

Application of Random Forest Algorithm on Feature Subset Selection and Classification and Regression

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Abstract: Feature subset selection becomes quite important and predominant in the case of data sets those are contained with higher number of variables. It discards insignificant variables and produces efficient and improved prediction performance on the class variables that is more cost effective and more reliable understanding of the data. Random forest has been emerged as a quite efficient and robust algorithm that can handle feature selection problem even with the higher number of variables. It is also very much efficient while dealing with Missing data imputation, classification, and regression problems. It can also handle outliers and noisy data very well. In this paper we applied the concept of random forest algorithm on the feature subset selection and classification and regression to perform the comparative study of the random forest algorithm in different perspectives.

Keywords: Random Forest; Feature Selection; Classification; Regression; Gini Index; Wrapper and Filter Methods.

I. INTRODUCTION

In the area of data processing and analysis, a dataset may have many numbers of variables or attributes which determine the applicability and usability of the data. It is obvious that, every attribute may not be contributing substantially for different applications rather than a subset of variables can provide us an equivalent and effective attention. Finding the subset or relevant features may be termed as feature selection or feature subset selection in the area of machine learning or statistics. This is also known as variable selection, attribute selection, variable or attribute subset selection. This approach may reduce the data training time and effort, rationalize the data interpretation, and reduce the overfitting scenario by enhanced data generalization [1].

In this paper we have considered the Chronic_Kidney_Disease data from UCI Machine Learning Repository [2]. For the determination of feature selection, we have followed the *Boruta* package in the R programming language [3]. This package is based on wrapper algorithms basically and works on the random forest method for the determination of the subset of the important features. This algorithm performs a top-down approach for relevant features with the comparison on the set of original attributes.

A. Literature Survey for Feature Selection and Random Forest Algorithm

The concept of feature selection came into picture after 1995 around. Blum and Langlay [5] had given a survey on two problems: issues of selecting relevant features and issues of selecting relevant examples, and produced a general framework to compare different algorithms.

Many works have been done on the ranking of variables for the features selection [6] [7]. Two well-known methods, Boosting [8] and Bagging [9] were proposed to generate many classifiers and aggregate their results for the classification tree.

We have elaborated random forest algorithm with different tools in section-II and applied it for the feature selection with the help of *Boruta* and *randomForest* packages from the R programming language. In the section-III, we have discussed about classification and regression techniques with the help of *randomForest* package from the R programming language. In the section-IV, we have summarized our paper work and proposed some future scope.

II. FEATURE SELECTION BY RANDOM FOREST

A forest is the collection of trees; a random forest is the collection of classification trees. Classification tree, sometimes also called as decision tree, is the construction of a tree which consist the members of the class variable on its leaf nodes and the entities of other dependent variables reside on the intermediate nodes. Class variables are also called as decision variables or predictor variables, which may comprise, for example, yes/no decision to predict a disease or loan approval, spam/no spam in the case of emails, good/bad/moderate for the product qualities, 0-9 for handwritten digits in the case pattern recognition, etc. Random forests develop many classification trees, and to add a new classification tree to the forest, add it down to the each of the trees in the forest. Each tree provides its classification and we consider it as its vote for that class. The forest considers the classification receiving the most votes from all the trees in the forest.

Construction of the Random Forest

1. If there are N cases in the training set, select all the cases randomly, as a separate set of data other than the original data set.
2. For T number of attributes in the training data set, select $t \ll T$ attributes at random such that at each node the best set of t variables is used to split the node. The value of t should be stable while tree growing.
3. Each tree will be growing to the extreme possible extent without pruning.

The error rate for the random forest depends on the following two factors:

- I. The error rate will increase if and only if the correlation between any two trees from the forest will be increasing.
- II. The strength of the tree is determined by the error rate that is lower the error rate stronger the tree and that will strengthen the forest.

Properties of the Random Forest:

- It has been considered as **unexcelled** algorithm in accuracy.
- It is very much efficient on huge data sets even with hundreds and thousands of input variables without overfitting and there is no requirement **data pruning**.
- It is applied for the feature subset selection and missing **data imputation** and performs very efficiently.
- An internal unbiased estimate of the generalization error is produced by the random forest algorithm in the process of forest construction.
- The generated forest can perform well for the future adding data.

Working Process of the Random Forest

There are two data objects generated by the random forest: random attribute data set and original data set. The training set is about two third of the original data set and rest are called as out-of-bag (*oob*) data, that is used to estimate unbiased classification error as trees are added to the forest.

The proximities are calculated for each pair of the cases after the built of the tree. If the two pairs compete for the same terminal node of the tree, their proximities are increased by one. Eventually the proximities are **normalized** by dividing by the total number of the trees in the forest.

The Error Estimation with *oob* Data

Out-of-bag estimation was proposed by Tibshirani [10], as an important ingredient for the calculation of **generalization error**. It is not required to cross-validate or a separate test to calculate an unbiased error estimate of the validation set in the random forest, since it performs eternally during the execution. Each tree is built using a random sampling with replacement from the original data. About one third of the cases are left out as *oob* data that are

not used in the built of the p -th tree. Put each case from *oob* data in the build of the p -th tree down to the p -th tree to get a classification. With this process a test classification is achieved for each case in about one-third of the trees. Eventually, consider q to be the class variable with maximum votes every time from m cases of *oob*. The *oob* error is estimated with the factor that q is not equal to the true class of m averaged over all cases. This estimation is unbiased for many cases.

Variable Importance

For the *oob* cases, let the number of vote cast for the correct class is x and for the permuted *oob* variables, it is y . the average of $(x-y)$ over all trees in the forest is considered as the raw importance score for variable x .

If we get these score values independent for every tree, then we compute standard error by standard computation, and the correlation for these scores are quite low. For a huge data set having many number of variables we first run this algorithm for all variables, and again execute same process for the considered variables from the first run.

Gini Importance

Gini index is the accuracy (or inaccuracy) measure of the decision trees. The Gini inaccuracy criterion for the parent node is always higher than the two descendent nodes that are split from the parent node. Improvement in the Gini decrease of each individual attribute for every tree in the forest provides surplus variable importance that is often quite consistent with the permutation importance measure.

Variables Interactions

Variables interaction is calculated at the terminal node with the split of variables either in left side or in right side. There may be k interaction on m variables on a terminal node that makes a split on k either systematically less possible or more possible. This interaction is calculated with Gini values for each tree in the forest. This is considered as rank for each tree for every two variables and the absolute differences of ranks are averaged over all trees.

The rank for each tree is also estimated with hypothesis that assumes the independence of two variables with each other. Subtract the lower rank value from higher rank value. Higher difference implies that a split on higher ranked variable inhibits a split on lower rank variable and vice versa.

Proximities Estimation

Proximity estimation is a very important tool in the random forest. It creates a $N \times N$ matrix. After growing a tree, put complete data down to this tree. If the two variables at the same terminal node are having proximities, increase it by one for both. Eventually, normalize it by taking average over the total number of trees in the forest.

With the large data set $N \times N$ matrix could not fit into the processing memory, so $N \times T$ matrix is processed, where T is the total number of trees in the forest.

Data Scaling

The proximity between the two variables p and q is a matrix $\{proximity(p, q)\}$ which is symmetric, positive definite, and bounded over by 1, with the diagonal elements 1. In the Euclidean space of dimension, the values $\{1-proximity(p, q)\}$ are squared distances and not exceeding the total number of cases.

Let the average value of $proximity(p, q)$ is $proximity(-, q)$ over the first coordinate, $proximity(p, -)$, over the second coordinate, and $proximity(-, -)$, the average over both coordinate. Then the proximity matrix

$$pm(p, q) = 0.5 * [proximity(p, q) - proximity(p, -) - proximity(-, q) + proximity(-, -)]$$

is the distance matrix of the inner product that is symmetric and positive definite. If the Eigen values and Eigen vectors of the proximity matrix pm are $l(i)$ and $p_i(p)$ respectively, then the vectors

$$x(p) = (\Theta l(1) p_1(p), \Theta l(2) p_2(p), \dots)$$

have squared distances between them with the value $\{1-proximity(p, q)\}$. The values $\Theta l(i) p_i(p)$ are considered as the i^{th} scaling coordinates.

Random forests perform the approximation of vectors $x(p)$ by extracting some of the largest values of Eigenvalues of the pm matrix and their corresponding values of the Eigenvectors.

Application of *Boruta* Package from R on the Data set Chronik_Kidney_Disease from the UCI machine learning repository:

```
library(Boruta)
boruta.train <- Boruta(class=., data = traindata, doTrace = 2)

plot(boruta.train, xlab = "", xaxt = "n")
lz <- lapply(1:ncol(boruta.train$ImpHistory), function(i)
  boruta.train$ImpHistory[is.finite(boruta.train$ImpHistory[,i]),i])
names(lz) <- colnames(boruta.train$ImpHistory)
labels <- sort(sapply(lz, median))
axis(side = 1, las=2, labels = names(labels),
  at = 1:ncol(boruta.train$ImpHistory), cex.axis = 0.7)
final.boruta <- TentativeRoughFix(boruta.train)
print(final.boruta)

##list of Confirmed attributes
getSelectedAttributes(final.boruta, withTentative = F)

##create a data frame of the final result derived from Boruta
boruta.df <- attStats(final.boruta)
print(boruta.df)

> print(boruta.df)
```

	meanImp	medianImp	minImp	maxImp	normHits	decision
Age	2.917592	2.938543	0.3785675	5.507572	0.757578	Confirmed
bp	5.800792	5.772647	4.7314161	7.555581	1.000000	Confirmed
sg	17.856400	17.868679	16.2750857	19.675943	1.000000	Confirmed
al	16.318842	16.284237	14.3290491	18.107874	1.000000	Confirmed
su	9.210438	9.236121	7.8593396	10.691650	1.000000	Confirmed
rbc	15.021551	14.996421	13.4547002	16.372840	1.000000	Confirmed
pc	7.159725	7.245119	5.9133154	8.131808	1.000000	Confirmed
pcc	3.873885	3.896815	2.4767305	5.030278	0.959596	Confirmed
ba	3.354710	3.367921	2.0758280	4.880679	0.919191	Confirmed
bgr	2.551377	2.498004	0.3918401	5.070106	0.626262	Rejected
bu	5.908567	5.928149	4.6354787	6.967415	1.000000	Confirmed
sc	18.525295	18.556597	16.0578113	20.198106	1.000000	Confirmed
sod	10.717466	10.739086	9.5744594	12.099973	1.000000	Confirmed
pot	8.940209	8.883427	7.5619009	10.373480	1.000000	Confirmed
hemo	11.218235	11.182024	9.3438088	12.616668	1.000000	Confirmed
pcv	17.580820	17.503315	16.1297163	19.316045	1.000000	Confirmed
wc	5.349204	5.377705	3.3470043	7.018811	0.989899	Confirmed
rc	16.149840	16.133833	14.1576808	18.082229	1.000000	Confirmed
htn	13.984560	13.948396	12.6689885	15.396414	1.000000	Confirmed
dm	13.201492	13.158996	11.4617186	15.207218	1.000000	Confirmed
cad	2.883597	2.860327	1.7331075	3.933949	0.767678	Confirmed
appet	8.932541	8.899613	7.3434304	10.636989	1.000000	Confirmed
pe	8.050709	8.037748	6.3734811	9.536482	1.000000	Confirmed
ane	6.335017	6.386672	5.0130262	7.427422	1.000000	Confirmed

```
library(randomForest)
traindata.rf <- randomForest(traindata[, -25], traindata[, 25], prox=TRUE)
traindata.p <- classcenter(traindata[, -25], traindata[, 25], traindata.rf$prox)

rf1 <- randomForest(class ~ ., traindata, ntree=150, norm.votes=FALSE)
rf2 <- randomForest(class ~ ., traindata, ntree=150, norm.votes=FALSE)
rf3 <- randomForest(class ~ ., traindata, ntree=150, norm.votes=FALSE)
rf4 <- randomForest(class ~ ., traindata, ntree=150, norm.votes=FALSE)
rf5 <- randomForest(class ~ ., traindata, ntree=150, norm.votes=FALSE)
rf.all <- combine(rf1, rf2, rf3, rf4, rf5)
print(rf.all)

##Extract a single tree from a forest.
getTree(randomForest(traindata[, -25], traindata[, 25], ntree=50), 3, labelVar=TRUE)

##Add trees to an ensemble
traindata.rf <- randomForest(class ~ ., traindata, ntree=500, norm.votes=FALSE)
traindata.rf <- grow(traindata.rf, 500)
print(traindata.rf)

> print(rf.all)

call:
randomForest(formula = class ~ ., data = traindata, ntree = 150, norm.votes = FALSE)
Type of random forest: classification
Number of trees: 750
No. of variables tried at each split: 4

> getTree(randomForest(traindata[, -25], traindata[, 25], ntree=50), 3, labelVar=TRUE)
left daughter right daughter split var split point status prediction
1 2 3 al 0.5 1 <NA>
2 4 5 sod 130.0 1 <NA>
3 0 0 <NA> 0.0 -1 ckd
4 0 0 <NA> 0.0 -1 ckd
5 0 0 <NA> 0.0 -1 notckd
> print(traindata.rf)

call:
randomForest(formula = class ~ ., data = traindata, ntree = 500, norm.votes = FALSE)
Type of random forest: classification
Number of trees: 1000
No. of variables tried at each split: 4
```

The package *Boruta* establishes an iterative comparison between randomly selected variables and the variables from the original data set. Those variables which are having significantly worst importance than the random data set are consecutively rejected.

III. CLASSIFICATION AND REGRESSION BY RANDOM FOREST

For the *categorical type* of class or target variables, decision trees are considered as classification decision trees, for example, the consumer behavior for buying the particular goods (binary target variables, yes/no). For the *continuous variables*, it is called as regression decision trees, for example deciding house prices, that can depend on different factors or variables like size (square ft.) and types (flat, independent) of houses.

A. Classification

Classification technique is applied to predict the decision values from the class variable for qualitative or categorical types of variables by the calculation with one or more independent or predictor variables. It is widely applied in the fields like computer science (Data Structure), medicine (diagnosis), botany (classification), and psychology (decision theory), etc. It can be very easily visualized as graphically that helps to interpret data more easily (mostly with the few number of variables) than numerical interpretation.

There are numerous applicable classification techniques, or classifiers that can be employed to predict a qualitative response. Some of the widely used classifiers are logistic regression, k-nearest neighbors, Bayes' theorem, etc.

Classification trees are getting attention due to two of its important features: hierarchical property and flexibility.

Construction of the Classification Tree

The split patterns of the members of the class variables and the class inaccuracy measure are the two important factors. A node is subjected as pure node if it is having the entities form the single class. The objective of the tree formation is to get the pure nodes eventually. We start with

the impure nodes with a function of relative frequencies of the classes at that node.

$$\eta(t) = \phi(v_1, v_2, \dots, v_j)$$

where v_j represents the relative frequencies of j different classes at the considered node. For the evenly distributed observations, the maximum inaccuracy measure will be $(1/j, 1/j, \dots, 1/j)$ and minimum inaccuracy measure will be $(1, 0, \dots, 0)$ for all the classes at the considered nodes. ϕ is a symmetric function of (v_1, v_2, \dots, v_j) .

There are different alternatives for inaccuracy measure and different algorithms for the tree implementation. Different tree implementation algorithms follow different inaccuracy measures. The inaccuracy measures are selected to reduce the inaccuracy that the split achieves on the considered node. Hence we can calculate the split performance s at node t as

$$\Delta \eta(s, t) = \eta(t) - \kappa(l)\eta(l) - \kappa(r)\eta(r)$$

where $\kappa(l)$ is left side proportion of the cases by the split, and for the right side, it is $\kappa(r)$.

Gini Index

One of the most important techniques for the inaccuracy measure is Gini index. For the two-class case it can be calculated as follows:

$$\eta(t) = v(0|t)v(1|t) = v(0|t)(1 - v(0|t)) = v(1|t)(1 - v(1|t))$$

where $v(0|t)$ or $v(1|t)$ is the frequency of the class label at the node.

The generalization of the Gini index with more than two classes can be produced as follows:

$$\eta(t) = \sum_j v(j|t)(1 - v(j|t))$$

where $v(j|t)$ is the relative frequency of the class j at the node t .

```
##classification
set.seed(45435)
traindata.rf <- randomForest(class ~ ., data=traindata, ntree=10000,
                             keep.forest=FALSE, importance=TRUE)
print(traindata.rf)
importance(traindata.rf)
importance(traindata.rf, type=1)
round(importance(traindata.rf), 2)

> print(traindata.rf)

call:
randomForest(formula = class ~ ., data = traindata, ntree = 10000,
              E, importance = TRUE)
Type of random forest: classification
Number of trees: 10000
No. of variables tried at each split: 4

OOB estimate of error rate: 0%
Confusion matrix:
      ckd notckd class.error
ckd    0      0      0
notckd 0    114      0
> importance(traindata.rf)
             ckd      notckd MeanDecreaseAccuracy MeanDecreaseGini
Age      2.0856854 0.3703602      1.838988      0.05652549
bp      -0.7402652 14.3327660      14.418921      0.21621131
sg      27.5527986 46.4607230      46.709829      4.27197080
al      42.2950739 59.4487124      56.828849      10.01968470
su      8.7153272 22.8058455      22.872639      0.39590224
rbc     8.9973296 19.6320465      19.702671      0.34083847
pc      8.7052999 24.0960751      24.183386      1.72893998
pcc     1.0820321 6.6146539      6.575736      0.06090716
ba      1.6697602 10.7517645      10.803262      0.05507508
bgr     13.3044470 29.0750129      29.197300      1.31505908
bu      11.2508816 31.6725976      31.852157      3.00807446
sc      34.1064908 52.7043503      51.249654      8.10160963
sod     7.9424880 21.3921823      21.995270      0.71998829
pot     0.3456195 6.2138897      6.086590      0.05272493
hemo    36.2518908 50.7866150      50.342742      8.54642018
pcv     35.3427548 51.6377361      50.935425      8.35699956
wc      13.9119626 29.6338077      29.789055      0.65285748
rc      31.7879112 47.7189057      46.978231      6.87189203
rtn     14.1375574 30.9945231      30.898444      3.01484491
dm      11.0305559 23.0031236      23.097786      1.39320682
cao     0.1273434 7.2683408      7.237820      0.02703383
appet   1.5198714 13.9376808      14.036472      0.34639856
pe      -0.8164332 13.2585467      13.274446      0.28379621
ane     0.9085953 9.3696561      9.313916      0.15214203
```

B. Regression

Random forest grows trees for the quantitative or numerical values of the class variable as opposite to the classification which grows trees for the qualitative class variables. As a result, output values are also numerical. It is also assumed that the training data is independently selected from the original data set. The mean-square error for any predictor variable X is estimated by $E_{X,y}(y - X)^2$, for the class variable y .

For the regression we have used “Air Quality” data from UCI Machine Learning Repository [4].

```
## Regression:
data(airquality)
set.seed(131)
ozone.rf <- randomForest(ozone ~ ., data=airquality, mtry=3,
                         importance=TRUE, na.action=na.omit)

print(ozone.rf)
## Show "importance" of variables: higher value mean more important:
round(importance(ozone.rf), 2)

> print(ozone.rf)

call:
randomForest(formula = ozone ~ ., data = airquality, mtry = 3,
              importance = TRUE, na.action = na.omit)
Type of random forest: regression
Number of trees: 500
No. of variables tried at each split: 3

Mean of squared residuals: 303.8304
% Var explained: 72.31
> round(importance(ozone.rf), 2)
      %IncMSE %IncNodePurity
solar.R    11.09    10534.24
wind       23.50     43833.13
Temp       42.03     55218.05
Month       4.07       2032.65
Day         2.63       7173.19
```

IV. CONCLUSION AND FURTHER APPLICATION

In this paper we considered ‘Chronic Kidney Disease’ data from UCI machine learning repository and applied random forest algorithm with help of the ‘Boruta’ package from R programming language for the feature subset selection and achieved the reduced set that is subset of the variables. We also applied the ‘randomForest’ package from R programming language for the classification and regression, and observed the functioning of random forest method in different perspectives. Further we can apply this random forest algorithm for the data sets with tens, hundreds, or thousands of variables and get the subset of important features.

REFERENCES

- [1]. Gareth James; Daniela Witten; Trevor Hastie; Robert Tibshirani, “An introduction to statistical learning”. Springer. p. 204 (2013).
- [2]. https://archive.ics.uci.edu/ml/datasets/Chronic_Kidney_Disease, Date: 5th-spt’2016, 11:00am.
- [3]. <https://cran.r-project.org/web/packages/Boruta/Boruta.pdf>, Date: 5th-spt’2016, 11:30am.
- [4]. <https://archive.ics.uci.edu/ml/datasets/Air+Quality>, Date: 6th-spt’2016, 11:30am.
- [5]. Avrim L. Blum, Pat Langley, “Selection of relevant features and examples in machine learning”, 0004-3702/97/1997 Elsevier Science B.V., Artificial Intelligence 97 (1997) 245-271.
- [6]. R. Bekkerman, R. El-Yaniv, N. Tishby, and Y. Winter, “Distributional word clusters vs. words for text categorization”. JMLR, 3:1183–1208(2003).
- [7]. R. Caruana and V. de Sa, “Benefitting from the variables that variable selection discards”. JMLR, 3:1245–1264(2003).
- [8]. R. Shapire, Y. Freund, P. Bartlett, and W. Lee, “Boosting the margin: A new explanation for the effectiveness of voting methods”. Annals of Statistics, 26 (5):1651–1686 (1998).
- [9]. L. Breiman, “Bagging predictors”, Machine Learning, 24 (2):123–140 (1996).
- [10]. Tibshirani, R. (1996), “Bias, Variance, and Prediction Error for Classification Rules”, Technical Report, Statistics Department, University of Toronto.