R Examples of Using Some Prediction Tools (Highlight: Random Forest)

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1 Introduction

We intend to advocate the prediction tool *Random Forest*, which is very powerful yet easy to use. To help understanding, we set it in a context of other tools and talk about them in the following sequence:

1. **Tree**: A building block.
2. **Bagging**: Improvement by tree *ensembles*.
3. **Random Forest**: Injecting more randomness into tree ensembles.
4. **Boosting**: A competing alternative to using the building block.

Demo Data For illustration, we use the Forensic Glass data in the `MASS` package. The goal is predict `type` (of glass fragments) with a set of predictors (of chemical properties). For illustration, we sample 10 data points as test sample and use the rest as training sample.

```
> library(MASS)
> data(fgl)
> str(fgl)
```

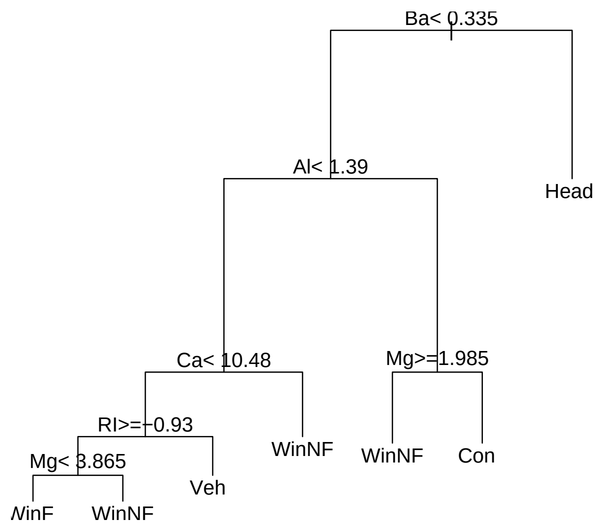
```
'data.frame':        214 obs. of  10 variables:
 $ RI  : num   3.01 -0.39 -1.82 -0.34 -0.58 ...
 $ Na  : num  13.6 13.9 13.5 13.2 13.3 ...
 $ Mg  : num  4.49 3.6 3.55 3.69 3.62 3.61 3.6 3.61 3.58 3.6 ...
 $ Al  : num  1.1 1.36 1.54 1.29 1.24 1.62 1.14 1.05 1.37 1.36 ...
 $ Si  : num  71.8 72.7 73.0 72.6 73.1 ...
 $ K   : num  0.06 0.48 0.39 0.57 0.55 0.64 0.58 0.57 0.56 0.57 ...
 $ Ca  : num  8.75 7.83 7.78 8.22 8.07 8.07 8.17 8.24 8.3 8.4 ...
 $ Ba  : num  0 0 0 0 0 0 0 0 0 0 ...
 $ Fe  : num  0 0 0 0 0 0.26 0 0 0 0.11 ...
 $ type: Factor w/ 6 levels "WinF","WinNF",..: 1 1 1 1 1 1 1 1 1 1 ...
```

```
> set.seed(1)
> s <- sample(dim(fgl)[1], 10)
> test <- fgl[s, ]
> train <- fgl[-s, ]
```

2 A Collection of Prediction Tools

Tree A tree-based prediction method (e.g. CART) partitions the feature (variables) space into a set of rectangles, on which fixed constants (predictions) are assigned. We can use the `rpart` function in the `rpart` package, which implements CART.

```
> library(rpart)
> p1 <- rpart(type ~ ., data = train)
> plot(p1)
> text(p1)
```



Bagging Bagging (Boostrap Aggregation) simply grows multiple trees, each tree growing on a differnt bootstrap sample. It then reports the majority vote or mean response (across all trees) as the prediction. We can use the `bagging` function in the `ipred` package.

```
> library(ipred)
> p2 <- bagging(type ~ ., data = fgl, coob = T)
> p2

Bagging classification trees with 25 bootstrap replications

Call: bagging.data.frame(formula = type ~ ., data = fgl, coob = T)

Out-of-bag estimate of misclassification error:  0.2477
```

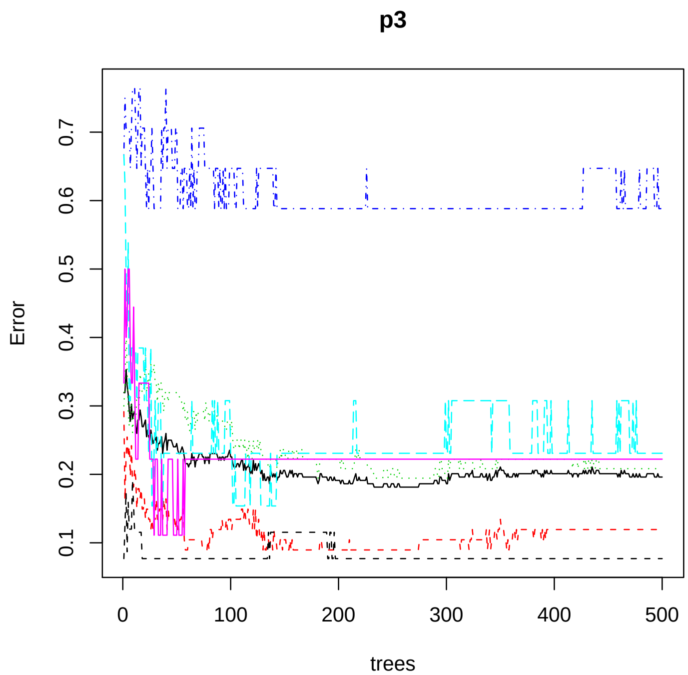
The `coob` option requests the out-of-bag estimate of the misclassification error.

Random Forest Random Forest injects additional randomness into the bagging procedure on trees: each node is split using the best among a *subset* of predictors randomly chosen at that node, instead of the full set. It has the following merits:

- Superior performance.
- Robust against overfitting.
- Easy to use, little tuning.

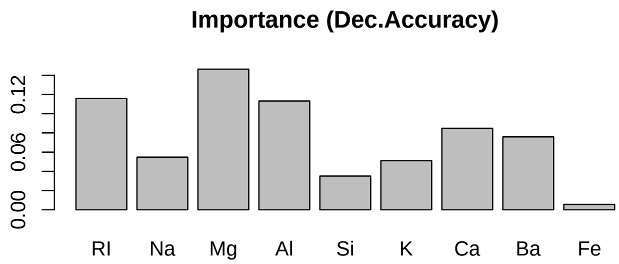
Thus this is a highly recommended prediction tool. My own hypothesis for its performance is that the additional randomness greatly *diversifies* the trees, resulting in expanded search space and noise profile, the former reduces the bias and the latter reduces the tendency for overfitting by keeping a healthy signal-noise ratio.

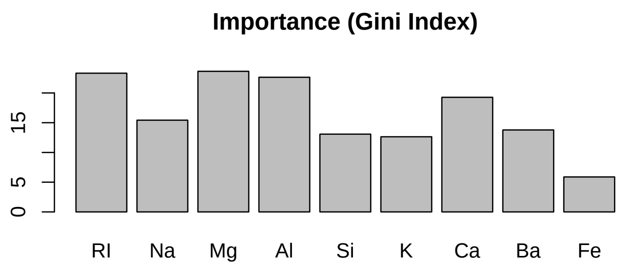
```
> library(randomForest)
> p3 <- randomForest(type ~ ., data = train, importance = T)
> p3

Call:
 randomForest(formula = type ~ ., data = train, importance = T)
               Type of random forest: classification
                     Number of trees: 500
No. of variables tried at each split: 3

        OOB estimate of  error rate: 19.12%
Confusion matrix:
      WinF WinNF Veh Con Tabl Head class.error
WinF    61     5   1   0    0    0  0.08955224
WinNF    8    57   2   2    2    1  0.20833333
Veh      6     4   7   0    0    0  0.58823529
Con      0     2   0  10    0    1  0.23076923
Tabl     0     2   0   0    7    0  0.22222222
Head     0     3   0   0    0   23  0.11538462

> plot(p3)
```



The `plot` method traces the error rates (out-of-bag, and by each response category) as the number of trees increases. The `importance` option in the `randomForest` function requests the assessment of predictor importances. There are two global measures: one is the mean descrease in accuracy over all classes, the other is the mean decrease in Gini index. Here is a plot of the two measures:

```
> par(mfrow = c(2, 1))
> barplot(p3$importance[, 7], main = "Importance (Dec.Accuracy)")
> barplot(p3$importance[, 8], main = "Importance (Gini Index)")
```





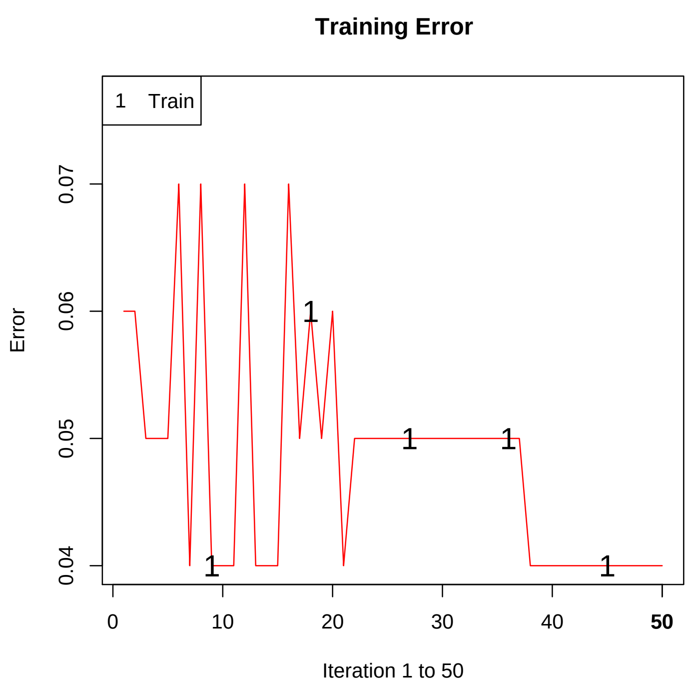
Boosting Boosting is a method for starting with a simple/weak classifier (e.g. a tree) and gradually improving it by refitting the data giving higher weight to misclassified samples. The prediction is *voted* by the resulting ensemble/committee of classifiers. In essence, boosting is a way of fitting an additive expansion in a set of elementary "basis" functions ([1]).

Unfortunately, currently no boosting package can deal directly with multinomial response (only continuos and binary). So we will use the Fisher's Iris Data (keep only two species) for illustration.

```
> data(iris)
> iris <- iris[iris$Species %in% c("versicolor", "virginica"),
+     ]
> iris$Species <- factor(iris$Species)
> library(ada)
> p4 <- ada(Species ~ ., data = iris)
> p4

Call:
ada(Species ~ ., data = iris)

Loss: exponential Method: discrete   Iteration: 50
```

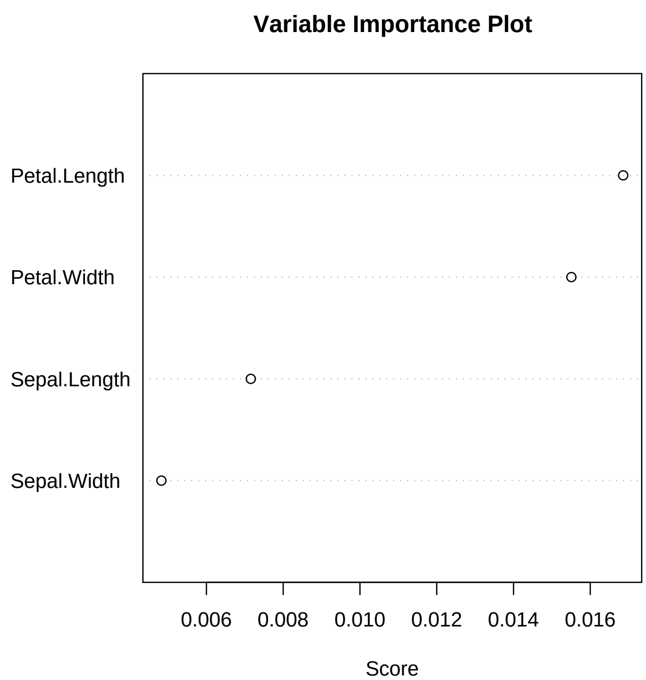
```
Final Confusion Matrix for Data:
            Final Prediction
True value   versicolor virginica
  versicolor         47         3
  virginica           2        48

Train Error: 0.05

Out-Of-Bag Error:  0.04  iteration= 14

Additional Estimates of number of iterations:

train.err1 train.kap1
         5          5
```

```
> plot(p4)
```



Following is the variable importance plot:

```
> varplot(p4)
```



3 Comparison

Prediction on the Test Sample The prediction accuracy on the test sample for Tree, Bagging, and Random Forest is:

```
> data.frame(Truth = test$type, Tree = predict(p1, test, type = "class"),
+     Bagging = predict(p2, test), Forest = predict(p3, test))
```

```
    Truth  Tree Bagging Forest
57   WinF   Veh    WinF   WinF
80  WinNF WinNF   WinNF  WinNF
122 WinNF WinNF   WinNF  WinNF
192  Head  Head    Head   Head
43   WinF  WinF    WinF   WinF
188  Head  WinF    Head   WinF
197  Head  Head    Head   Head
137 WinNF  WinF   WinNF   WinF
130 WinNF   Con   WinNF  WinNF
13   WinF WinNF    WinF  WinNF
```

Incidentally, Bagging performs better than Forest on this test sample. Note Bagging is a special case of Forest. For a more rigorous check, we shall estimate the *test error* rate.

Error Rate Estimation To compare the performances of different prediction tools, we can do a 10-fold *cross validation* to estimate the test error, using the `errorest` function in the `ipred` package. This function requires a `predict` function that specifies only two arguments (`object` and `newdata`) and returns a predicted class (or scalar). So we first need to write a wrapper function for `predict.rpart`:

```
> mypredict.rpart <- function(object, newdata) {
+     predict(object, newdata = newdata, type = "class")
+ }
```

We can see a significant improvement by Random Forest in the following error rate comparison:

```
> c(Tree = errorest(type ~ ., data = train, model = rpart, predict = mypredict.rpart)$error,
+     Bagging = errorest(type ~ ., data = train, model = bagging)$error,
+     Forest = errorest(type ~ ., data = train, model = randomForest)$error)

     Tree   Bagging    Forest
0.3186275 0.2303922 0.1911765
```

Following is the error rate comparison for the Fisher's Iris data:

```
> c(Tree = errorest(Species ~ ., data = iris, model = rpart, predict = mypredict.rpart)$erro
+     Bagging = errorest(Species ~ ., data = iris, model = bagging)$error,
+     Forest = errorest(Species ~ ., data = iris, model = randomForest)$error,
+     Boosting = errorest(Species ~ ., data = iris, model = ada)$error)

    Tree  Bagging   Forest Boosting
    0.10     0.09     0.07     0.08
```

4 Conclusion

We introduced a set of prediction tools(Tree, Bagging, Forest, Boosting). Tree is a nonlinear method and serves as the building block for the other three tools. The drawback of Tree is that it is instable (sensitive to data noise) and has high variance in the prediction. Bagging reduces such variance by bootstrapping the samples. In contrast, Boosting can be think of as a bias reduction tool.

We recommend the Random Forest for routine prediction tasks.

References

[1] T. Hastie, R. Tibshirani, and J. H. Friedman. *The Elements of Statistical Learning*. Springer, August 2001.