ggRandomForests: Exploring Random Forests in **R**

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Abstract

Random Forests (Breiman 2001) (RF) are a fully non-parametric statistical method requiring no distributional assumptions on covariate relation to the response. RF are a robust, nonlinear technique that optimizes predictive accuracy by fitting an ensemble of trees to stabilize model estimates. Random Forests for survival (Ishwaran and Kogalur 2007; Ishwaran, Kogalur, Blackstone, and Lauer 2008) (RF-S) are an extension of Breiman's RF techniques to survival settings, allowing efficient non-parametric analysis of time to event data. The **randomForestSRC** package (Ishwaran and Kogalur 2014) is a unified treatment of Breiman's random forests for survival, regression and classification problems.

Predictive accuracy make RF an attractive alternative to parametric models, though complexity and interpretability of the forest hinder wider application of the method. We introduce the **ggRandomForests** package, tools for creating and plotting data structures to visually understand random forest models grown in R with the **randomForestSRC** package. The **ggRandomForests** package is structured to extract intermediate data objects from **randomForestSRC** objects and generate figures using the **ggplot2** (Wickham 2009) graphics package.

Using both classification (RF-C) and survival (RF-S) examples from our research at the Cleveland Clinic, we will demonstrate the **randomForestSRC** package. We use Variable Importance measure (VIMP) (Breiman 2001) as well as Minimal Depth (Ishwaran, Kogalur, Gorodeski, Minn, and Lauer 2010), a property derived from the construction of each tree within the forest, to assess the impact of variables on forest prediction. We will also demonstrate the use of variable dependence plots (Friedman 2000) to aid interpretation RF results in different response settings.

Keywords: random forest, survival, classification, regression, VIMP, minimal depth.

1. About this document

This document is an introduction to the **ggRandomForests** R package. The aim of this introduction is to provide a detailed user guide to **ggRandomForests** as well as provide a tutorial to building Random Forest models with the **randomForestSRC** package. Our attempt is to use simple, reproducible worked examples with open dataset available with base R or the **randomForestSRC** package.

This document is available as a vignette within **ggRandomForests** package, available from the Comprehensive R Archive Network via http://CRAN.R-project.org/package=ggRandomForests.

2. Introduction

Random Forests (Breiman 2001) (RF) are a robust statistical method that utilizes all variables in predicting the specified outcome. It does not require prior knowledge of the relation of variables (linearity or non-linearity) to the response, or of interactions between variables. RF does not eliminate any risk factor, but rather chooses the most important variables by assessing variable impact on the predictive ability of the forest of trees. Each tree is created with a random sub-group of patients. Each tree is designed to be independent of the others within the forest. This is achieved within the tree growing process by evaluating a split variable candidates from a random subset of covariates.

A Random Forest is built up by bagging (Breiman 1996a) a collection of classification and regression trees (Breiman, Friedman, Olshen, and Stone 1984) (CART). The method uses a set of B bootstrap (Efron and Tibshirani 1994) samples, growing a single tree on each sample. The strength of RF is in ensuring that each tree is independent by subsampling a set of $m \leq p$ input variables for evaluation at each node split of the tree growing process. This independence property ensures that RF minimizes the variance of the aggregated tree estimates. Each node is split into two groups by maximizing the separation of observations according to a measure of the response variable until reaching a stopping criteria of terminal node purity or member size. Each observation is uniquely sorted into only one terminal node per tree. The Random Forest estimate for each observation is obtained by simple averaging (regression) or vote aggregating (classification) the terminal node results across the collection of trees.

Random Forests also have a built in estimate of prediction error. Each bootstrap sample selects approximately 63.2% of data set ibservations on average. The remaining 36.8% observations are left Out-of-Bag (Breiman 1996b) (OOB) which can be used as a hold out test set for each tree. The OOB error rate is calculated for each observation by predicting a response for each observation over the set of trees NOT trained on that particular observation. The OOB prediction error estimates are nearly identical to k–fold cross validation estimates. This RF feature allows us to obtain both model fit and validation in one pass of the algorithm.

RF utilizes all variables in predicting the specified outcome, effectively weighting the most important covariates by assessing their impact on separating dissimilar groups of observations.

2.1. Random Forests for Survival

Random Forests for survival (Ishwaran 2007; Ishwaran *et al.* 2008) (RF-S) are an extension of Random Forests (Breiman 2001) to survival settings, creating a forest of survival trees. Each node tests a random selection of candidate variables, splitting of the node is chosen by maximizing the log-rank statistic to select the optimal candidate variable. The process continues down each branch of the tree until all observations are sorted into a unique terminal node for each tree. This approach produces extensively grown trees where each terminal node includes a small group of observations having similar characteristics and survival outcomes. The survival estimate for each observation is constructed within each terminal node at all population event times, and averaged over the entire forest of trees.

2.2. randomForestSRC package

We use the **randomForestSRC** package (Ishwaran and Kogalur 2014) (RF-SRC) for all ran-

domForest methods. This package combines the different random forest outcomes (survival, regression and classification) in one package with consistent function calls and interfaces.

2.3. ggRandomForests package

The **randomForestSRC** package is a mature analysis and research randomForest implementation under rapid development. The package includes diagnostic and postprocessing functions for anlaysis and visualizations of randomForest model properties. However, in our research we frequently found it difficult to manipulate the standard figures directly produced with the **randomForestSRC** package.

In order to simplify these manipulations, we developed the **ggRandomForests** package. We attempted to follow two design principles in this development:

- Model/View separation: The package originally designed to generating **ggplot2** Wickham (2009) figures for random forest objects. However, some users would prefer to use other graphing methods within R or outside of it. To help users, we separate the data generation and the figure generation into two separate operations.

- Modularity: We strive to create a modular design by following the *do one thing well* philosphy. Each function operates on one **randomForestSRC** object to create only one data object or figure type.

To demonstrate using the **ggRandomForests** package, we organize this document as follows. In Section 3 we outline growing a random forest for each of the classification, regression and survival settings with the **randomForestSRC** package. We use the **ggRandomForests** package to begin exploring random forest convergence and prediction. In Section 4 we discuss how variables contribute to the random forest prediction using the Variable Importance (VIMP) and Minimal Depth measures.

Once we have an idea which variables are most informative in minimizing forest prediction error, we turn our focus to how the variables are related to the forest prediction. Because Random Forests are non-linear and non-parametric predictors, we can use variable dependence (Section 5.1) to examine where each observation contributes to model prediction as a function of specific covariate values. Partial dependence (Section 5.2) gives us a risk adjust view of the preditor dependence on a variable. We then find two way interactions using minimal depth in Section 5.3 and use conditional plots in Section 5.5 to look variable interactions in an intuitive manner.

3. Growing a Random Forest

3.1. Classification Forests

```
R> # Grow the classification forest
R> iris_rf <- rfsrc(Species ~., data = iris)
R>
R> # Plot the error convergence rate for the forest growth
R> plot.gg_error(iris_rf)
```

```
R>
R> # Plot predicted class probabilities for the training data
R> plot.gg_rfsrc(iris_rf)
R>
R> # Plot predicted class ROC curves
R> plot.gg_roc(iris_rf)
```

```
                        Sample size: 150
          Frequency of class labels: 50, 50, 50
                     Number of trees: 1000
         Minimum terminal node size: 1
       Average no. of terminal nodes: 8.821
No. of variables tried at each split: 2
               Total no. of variables: 4
                            Analysis: RF-C
                              Family: class
                       Splitting rule: class
                         Brier score: 2.51
                          Error rate: 0.04, 0, 0.08, 0.04

Confusion matrix:

           predicted
 observed    setosa versicolor virginica class.error
 setosa          50          0         0        0.00
 versicolor       0         46         4        0.08
 virginica        0          2        48        0.04

Overall error rate: 4%
```
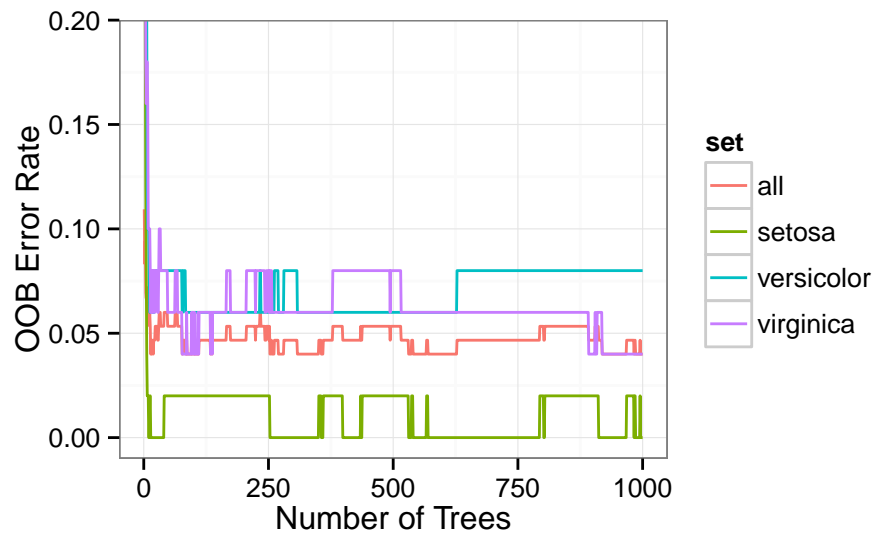

Figure 1: Classification Forest: Forest error convergence rate.
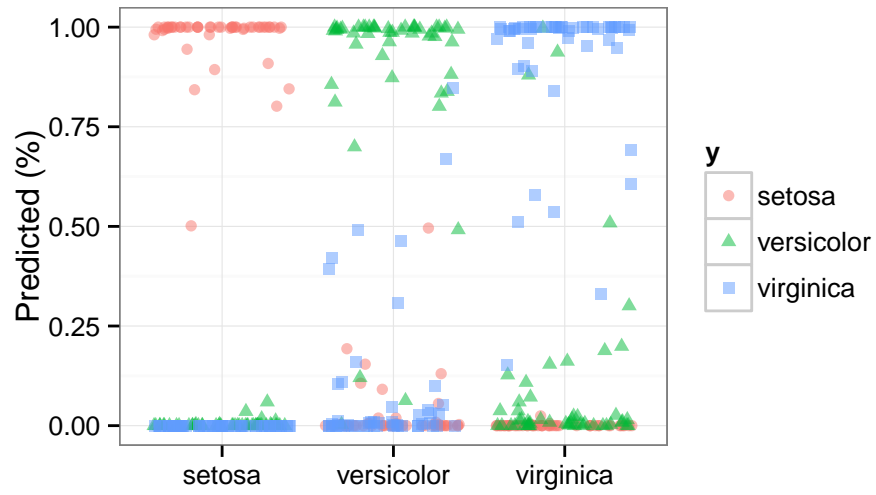
3.2. Regression Forests

Figure 2: Classification Forest: Predicted probability of IRIS class.
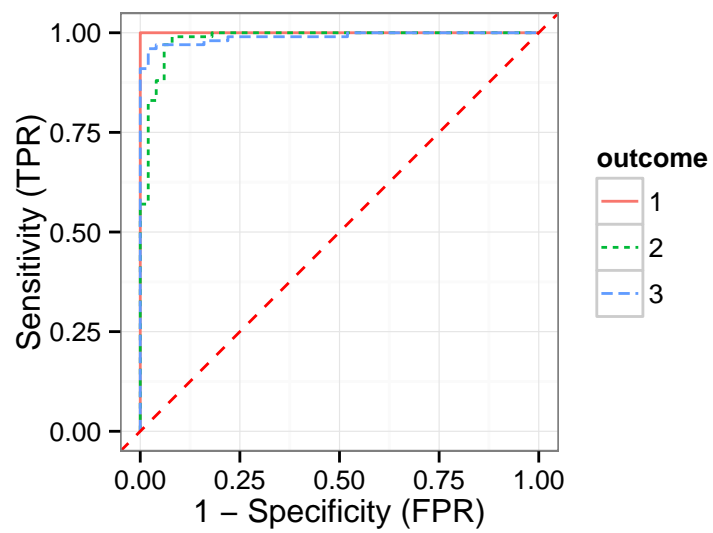

Figure 3: Classification Forest: ROC curves.

```
R> # Grow the regression forest
R> airq_rf <- rfsrc(Ozone ~ ., data = airquality, na.action = "na.impute")
R>
R> # Plot the error convergence rate for the forest growth
R> gg_err <- gg_error(airq_rf)
R> plot(gg_err)
R>
R> # Plot predicted values for the training data
R> gg_rfr <- gg_rfsrc(airq_rf)
R> plot(gg_rfr)
```

```
                      Sample size: 153
                 Was data imputed: yes
                      Missingness: 27.45%
                  Number of trees: 1000
        Minimum terminal node size: 5
     Average no. of terminal nodes: 17.74
No. of variables tried at each split: 2
             Total no. of variables: 5
                          Analysis: RF-R
                            Family: regr
                    Splitting rule: regr
              % variance explained: 75.99
                        Error rate: 261.3
```
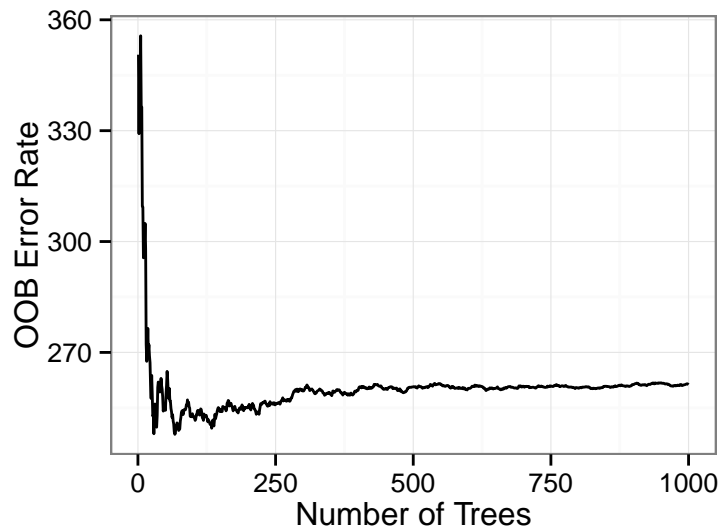

Figure 4: Regression forest: Forest error convergence rate.

3.3. Survival Forests

Similar to RF, RF-S is a collection of B survival trees. At each node of the tree, we randomly selected a subset of $m \leq p$ candidate variables. The node is then split into two groups by constructing Kaplan–Meier survival curves and choosing the variable that maximizing
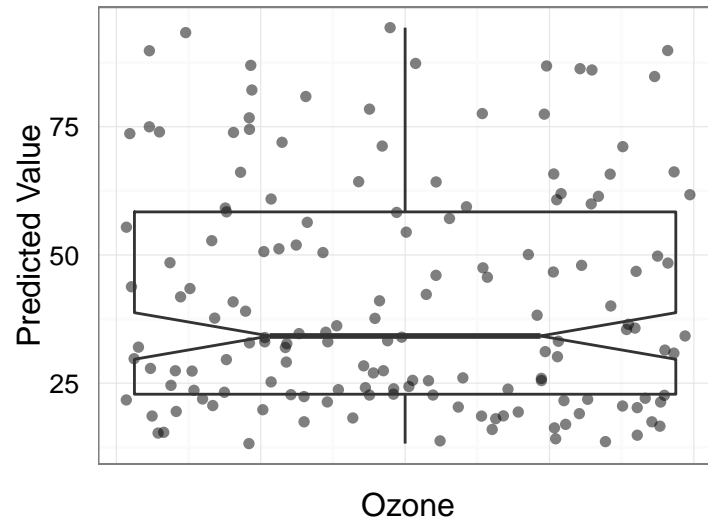
Figure 5: Regression forest: Predicted Ozone level.

the log-rank statistic. We split categorical variables according to their natural categories and continuous variables by comparing 10 randomly selected cut points. For each subsequent node of the tree, we repeated the same process: random selection of candidate variables, splitting of each variable with construction of survival plots and calculation of log-rank statistic, and selection of the best splitting variable. The process continued down each branch of the tree until we reached a unique subset of observations that contain no fewer than 3 deaths within a terminal node. This approach produces extensively grown trees where each terminal node includes a group of observations having similar characteristics and survival outcomes.

```
R> # Load the dataset,
R> data(pbc, package = "randomForestSRC")
R>
R> # Grow the survival forest
R> pbc_rf <- rfsrc(Surv(days, status) ~ ., pbc, nsplit = 10, ntree=500)
R>
R> # Plot the error convergence rate for the forest growth
R> plot.gg_error(pbc_rf)
R>
R> # Plot predicted survival probabilities for the training data
R> plot.gg_rfsrc(pbc_rf) +
+    theme(legend.position=c(.8,.8))
```

```
                    Sample size: 276
                Number of deaths: 111
                 Number of trees: 500
       Minimum terminal node size: 3
     Average no. of terminal nodes: 54.3
No. of variables tried at each split: 5
           Total no. of variables: 17
                        Analysis: RSF
                          Family: surv
```

```
                     Splitting rule: logrank *random*
        Number of random split points: 10
                         Error rate: 16.67%
```
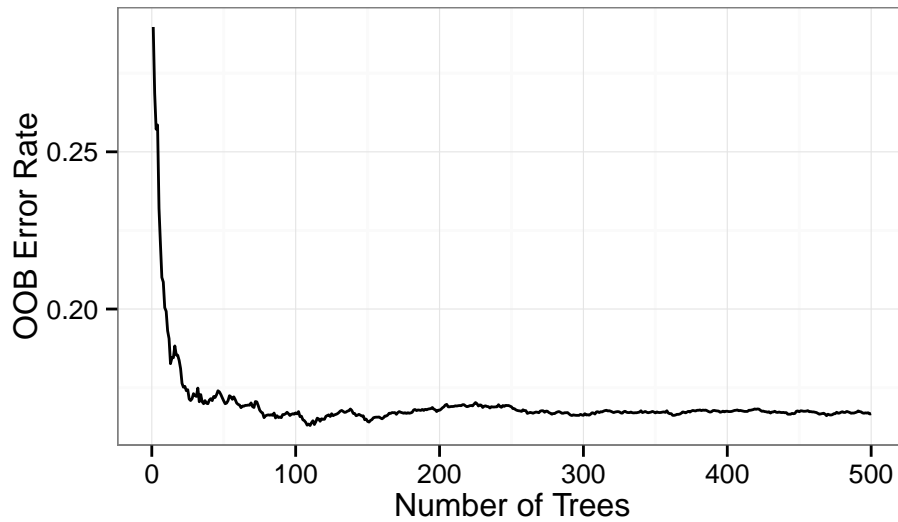

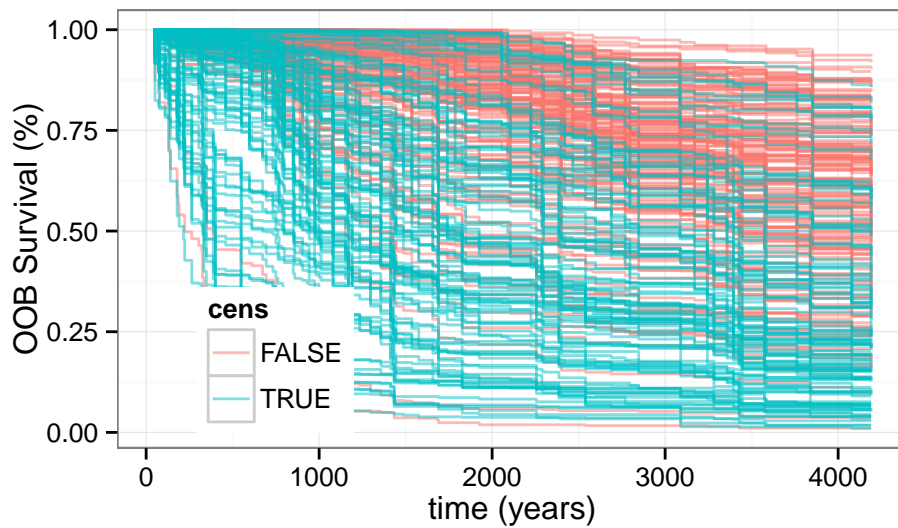Figure 6: Survival Forest: Predicted probability of survival.

Figure 7: Survival Forest: Predicted probability of survival.

4. Identification of Predictive Variables

Unlike the linear model settings, RF does not explicity specify the functional form of the

covariate response relation. We use two seperate methods in order to determine how the RF has built the response prediction, the standard method of Variable Importance (VIMP) as well as the forest minimal depth.

4.1. Variable Importance

Variable importance (VIMP) was originally defined in CART using a measure involving surrogate variables (see Chapter 5 of Breiman *et al.* (1984)). Definitions in terms of mean overall improvement in node impurity for a tree have also been proposed. In regression trees, node impurity is measured by mean squared error, whereas in classification problems, the Gini index is used (**?**). The most popular VIMP method to date, however, adopts a prediction error approach involving "noising-up" a variable. In random forests, for example, VIMP for a variable x_v is the difference between prediction error when x_v is noised up by permuting its value randomly, compared to prediction error under the original predictor (Breiman 2001; Liaw and Wiener 2002; Ishwaran 2007; Ishwaran *et al.* 2008).

Given that VIMP is the absolute difference between prediction errors before and after permutation, a large VIMP value indicates that misspecification of that variable detracts from the predictive accuracy of the forest. VIMP close to zero indicates the variable has no impact on predictive accuracy, and negative values indicate the predictive accuracy improves when the variable is mispecified. In the later case, we assume noise is more informative than the variable. As such, we ignore variables with negative and zero values of VIMP, relying on large positive values to indicate that the predictive power of the forest is dependent on those variables.
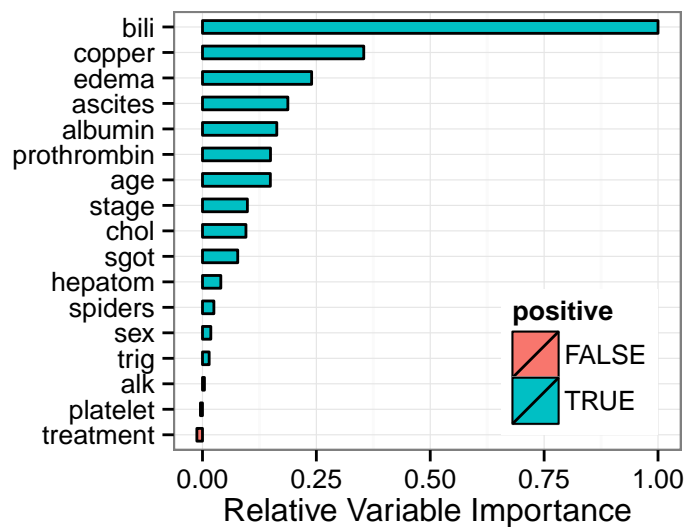
```
R> plot.gg_vimp(iris_rf)+
+    theme(legend.position="none")
```
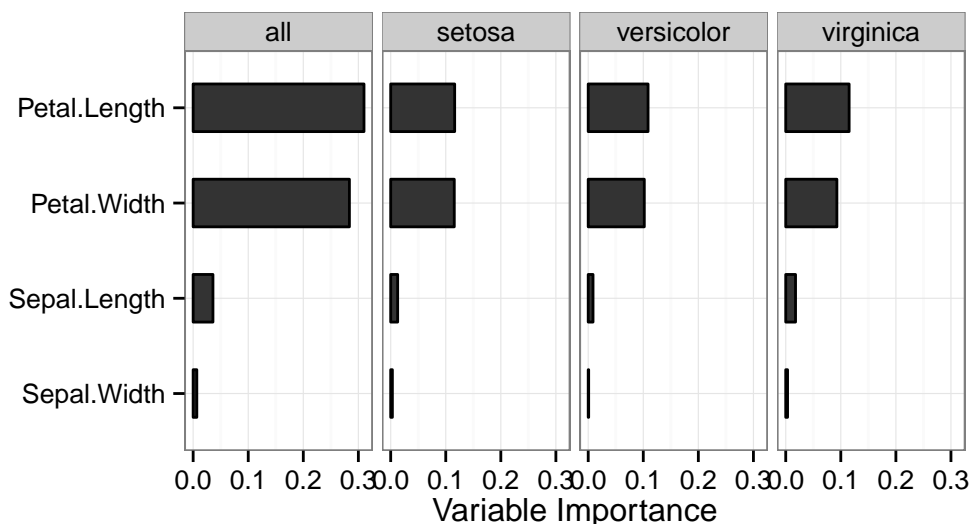


```
R> plot.gg_vimp(airq_rf)
```
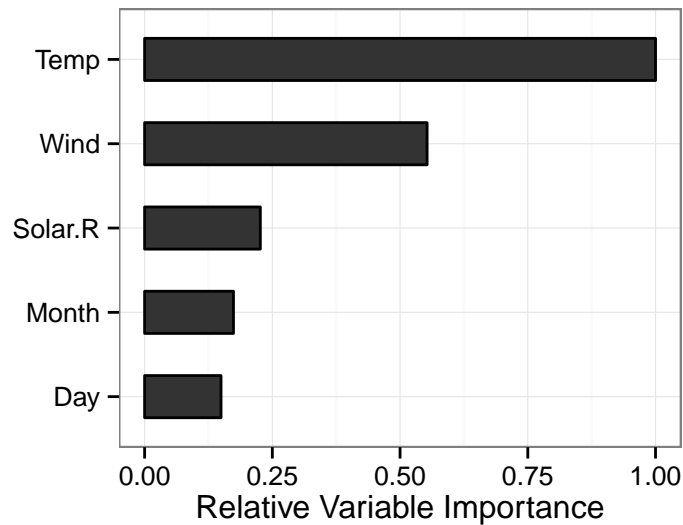
```
R> plot.gg_vimp(pbc_rf)+
+    theme(legend.position=c(.8,.2))
```
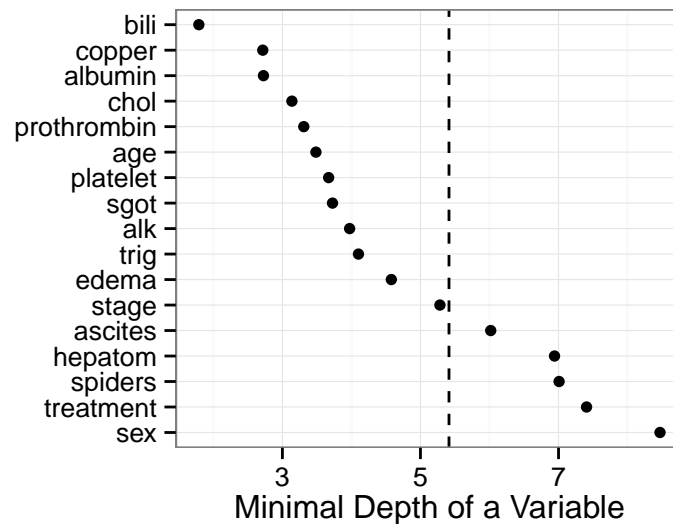

4.2. Minimal Depth

In VIMP, prognostic risk factors are determined by inspection of the forest, ranking the most important variables according to impact on predictive ability of the forest. An alternative method recognizes that most important variables for prediction are those that most frequently split nodes nearest to the trunks of the trees (ie, at the root node). Node levels are numbered based on their relative distance to the trunk of the tree (ie. 0, 1, 2). A measure of important risk factors is determined by averaging the depth of first split for each variable over all trees within the forest. Lower values of this measure indicate those variables that split larger groups of patients. This method has been shown to successfully identify the strongest predictors, with no loss of overall model accuracy because of excessive parsimony.

The maximal subtree for a variable x is the largest subtree whose root node splits on x. Thus, all parent nodes of x's maximal subtree have nodes that split on variables other than x. The largest maximal subtree possible is the root node. In general, however, there can be more than one maximal subtree for a variable. A maximal subtree may also not exist if there are no splits on the variable.

The minimal depth of a maximal subtree (the first order depth) measures predictiveness of a variable x. It equals the shortest distance (the depth) from the root node to the parent node of the maximal subtree (zero is the smallest value possible). The smaller the minimal depth, the more impact x has on prediction. The mean of the minimal depth distribution is used as the threshold value for deciding whether a variable's minimal depth value is small enough for the variable to be classified as strong.

```
R> data(pbc_vs, package="ggRandomForests")
R> plot.gg_minimal_depth(pbc_vs)
```


4.3. Variable Importance and Minimal Depth

```
R> plot.gg_minimal_vimp(pbc_rf)
minimal depth variable selection ...


-----------------------------------------------------------
family             : surv
var. selection     : Minimal Depth
conservativeness   : medium
x-weighting used?  : TRUE
dimension          : 17
sample size        : 276
ntree              : 500
nsplit             : 10
mtry               : 5
nodesize           : 3
```
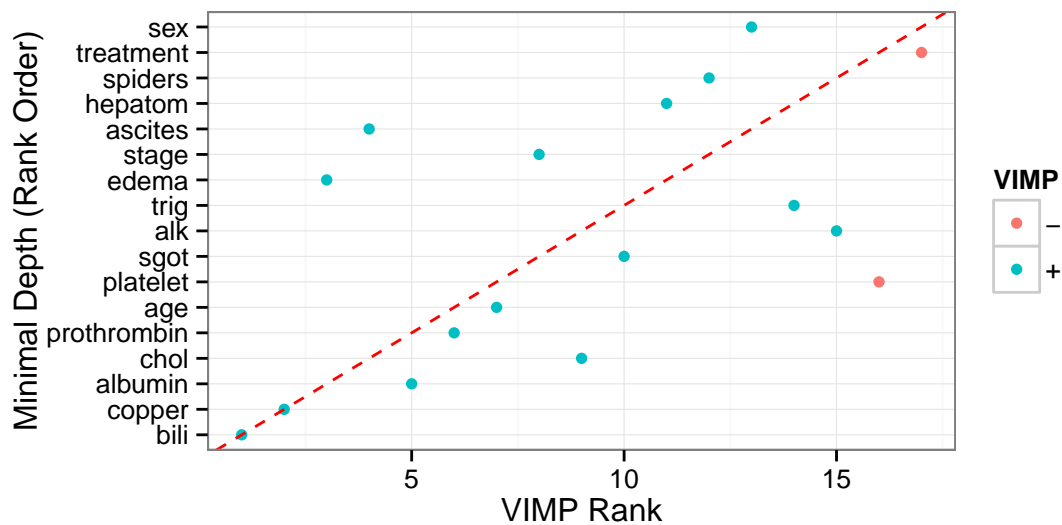
```
refitted forest    : FALSE
model size         : 12
depth threshold    : 5.414
PE (true OOB)      : 16.67


Top variables:
            depth  vimp
bili        1.790 0.067
copper      2.716 0.024
albumin     2.726 0.011
chol        3.138 0.006
prothrombin 3.310 0.010
age         3.486 0.010
platelet    3.670 0.000
sgot        3.726 0.005
alk         3.974 0.000
trig        4.102 0.001
edema       4.578 0.016
stage       5.282 0.007
-------------------------------------------------------------
```
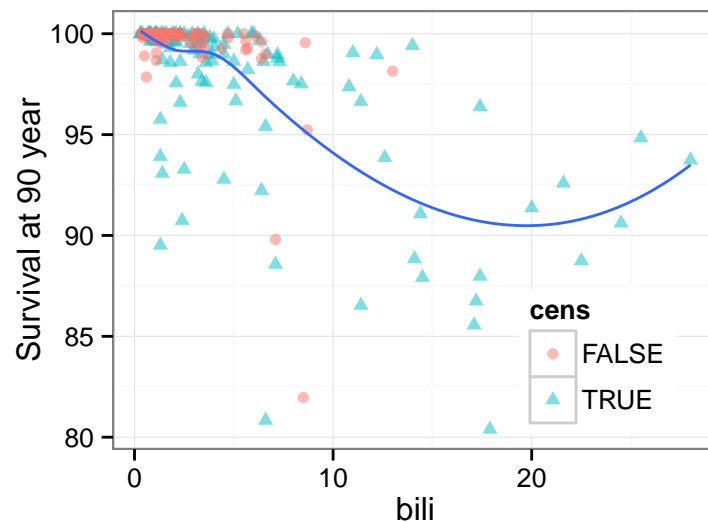

5. Variable Dependence

Once we have an idea of which variables contribute to the predictive accuracy of the forest, it is useful to get some idea of form of this contribution. We use graphical methods to show the predicted response given dependence on covariates. We can plot the marginal effect of an covariate on the class probability (classification), response (regression), mortality (survival), or the expected years lost (competing risk) for a RF analysis. We plot the ensemble predicted value on the vertical axis and covariates along the horizontal axis.
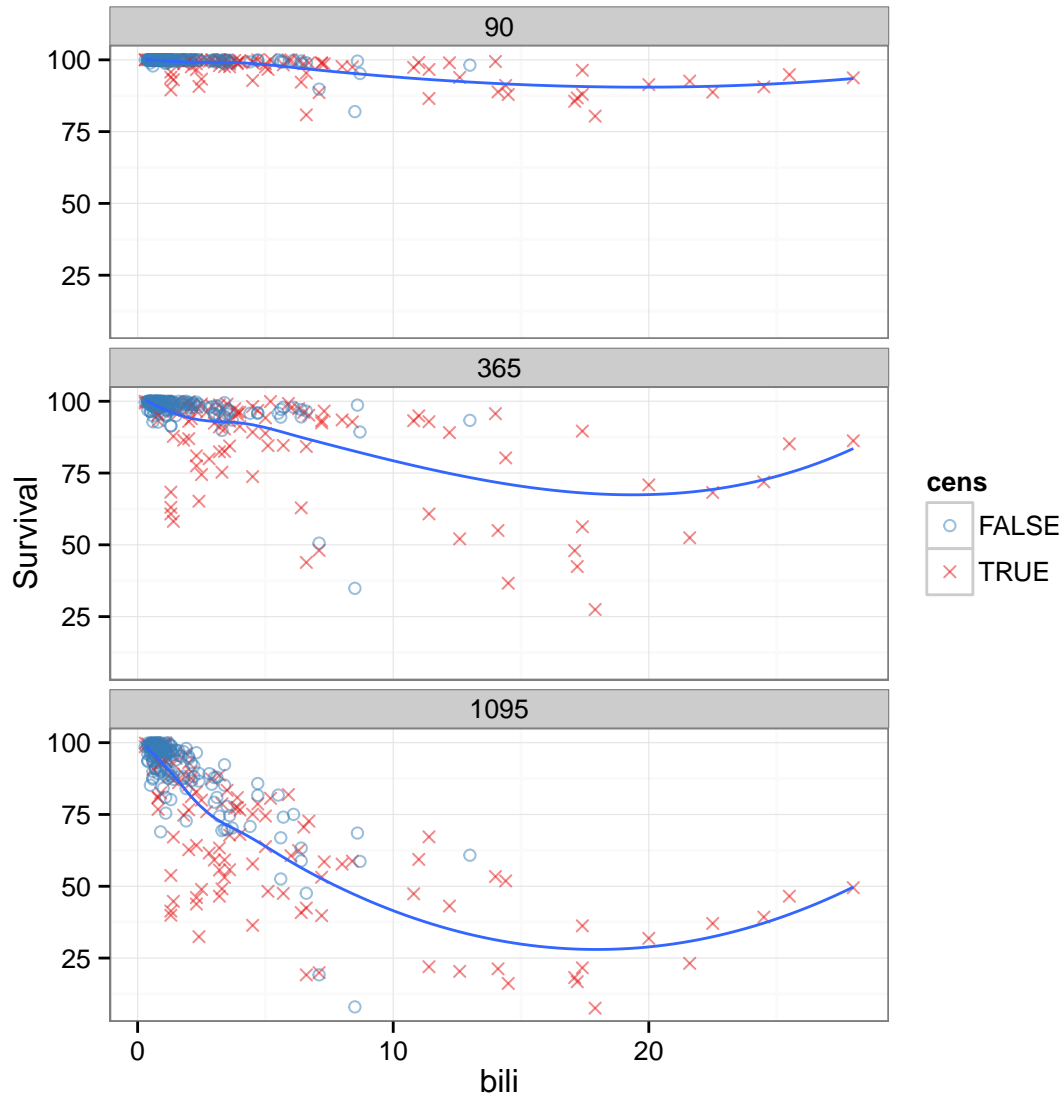
5.1. Marginal Dependence

Marginal variable dependence plots the predicted response as a function of the covariate, showing each subject as a point on the plot. For classification and regression, this is straight forward predicting the response. In survival settings, we must account for the additional dimension of time. In this case, we plot the response at a specific time point of interest, for example survival at one year. Each predicted point is dependent on the full combination of all covariates, not only on the covariate displayed in the dependence plot. So interpretation can only be in general terms.

```
R> ggrf <- gg_variable(pbc_rf, time=90)
R>
R> plot(ggrf, x_var = "bili") +
+    theme(legend.position=c(.8,.2))
```



```
R> ggrf <- gg_variable(pbc_rf, time=c(90,  365, 3*365))
R>
R> plot(ggrf, x_var = "bili")+
+    scale_shape_manual(values=event.marks, labels=event.labels)+
+    scale_color_manual(values=strCol, na.value="lightgrey", drop=FALSE,
+                       labels=event.labels)
```

5.2. Partial Dependence

An alternative to marginal variable dependence is to integrate out the effects of varaibles beside the covariate of interest. For these *partial variable dependence* plots, the y-value for a variable X, evaluated at X=x, is
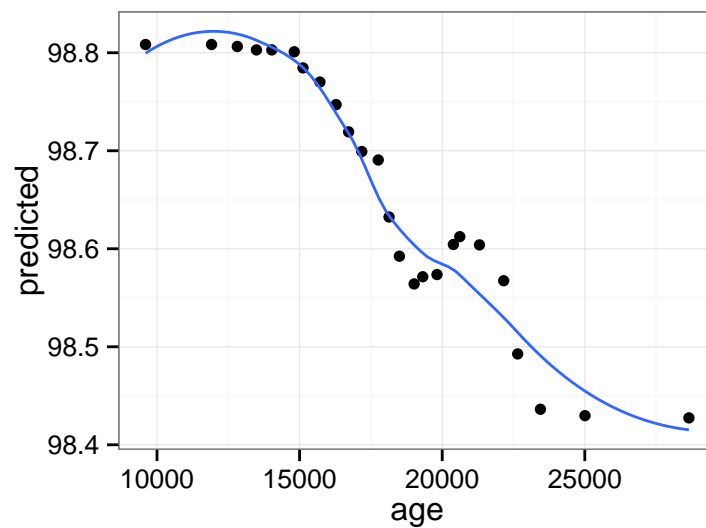
$$\tilde{f}(x) = \frac{1}{n} \sum_{i=1}^{n} \hat{f}(x, x_{i,o}),$$

where $\hat{f}$ is the predicted response and $x_{i,o}$ represents the value for all other covariates other than X for the observation i (**?**). The partial plot can be viewed as a risk adjusted estimate of the response as a function of the covariate X.

```
R> data(pbc_prtl, package="ggRandomForests")
R> ggprtl <- gg_partial(pbc_prtl)
R>
R> plot(ggprtl[[1]])
```
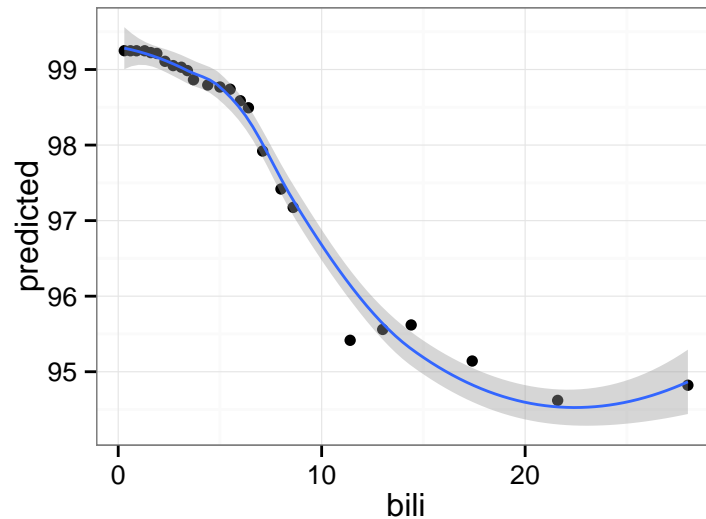


```
R> plot(ggprtl[[4]], se=FALSE)
```


5.3. Variable Interactions and Conditional Plots

Using the different variable dependence measures, we can calculate pairwise interactions for any pair of variables.

Using minimal depth, we calculate the maximal subtree using the normalized minimal depth of variable i relative to the root node (normalized wrt the size of the tree) the maximal

subtree interaction measure is the normalized minimal depth of a variable j wrt the maximal subtree for variable i (normalized wrt the size of i's maximal subtree). Smaller diagonal entries indicate predictive variables. Small interaction entries having small diagonal entries are a sign of an interaction between variable i and j (**??**)

A joint-VIMP approach is also available where two variables are paired and their paired VIMP calculated (refered to as 'Paired' importance). The VIMP for each separate variable is also calculated. The sum of these two values is refered to as 'Additive' importance. A large positive or negative difference between 'Paired' and 'Additive' indicates an association worth pursuing if the univariate VIMP for each of the paired-variables is reasonably large (Ishwaran 2007).

By plotting the resulting interaction measures for each variable, we can detect the "most interactive" pairs, and develop conditonal plots . These plots are similar to stratifed results, arranged in a set of panels by the interactive variable of interest.

5.4. Variable Interactions

5.5. Conditional Dependence

6. Conclusions

7. Acknowledgments

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