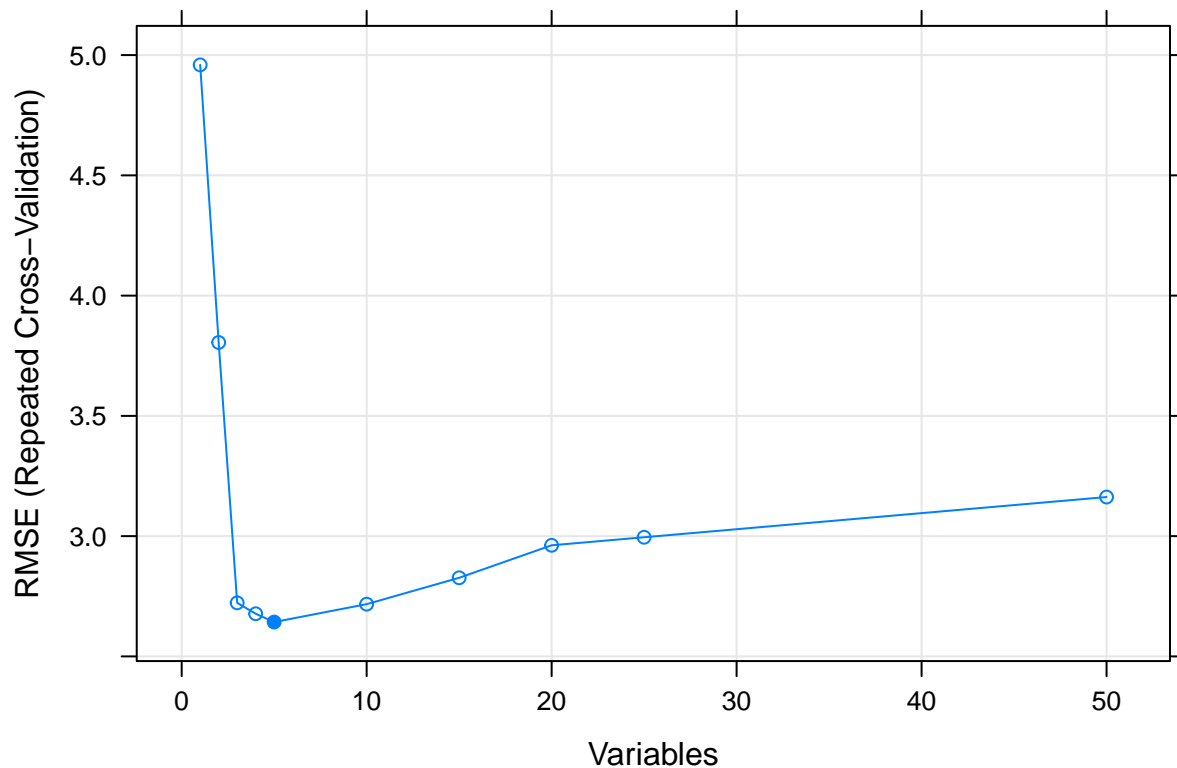
control <- rfeControl(functions = rfFuncs, method = "repeatedcv", number=10, repeats = 5)
rf.sim <- rfe(x, y, sizes=subsets, rfeControl=control)
rf.sim

##
## Recursive feature selection
##
## Outer resampling method: Cross-Validated (10 fold, repeated 5 times)
##
## Resampling performance over subset size:
##
## Variables RMSE Rsquared MAE RMSESD RsquaredSD MAESD Selected
##          1 4.96   0.0732 4.05  0.707   0.0760 0.587
##          2 3.81   0.3352 3.12  0.479   0.1530 0.451
```

```
##      3 2.72   0.6762 2.17  0.376   0.1120 0.325
##      4 2.68   0.7201 2.20  0.371   0.1176 0.348
##      5 2.64   0.7890 2.15  0.391   0.0834 0.329      *
##     10 2.72   0.7698 2.20  0.380   0.0834 0.311
##     15 2.83   0.7399 2.29  0.414   0.0978 0.343
##     20 2.96   0.7269 2.41  0.422   0.1028 0.339
##     25 3.00   0.7166 2.43  0.433   0.1102 0.353
##     50 3.16   0.6810 2.57  0.423   0.1214 0.335
```

```
##
## The top 5 variables (out of 5):
##   real1, real2, real4, real5, real3
```

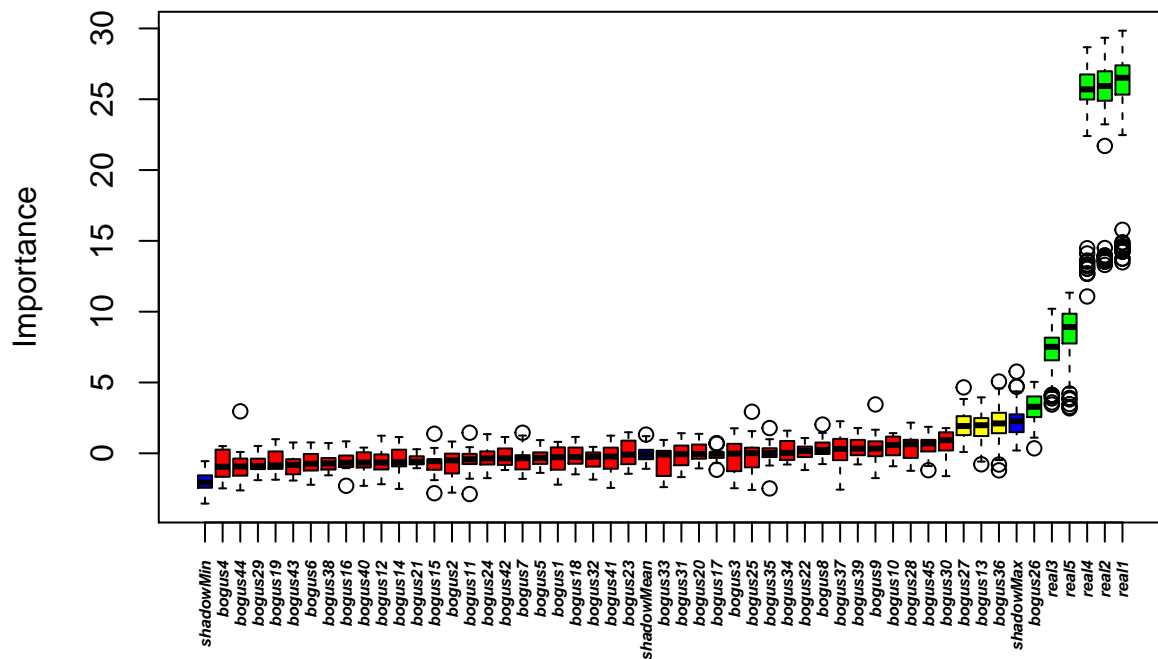
```
plot(rf.sim, type = c("g", "o"))
```



```
boruta.sim <- Boruta(x, y)
boruta.sim
```

```
## Boruta performed 99 iterations in 3.36 secs.
## 6 attributes confirmed important: bogus26, real1, real2, real3, real4 and 1 more;
## 41 attributes confirmed unimportant: bogus1, bogus10, bogus11, bogus12, bogus14 and 36
## more;
## 3 tentative attributes left: bogus13, bogus27, bogus36;
```

```
plot(boruta.sim, xlab="", xaxt="n")
lz<-lapply(1:ncol(boruta.sim$ImpHistory), function(i)
boruta.sim$ImpHistory[is.finite(boruta.sim$ImpHistory[, i]), i])
names(lz)<-colnames(boruta.sim$ImpHistory)
lb<-sort(sapply(lz, median))
axis(side=1, las=2, labels=names(lb), at=1:ncol(boruta.sim$ImpHistory), cex.axis=0.5, font = 4)
```



```
attStats(boruta.sim)
```

##		meanImp	medianImp	minImp	maxImp	normHits	decision
##	real1	25.053076	26.5155	13.4857	29.840	1.0000	Confirmed
##	real2	24.560321	25.9342	13.2992	29.340	1.0000	Confirmed
##	real3	7.220585	7.5180	3.4442	10.206	0.9899	Confirmed
##	real4	24.368496	25.6965	11.0746	28.673	1.0000	Confirmed
##	real5	8.566450	8.9142	3.1754	11.342	0.9899	Confirmed
##	bogus1	-0.404292	-0.2789	-2.2098	0.809	0.0000	Rejected
##	bogus2	-0.832059	-0.4985	-2.7748	0.833	0.0000	Rejected
##	bogus3	-0.267769	-0.0209	-2.4676	1.766	0.0000	Rejected
##	bogus4	-0.827315	-0.9488	-2.4737	0.507	0.0000	Rejected
##	bogus5	-0.282409	-0.3281	-1.3830	0.931	0.0000	Rejected
##	bogus6	-0.653863	-0.7346	-2.2195	0.768	0.0000	Rejected
##	bogus7	-0.386086	-0.3479	-1.8040	1.454	0.0000	Rejected
##	bogus8	0.415413	0.2368	-0.7636	2.029	0.0000	Rejected
##	bogus9	0.375869	0.3359	-1.7517	3.450	0.0101	Rejected
##	bogus10	0.471256	0.5885	-0.9141	1.424	0.0000	Rejected
##	bogus11	-0.466887	-0.4217	-2.8748	1.454	0.0000	Rejected
##	bogus12	-0.585345	-0.6544	-2.1831	1.244	0.0000	Rejected
##	bogus13	1.776393	1.9851	-0.7756	3.950	0.4242	Tentative
##	bogus14	-0.482675	-0.6288	-2.5130	1.148	0.0000	Rejected
##	bogus15	-0.745976	-0.5519	-2.8194	1.381	0.0000	Rejected
##	bogus16	-0.548214	-0.6603	-2.2924	0.845	0.0000	Rejected
##	bogus17	-0.075336	-0.0288	-1.1625	0.711	0.0000	Rejected
##	bogus18	-0.241221	-0.2671	-1.4838	1.158	0.0000	Rejected
##	bogus19	-0.626955	-0.8546	-1.8638	0.995	0.0000	Rejected
##	bogus20	0.077822	-0.0491	-1.0636	1.374	0.0000	Rejected
##	bogus21	-0.502531	-0.5947	-1.0513	0.289	0.0000	Rejected
##	bogus22	0.124647	0.1656	-1.1825	1.080	0.0000	Rejected
##	bogus23	-0.000906	-0.0929	-1.4442	1.487	0.0000	Rejected
##	bogus24	-0.335973	-0.3608	-1.7523	1.353	0.0000	Rejected
##	bogus25	-0.034877	0.0117	-2.5847	2.935	0.0101	Rejected

## bogus26	3.238152	3.2876	0.3516	5.045	0.7677	Confirmed
## bogus27	2.006880	1.9267	0.0885	4.655	0.4040	Tentative
## bogus28	0.393491	0.6451	-1.2355	2.166	0.0000	Rejected
## bogus29	-0.780894	-0.8982	-1.8962	0.520	0.0000	Rejected
## bogus30	0.728078	0.9278	-1.6100	1.778	0.0000	Rejected
## bogus31	-0.166516	-0.0602	-1.6803	1.419	0.0000	Rejected
## bogus32	-0.431643	-0.2485	-1.8541	0.456	0.0000	Rejected
## bogus33	-0.470244	-0.0833	-2.3879	0.945	0.0000	Rejected
## bogus34	0.171497	0.0330	-0.7908	1.600	0.0000	Rejected
## bogus35	0.008024	0.0151	-2.4785	1.783	0.0000	Rejected
## bogus36	2.066192	2.1096	-1.2037	5.068	0.4646	Tentative
## bogus37	0.296761	0.3103	-2.5647	2.266	0.0000	Rejected
## bogus38	-0.589869	-0.7163	-1.5509	0.725	0.0000	Rejected
## bogus39	0.450585	0.3356	-0.7814	1.791	0.0000	Rejected
## bogus40	-0.627772	-0.6582	-2.2954	0.403	0.0000	Rejected
## bogus41	-0.279155	-0.2293	-2.4399	1.248	0.0000	Rejected
## bogus42	-0.228526	-0.3534	-1.1796	1.154	0.0000	Rejected
## bogus43	-0.769450	-0.8143	-1.9202	0.765	0.0000	Rejected
## bogus44	-0.750402	-0.9276	-2.6177	2.963	0.0000	Rejected
## bogus45	0.371304	0.6918	-1.1921	1.871	0.0000	Rejected