

A University of Queensland Advanced Workshop

Session 9: Machine Learning Approaches

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1 The Swiss credit card data set

For this section, we use one data set which we prepare from original sources, namely the file creditCard.csv.

- Response: credit.card.owner, binary with levels c("no", "yes").
- Predictors: mostly numeric, to do with banking activity.
 - profession is a sparse factor which we re-group into three densely populated levels (as factor pclass).
 - nationality which we re-group into two levels, "Swiss" and "Foreigner".
 - **sex** is the only other factor.
- Entries have a numerical *ident* which we zero-fill and move to the *rownames* rather than have it as a potentially active variable.

Read in the data and

```
library(WWRCourse)
CCf <- system.file("extdata", "creditCard.csv", package = "WWRCourse")
CC <- read.csv(CCf, na.strings="", stringsAsFactors = TRUE)
row.names(CC) <- fillo(CC$ident)

with(CC, c(cases = nrow(CC), known = sum(!is.na(credit.card.owner))))
cases known
10893 2085</pre>
```

The data is mostly *unknown*: for building predictive models we only have two thousand and eighty-five *at most* from ten thousand eight hundred and ninety-three cases.

```
CC <- CC %>% within({
  p2 <- c("doctor", "engineer", "lawyer", "professor", "business")</pre>
  p1 <- c("teacher", "police", "service", "chemist", "nurse",
           "postman", "physical")
  p0 <- "none"
  pclass <- rep("", length(profession))</pre>
  pclass[profession %in% p0] <- "p0"</pre>
  pclass[profession %in% p1] <- "p1"</pre>
  pclass[profession %in% p2] <- "p2"</pre>
  pclass <- factor(pclass, levels = paste0("p", 0:2))</pre>
  swiss <- ifelse(nationality == "CH", "Swiss", "Foreigner")</pre>
  sex <- factor(sex)</pre>
  swiss <- factor(swiss)</pre>
  pclass <- factor(pclass)</pre>
  ident <- profession <- nationality <- p0 <- p1 <- p2 <- NULL
})
CCKnown <- na.omit(CC)</pre>
dim(CCKnown)
[1] 1620 55
```

For model building we have just one thousand six hundred and twenty

cases and fifty-four potential predictors.

For demonstration purposes we split these into *Training* and Test data sets.

```
set.seed(20200202) ## for reproducibility
train <- sample(nrow(CCKnown), nrow(CCKnown)/2)

CCTrain <- CCKnown[train, ]
CCTest <- CCKnown[-train, ]
Store(CC, CCKnown, CCTrain, CCTest, train, remove = FALSE) ## for saftey</pre>
```

2 Trees and forests

- A technique that developed in machine learning and now widely used in data mining.
- The model uses *recursive partitioning* of the data and is a greedy algorithm.
- The two main types of tree models are
 - Regression trees response is a continuous variable and fitting uses a least squares criterion,
 - Classification trees response is a factor variable and fitting uses an entropy (multinomial likelihood) criterion.

- Model fitting is easy. Inference poses more of a dilemma.
- The tree structure is very unstable. *boosting* and *bagging* (random forests) can be useful ways around this.
- Two packages for tree models: **rpart** (which is part of **R** itself) and the older **tree**, (**Ripley**., 2012), which has an **S-PLUS** flavour and a few advantages for teaching.

Use rpart in practice.

3 Do you want a credit card?

Our plan is to build predictive models on the *Training* set, and use the *Test* set to see how well they fared. We employ a number of techniques, mostly of the "black box" kind.

3.1 An initial tree model

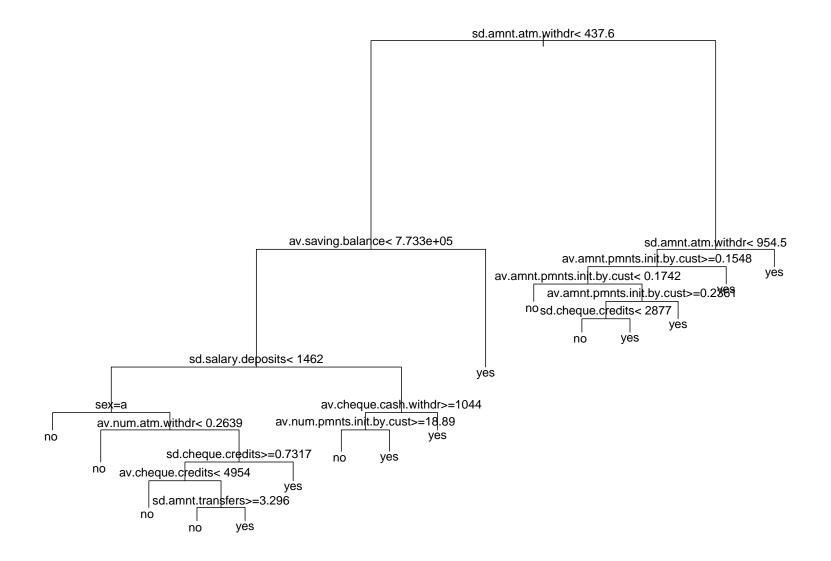
```
requireData(rpart)
CCTree <- rpart(credit.card.owner ~ ., CCTrain)
Store(CCTree, remove = FALSE)

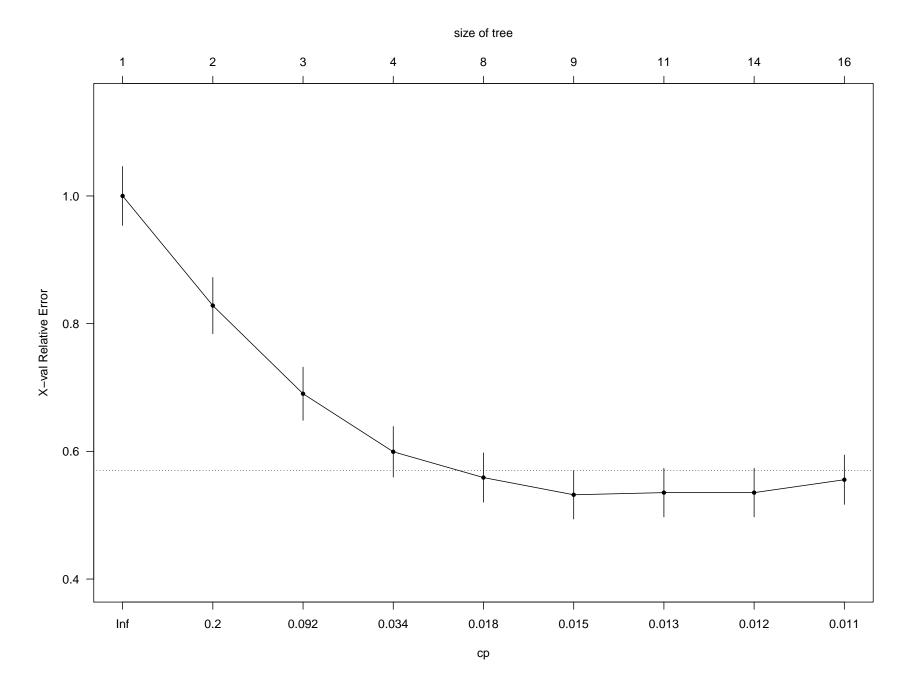
## The first graphic shows the initial fitted tree:

plot(CCTree)
text(CCTree, xpd = NA)

## The next graphic is to check for the need to prune:

plotcp(CCTree)</pre>
```





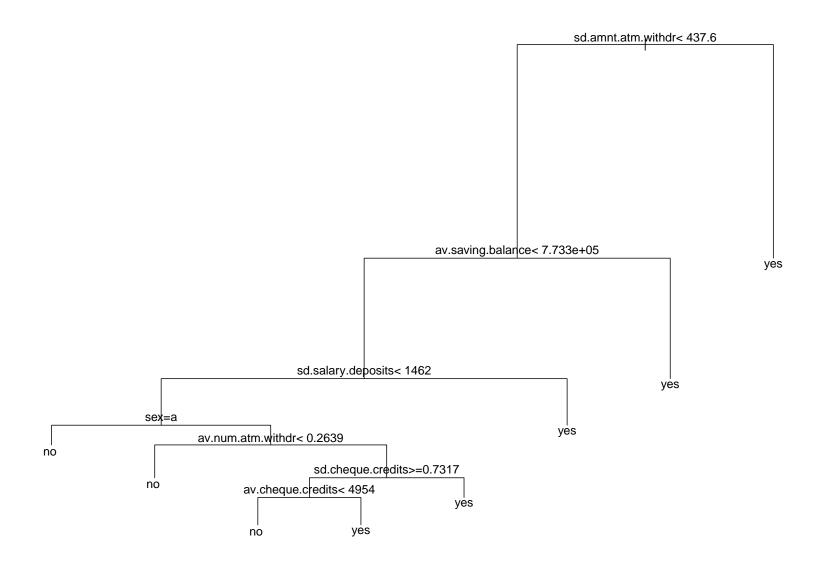
Pruning is suggested by the "one standard error" rule. Get the pruned tree:

```
oneSERule(CCTree) ## optimal tuning paramater

[1] 0.01683502

CCPTree <- prune(CCTree, cp = oneSERule(CCTree))
Store(CCPTree, remove = FALSE)

plot(CCPTree) ## should have 10 terminal nodes
text(CCPTree, xpd = NA)</pre>
```



The "one standard error rule" function(s) are listed here for completeness. (The coding details are not important for our primary purpose here.)

```
WWRCourse::oneSERule
function (tree, f, ...)
    UseMethod("oneSERule")
}
<bytecode: 0x5641497423b8>
<environment: namespace:WWRCourse>
methods("oneSERule")
[1] oneSERule.rpart*
see '?methods' for accessing help and source code
WWRCourse:::oneSERule.rpart
function (tree, f = 1, ...)
{
    cp <- data.frame(tree$cptable)</pre>
    imin <- with(cp, which(xerror == min(xerror))[1])</pre>
    with(cp, CP[which(xerror <= xerror[imin] + f * xstd[imin])[1]])</pre>
}
<bytecode: 0x56414d4708c0>
```

<environment: namespace:WWRCourse>

3.2 Simple bagging

"Bootstrap aggregation" — invented by Leo Breimann as a device to stabilize tree methods and improve their predictive capacity. Very much a "black box" technique.

- Grow a forest of trees using bootstrap samples of the training data.
- For predictions average over the forest:
 - For classification trees, take a majority vote,
 - For regression trees, take an average.

'Random forests', (Liaw and Wiener, 2002), is a development of bagging with extra protocols imposed.

Consider bagging "by hand".

```
bagRpart <- local({</pre>
  bsample <- function(dataFrame) # bootstrap sampling</pre>
    dataFrame[sample(nrow(dataFrame), rep = TRUE), ]
  function(object, data = eval.parent(object$call$data),
            nBags=200, type = c("standard", "bayesian"), ...) {
    type <- match.arg(type)</pre>
    bagsFull <- vector("list", nBags)</pre>
    if(type == "standard") {
      for(j in 1:nBags)
          bagsFull[[j]] <- update(object, data = bsample(data))</pre>
      } else {
        nCases <- nrow(data)</pre>
        for(j in 1:nBags)
             bagsFull[[j]] <- update(object, data = data, weights = rexp(nCases))</pre>
    class(bagsFull) <- "bagRpart"</pre>
    bagsFull
## a prediction method for the objects (somewhat tricky!)
```

```
predict.bagRpart <- function(object, newdata, ...) {
   X <- sapply(object, predict, newdata = newdata, type = "class")
   candidates <- levels(predict(object[[1]], type = "class"))
   X <- t(apply(X, 1, function(r) table(factor(r, levels = candidates))))
   factor(candidates[max.col(X)], levels = candidates)
}
Store(bagRpart, lib = .Robjects)</pre>
```

An alternative coding using replicate:

```
bagRpart <- local({</pre>
###
  bsample <- function(dataFrame) # bootstrap sampling</pre>
    dataFrame[sample(nrow(dataFrame), rep = TRUE), ]
###
  function(object, data = eval.parent(object$call$data),
           nBags=200, type = c("standard", "bayesian"), ...) {
    type <- match.arg(type)</pre>
    bagsFull <- if(type == "standard") {</pre>
      replicate(nBags, update(object, data = bsample(data)),
                 simplify = FALSE)
    } else {
      nCases <- nrow(data)</pre>
      replicate(nBags, update(object, data = data, weights = rexp(nCases)),
                 simplify = FALSE)
    class(bagsFull) <- "bagRpart"</pre>
    bagsFull
```

Now for an object or two:

3.3 A parallel version

Some preliminaries first:

```
## parallel backend; includes other pkgs
suppressPackageStartupMessages({
    library(doParallel)
})

(nc <- detectCores()) ## how many CPUs has your computer?

[1] 12

cl <- makeCluster(nc-1)
registerDoParallel(cl)</pre>
```

A modified version of the fitting function. Some care needed:

```
bagRpartParallel <- local({</pre>
  bsample <- function(dataFrame) # bootstrap sampling</pre>
    dataFrame[sample(nrow(dataFrame), rep = TRUE), ]
  function(object, data = eval.parent(object$call$data),
           nBags = 200, type = c("standard", "bayesian"), ...,
           cores = detectCores() - 1, seed0 = as.numeric(Sys.Date())) {
    type <- match.arg(type)</pre>
    bagsFull <- foreach(j = idiv(nBags, chunks=cores), seed = seed0+seq(cores),</pre>
                         .combine = c, .packages = c("rpart", "stats"),
                         .inorder = FALSE, .export = c("bsample")) %dopar% {
                           ## now inside a single core
                           set.seed(seed = seed)
                           if(type == "standard") {
                             replicate(j, simplify = FALSE,
                                       update(object, data = bsample(data)))
                           } else {
                             replicate(j, simplify = FALSE,
                                       update(object, data = data,
                                               weights = rexp(nrow(data))))
```

A timing comparison

```
Obj <- update(CCTree, cp = 0.005, minsplit = 9) ## expand the tree
rbind(one.
     standardP = system.time(CCSBagP <- bagRpartParallel(Obj, nBags = 200)),</pre>
     BayesP = system.time(CCBBagP <- bagRpartParallel(Obj, nBags = 200,</pre>
                                                      type = "bayes")))
         user.self sys.self elapsed user.child sys.child
standard
            11.333 0.008 11.342
                                       0.000
                                                    0
           11.561 0.004 11.565 0.000
Bayes
standardP 0.156 0.016 1.993 0.002
                                                    0
BayesP 0.152 0.008 1.924 0.003
                                                    0
rm(Obj, one)
Store(CCSBagP, CCBBagP, remove = FALSE)
```

3.4 The actual random forest

The random forest package, (Liaw and Wiener, 2002), implements this technology, and more, automatically. The number of trees is set to 500 by default. How many times does each observation get sampled if we restrict it to 200 trees?

So in this simulation the cases were sampled between one hundred and four and one hundred and fifty times. This seems about enough.

We now fit the random forest.

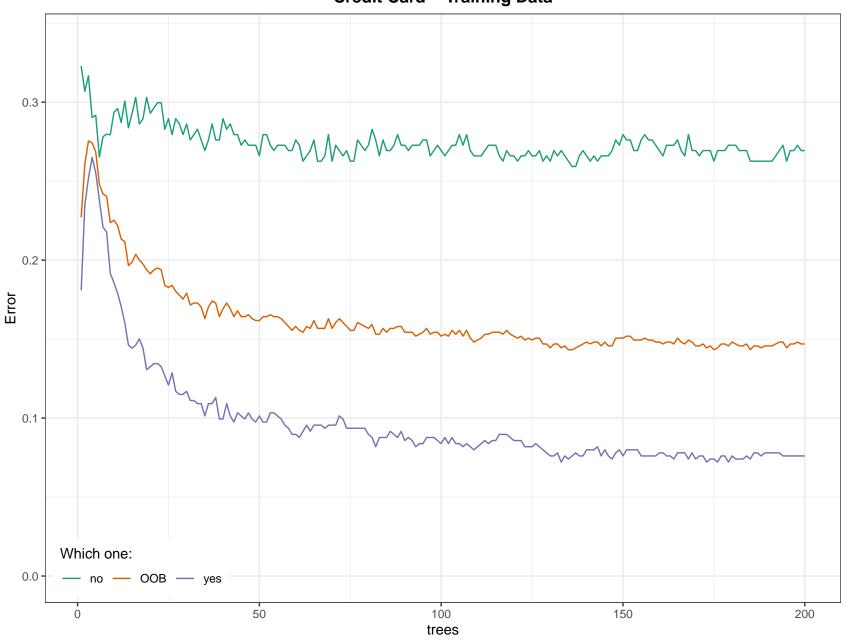
```
requireData(randomForest)
(CCRf <- randomForest(credit.card.owner ~ ., CCTrain, ntree = 200))
Call:
 randomForest(formula = credit.card.owner ~ ., data = CCTrain, ntree = 200)
              Type of random forest: classification
                    Number of trees: 200
No. of variables tried at each split: 7
        OOB estimate of error rate: 14.69%
Confusion matrix:
    no yes class.error
no 217 80 0.26936027
yes 39 474 0.07602339
Store(CCRf, remove = FALSE)
```

The "out of bag" (OOB) error rate is estimated as 14.69%. We check later how this compares with the observed error rate in the reserved *Test* data.

3.5 Progressive error rate

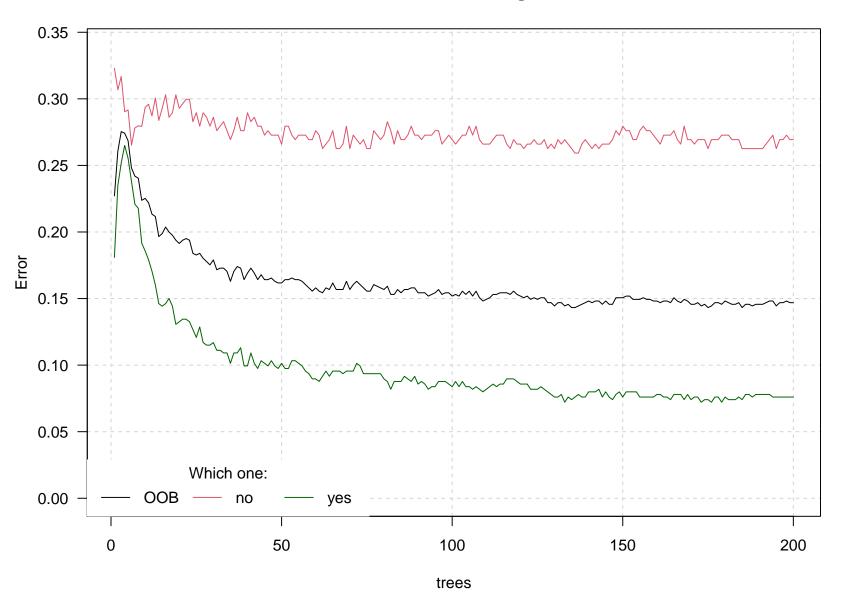
The random forest technology keeps a tally of the OOB error rate as the forest grows.

Credit Card – Training Data



We can do this more directly with the plot method for random forest objects. As is our custom, we add a few little aesthetic enhancements:

Credit Card – Training Data



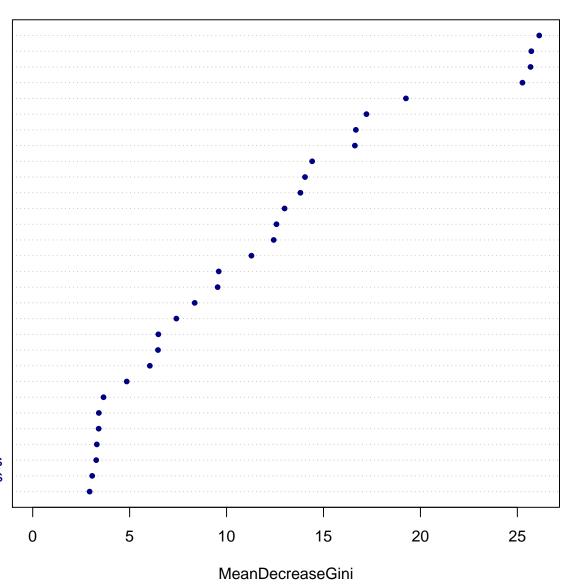
3.6 Variable importances

One other nice by-product is variable importances.

```
par(family="sans")
varImpPlot(CCRf, pch = 20, col = "navy") ## causes a plot
```

CCRf

av.amnt.atm.withdr av.salary.deposits av.cheque.credits sd.amnt.atm.withdr sd.cheque.credits av.saving.balance av.cheque.debits age sd.amnt.transfers av.cheque.cash.withdr sd.cheque.debits av.num.atm.withdr sd.salary.deposits sd.cheque.cash.withdr sex sd.num.atm.withdr sd.amnt.pmnts.init.by.cust av.amnt.transfers av.num.cheque.cash.withdr av.num.pmnts.init.by.cust sd.num.pmnts.init.by.cust av.amnt.pmnts.init.by.cust sd.saving.balance av.num.salary.deposits sd.num.cheque.cash.withdr sd.num.saving.cash.deposits av.num.saving.cash.deposits av.amnt.saving.cash.deposits sd.amnt.saving.cash.deposits pclass



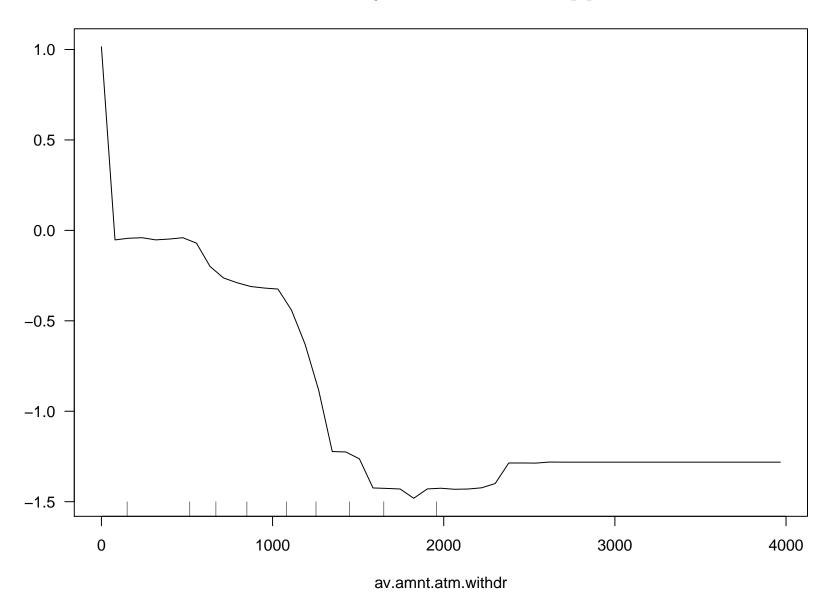
```
(v <- sort(drop(importance(CCRf)), decreasing = TRUE))[1:6]</pre>
av.amnt.atm.withdr av.salary.deposits av.cheque.credits
          26.12861
                             25.72058
                                                 25.68204
sd.amnt.atm.withdr sd.cheque.credits av.saving.balance
          25.26308
                              19.25392
                                                 17.21673
best_few <- names(v)[1:20] %>% print ## used later
 [1] "av.amnt.atm.withdr"
                                   "av.salary.deposits"
 [3] "av.cheque.credits"
                                   "sd.amnt.atm.withdr"
     "sd.cheque.credits"
                                   "av.saving.balance"
 [7] "av.cheque.debits"
                                   "age"
 [9] "sd.amnt.transfers"
                                   "av.cheque.cash.withdr"
                                   "av.num.atm.withdr"
[11] "sd.cheque.debits"
[13] "sd.salary.deposits"
                                   "sd.cheque.cash.withdr"
[15] "sex"
                                   "sd.num.atm.withdr"
[17] "sd.amnt.pmnts.init.by.cust" "av.amnt.transfers"
[19] "av.num.cheque.cash.withdr"
                                   "av.num.pmnts.init.by.cust"
```

3.6.1 Partial plots for predictor variables

These look at the way predictors appear to influence the response, mutatis mutandis.

```
partialPlot(CCRf, pred.data = CCTrain, x.var = best_few[1], xlab = best_few[1])
```

Partial Dependence on best_few[1]



3.7 Parametric models

Tree models and random forests are natural competitors to the standard parametric models, notably GLMs. We begin with a naive model based only on what appear good variables in the random forest, and then consider other modest versions, but automatically produced.

3.8 Boosting other models

The *mboost* package is an implementation of the boosting idea for a suite of different models. It is described in Buehlmann and Hothorn (2007). We consider two different kinds of boosted models, namely a boosted GLM and a boosted TREE version.

The package is profligate in the number of others it requires!

3.9 Weird science: C5.0

This is a development of a previously proprietary algorithm of Quinlan (1993); Kuhn and Quinlan (2020). It yields a rule-based classifier that might be considered intermediate between trees and forests.

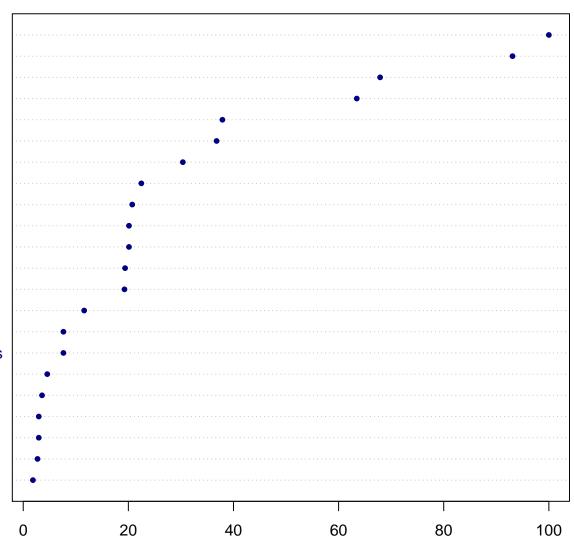
```
requireData(C50) ## NB C-5-Zero
(CCc50 <- C5.0(credit.card.owner ~ ., CCTrain))
Call:
C5.0.formula(formula = credit.card.owner ~ ., data = CCTrain)
Classification Tree
Number of samples: 810
Number of predictors: 54
Tree size: 37
Non-standard options: attempt to group attributes
Store(CCc50)
```

The C50 package, like randomForest, has some tools that allow the fitted model object to be investigated.

These include tools to assess *variable importance*, where the measure itself is somewhat obscure, but it expressed as a percentage.

```
obj <- C5imp(CCc50)
data.frame(importance = obj$Overall, variable = rownames(obj)) %>%
  filter(importance > 0) %>%
  arrange(importance) %>%
  with(., dotchart(importance, as.character(variable), pch = 20, col = "navy"))
rm(obj)
```

av.num.cheque.cash.withdr sd.amnt.atm.withdr av.num.saving.cash.deposits sex sd.amnt.pmnts.init.by.cust av.salary.deposits av.num.reg.pmnt.init.by.cust av.amnt.transfers sd.num.reg.pmnt.init.by.cust sd.amnt.transfers av.saving.balance av.num.atm.withdr av.amnt.pmnts.init.by.cust sd.saving.balance sd.cheque.credits sd.num.cheque.cash.deposits av.amnt.atm.withdr sd.cheque.cash.withdr av.num.security.pur.ord age sd.num.saving.cash.deposits sd.cheque.debits



3.10 Gradient boosting models, GBM

Like C5.0 this method was proprietary but for some time now there has been an R implementation by Greg Ridgeway, (Greenwell et al., 2020).

It offers a powerful machine learning method for several classes of models, including 'bernoulli' (binary data, but **not** multinomial, unlike randomForest or even C5.0.)

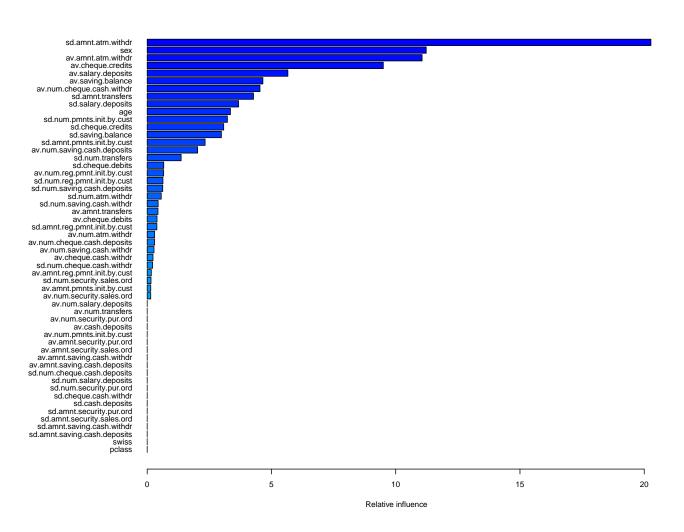
Bernoulli models need to be fitted with a numeric response confined to the values $\{0,1\}$, which can be a bit awkward:

There are several useful tools for investigating the fit and efficacy of a GBM. The first of these is one for looking at the relative influence of the predictors:

```
summary(CCgbm, plotit = FALSE) %>% filter(rel.inf > 0)
                                                                 rel.inf
                                                          var
sd.amnt.atm.withdr
                                          sd.amnt.atm.withdr 20.2703539
                                                          sex 11.2280381
sex
av.amnt.atm.withdr
                                          av.amnt.atm.withdr 11.0621992
av.cheque.credits
                                           av.cheque.credits
                                                              9.5013640
av.salary.deposits
                                          av.salary.deposits
                                                               5.6615081
av.saving.balance
                                           av.saving.balance
                                                               4.6562862
av.num.cheque.cash.withdr
                                   av.num.cheque.cash.withdr
                                                               4.5393055
av.num.saving.cash.withdr
                                   av.num.saving.cash.withdr
                                                               0.2743822
av.cheque.cash.withdr
                                       av.cheque.cash.withdr
                                                               0.2336712
sd.num.cheque.cash.withdr
                                   sd.num.cheque.cash.withdr
                                                               0.2199467
av.amnt.reg.pmnt.init.by.cust av.amnt.reg.pmnt.init.by.cust
                                                               0.1665780
                                   sd.num.security.sales.ord
                                                               0.1537358
sd.num.security.sales.ord
av.amnt.pmnts.init.by.cust
                                  av.amnt.pmnts.init.by.cust
                                                               0.1441431
av.num.security.sales.ord
                                   av.num.security.sales.ord
                                                               0.1435577
```

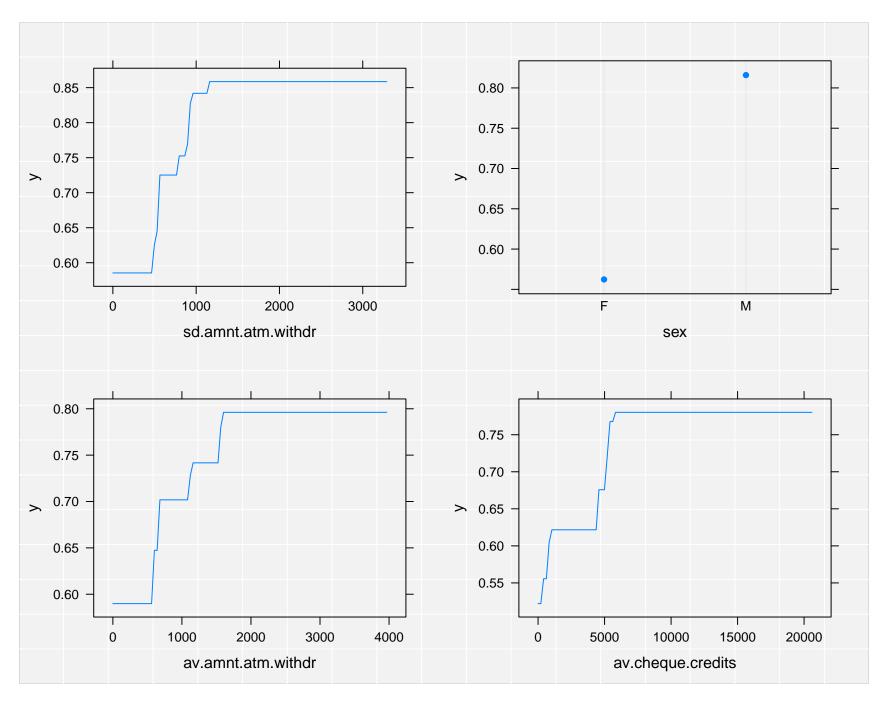
But wait, there's more. You can get a barplot of the result using same function

```
par(mar = c(4,12,1,1), cex = 0.7)
tmp <- summary(CCgbm) ## tmp is now the data frame displayed above.</pre>
```



Partial dependency plots are also available.

Look at the four "most influential" variables



4 The final reckoning

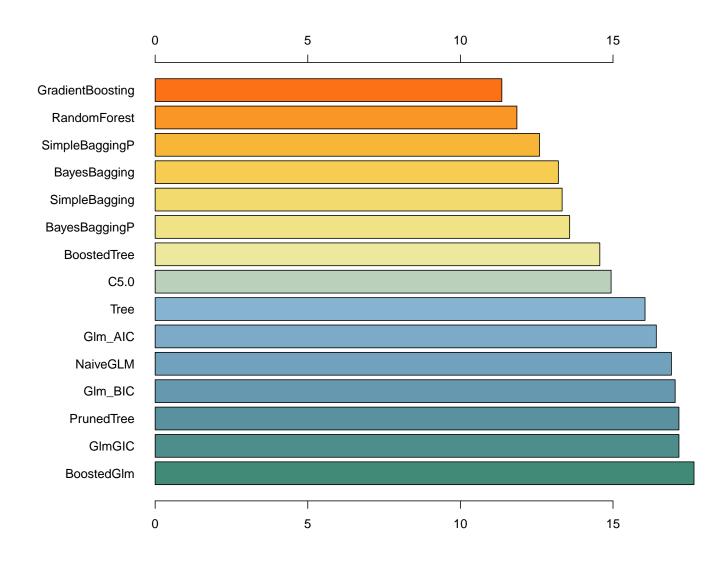
Now to see how things worked out this time. First a helper function

```
Class <- function(object, newdata, ...)</pre>
    UseMethod("Class")
Class.rpart <- function(object, newdata, ...)</pre>
    predict(object, newdata, type = "class")
Class.bagRpart <- function(object, newdata, ...)</pre>
    predict(object, newdata)
Class.randomForest <- Class.C5.0 <- predict
Class.glm <- Class.mboost <- Class.gbm <- function(object, newdata, ...) {
  ## only applies for binomial GLMs with symmetric links
  suppressMessages(predict(object, newdata) > 0)
```

The helper function *Class* streamlines things a bit:

```
errorRate <- function(tab) 100*(1 - sum(diag(tab))/sum(tab))
true <- CCTest$credit.card.owner #$</pre>
(res <- sort(sapply(list(Tree = CCTree,</pre>
                                         PrunedTree = CCPTree,
                        SimpleBagging = CCSBag, BayesBagging = CCBBag,
                        SimpleBaggingP = CCSBagP, BayesBaggingP = CCBBagP,
                        RandomForest = CCRf, C5.0 = CCc50,
                        GradientBoosting = CCgbm, BoostedGlm = CCglmboost,
                        NaiveGLM = CCGlmNaive, BoostedTree = CCblackboost,
                        Glm_AIC = CCGlmAIC, GlmGIC = CCGlmGIC,
                        Glm BIC = CCGlmBIC),
                   function(x) errorRate(table(Class(x, CCTest), true)))))
GradientBoosting
                    RandomForest
                                   SimpleBaggingP
                                                      BayesBagging
       11.35802
                        11.85185
                                         12.59259
                                                          13.20988
  SimpleBagging
                   BayesBaggingP
                                      BoostedTree
                                                              C5.0
       13.33333
                        13.58025
                                         14.56790
                                                          14.93827
                                         NaiveGLM
           Tree
                         Glm_AIC
                                                          Glm_BIC
                        16.41975
                                                          17.03704
       16.04938
                                         16.91358
     PrunedTree
                          GlmGIC
                                       BoostedGlm
       17.16049
                        17.16049
                                         17.65432
```

```
par(mar = c(3,8,3,1))
barplot(rev(res), horiz=TRUE, las=1, fill = pal_green2brown)
axis(3)
```



References

- Buehlmann, P. and T. Hothorn (2007). Boosting algorithms: Regularization, prediction and model fitting (with discussion). *Statistical Science 22*, 477–505.
- Greenwell, B., B. Boehmke, J. Cunningham, and G. Developers (2020). *gbm: Generalized Boosted Regression Models*. R package version 2.1.8.
- Kuhn, M. and R. Quinlan (2020). *C50: C5.0 Decision Trees and Rule-Based Models*. R package version 0.1.3.1.
- Liaw, A. and M. Wiener (2002). Classification and regression by randomForest. R News 2(3), 18-22.
- Quinlan, R. (1993). *C4.5: Programs for Machine Learning*. Morgan Kaufmann Publishers.
- Ripley., B. (2012). *tree: Classification and Regression Trees.* CRAN. R package version 1.0–29.

Session information

Date: 2021-01-29

• R version 4.0.3 (2020-10-10), x86_64-pc-linux-gnu

• Running under: Ubuntu 20.04.1 LTS

• Matrix products: default

• BLAS: /usr/lib/x86_64-linux-gnu/blas/libblas.so.3.9.0

• LAPACK: /usr/lib/x86_64-linux-gnu/lapack/liblapack.so.3.9.0

• Base packages: base, datasets, graphics, grDevices, methods, parallel, stats, utils

- Other packages: C50 0.1.3.1, doParallel 1.0.16, dplyr 1.0.3, english 1.2-5, forcats 0.5.1, foreach 1.5.1, gbm 2.1.8, GGally 2.1.0, ggplot2 3.3.3, ggthemes 4.2.4, gridExtra 2.3, haven 2.3.1, iterators 1.0.13, knitr 1.31, lattice 0.20-41, lme4 1.1-26, Matrix 1.3-2, mboost 2.9-4, mgcv 1.8-33, microbenchmark 1.4-7, nlme 3.1-151, patchwork 1.1.1, purrr 0.3.4, randomForest 4.6-14, rbenchmark 1.0.0, Rcpp 1.0.6, readr 1.4.0, rpart 4.1-15, scales 1.1.1, SOAR 0.99-11, stabs 0.6-3, stringr 1.4.0, tibble 3.0.5, tidyr 1.1.2, tidyverse 1.3.0, visreg 2.7.0, WWRCourse 0.2.3, WWRData 0.1.0, WWRGraphics 0.1.2, WWRUtilities 0.1.2, xtable 1.8-4
- Loaded via a namespace (and not attached): assertthat 0.2.1, backports 1.2.1, boot 1.3-26, broom 0.7.3, cellranger 1.1.0, cli 2.2.0, codetools 0.2-18, colorspace 2.0-0, compiler 4.0.3, crayon 1.3.4, Cubist 0.2.3, DBI 1.1.1, dbplyr 2.0.0, digest 0.6.27, ellipsis 0.3.1, evaluate 0.14, fansi 0.4.2, farver 2.0.3, Formula 1.2-4, fractional 0.1.3, fs 1.5.0, generics 0.1.0, glue 1.4.2, grid 4.0.3, gtable 0.3.0, highr 0.8, hms 1.0.0, httr 1.4.2, inum 1.0-1, jsonlite 1.7.2, labeling 0.4.2, lazyData 1.1.0, libcoin 1.0-7, lifecycle 0.2.0, lubridate 1.7.9.2, magrittr 2.0.1, MASS 7.3-53, minqa 1.2.4, modelr 0.1.8, munsell 0.5.0, mvtnorm 1.1-1, nloptr 1.2.2.2, nnls 1.4, partykit 1.2-11, PBSmapping 2.73.0, pillar 1.4.7, pkgconfig 2.0.3, plyr 1.8.6, quadprog 1.5-8, R6 2.5.0, RColorBrewer 1.1-2, readxl 1.3.1, reprex 1.0.0, reshape 0.8.8, reshape 2 1.4.4, rlang 0.4.10, rstudioapi 0.13, rvest 0.3.6, splines 4.0.3, statmod 1.4.35, stringi 1.5.3, survival 3.2-7, tidyselect 1.1.0, tools 4.0.3, vctrs 0.3.6, withr 2.4.1, xfun 0.20, xml2 1.3.2