

# **A Handbook of Statistical Analyses Using R**

---

Brian S. Everitt and Torsten Hothorn



## Recursive Partitioning: Large Companies and Glaucoma Diagnosis

### 8.1 Introduction

### 8.2 Recursive Partitioning

### 8.3 Analysis Using R

#### 8.3.1 Forbes 2000 Data

For some observations the profit is missing and we first remove those companies from the list

```
R> data("Forbes2000", package = "HSAUR")
R> Forbes2000 <- subset(Forbes2000, !is.na(profits))
```

The `rpart` function from *rpart* can be used to grow a regression tree. The response variable and the covariates are defined by a model formula in the same way as for `lm`, say. By default, a large initial tree is grown.

```
R> library("rpart")
R> forbes_rpart <- rpart(profits ~ assets + marketvalue + sales,
+                       data = Forbes2000)
```

A `print` method for *rpart* objects is available, however, a graphical representation shown in Figure 8.1 is more convenient. Observations which satisfy the condition shown for each node go to the left and observations which don't are element of the right branch in each node. The numbers plotted in the leaves are the mean profit for those observations satisfying the conditions stated above. For example, the highest profit is observed for companies with a market value greater than 89.33 billion US dollars and with more than 91.92 US dollars sales.

To determine if the tree is appropriate or if some of the branches need to be subjected to pruning we can use the `cptable` element of the *rpart* object:

```
R> print(forbes_rpart$cptable)
      CP nsplit rel error   xerror   xstd
1 0.23748446    0 1.0000000 1.0006021 0.1946415
2 0.04600397    1 0.7625155 0.8445024 0.2184820
3 0.04258786    2 0.7165116 0.8158351 0.2132917
4 0.02030891    3 0.6739237 0.7930997 0.2114658
5 0.01854336    4 0.6536148 0.8254006 0.2130313
6 0.01102304    5 0.6350714 0.8273236 0.2134337
7 0.01076006    6 0.6240484 0.8382426 0.2153916
8 0.01000000    7 0.6132883 0.8352144 0.2153901
```

```
R> opt <- which.min(forbes_rpart$cptable[, "xerror"])
```

```
R> plot(forbes_rpart, uniform = TRUE, margin = 0.1, branch = 0.5,
+       compress = TRUE)
R> text(forbes_rpart)
```

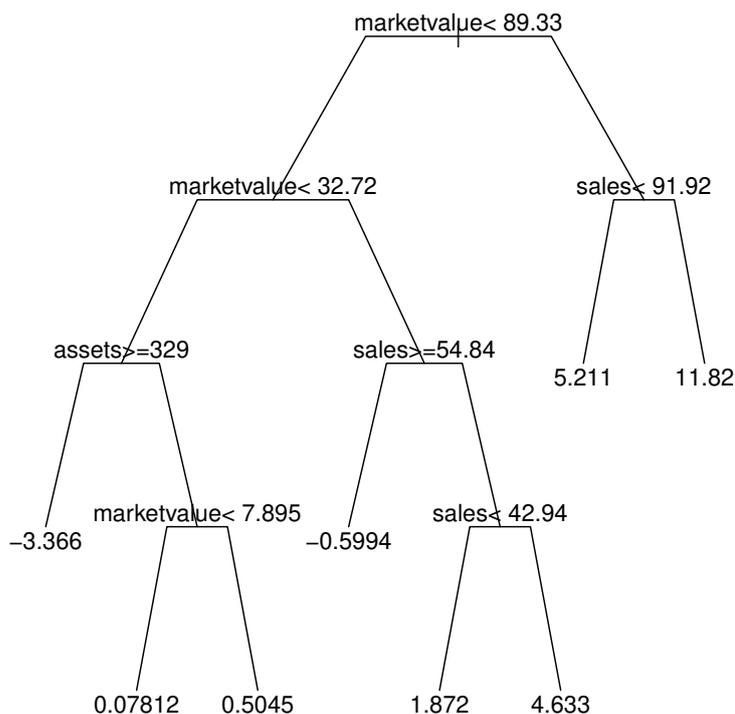


Figure 8.1 Large initial tree for Forbes 2000 data.

The `xerror` column contains estimates of cross-validated prediction error for different numbers of splits (`nsplit`). The best tree has three splits. Now we can prune back the large initial tree using

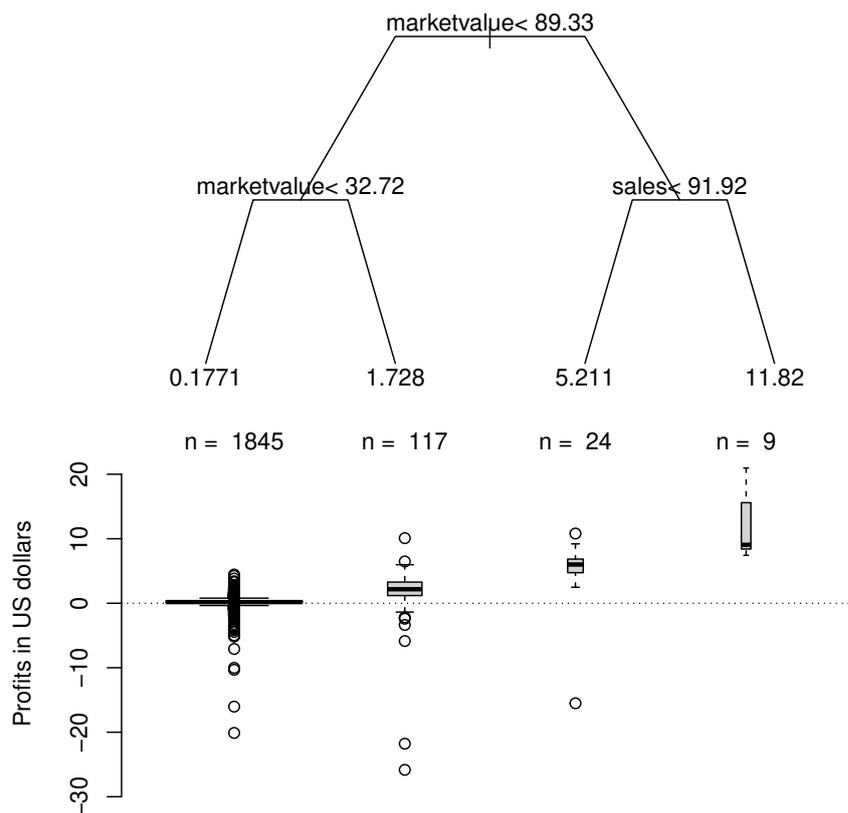
```
R> cp <- forbes_rpart$cptable[opt, "CP"]
R> forbes_prune <- prune(forbes_rpart, cp = cp)
```

The result is shown in Figure 8.2. This tree is much smaller. From the sample sizes and boxplots shown for each leaf we see that the majority of companies is grouped together. However, a large market value, more than 32.72 billion US dollars, seems to be a good indicator of large profits.

```

R> layout(matrix(1:2, nc = 1))
R> plot(forbes_prune, uniform = TRUE, margin = 0.1, branch = 0.5,
+       compress = TRUE)
R> text(forbes_prune)
R> rn <- rownames(forbes_prune$frame)
R> lev <- rn[sort(unique(forbes_prune$where))]
R> where <- factor(rn[forbes_prune$where], levels = lev)
R> n <- tapply(Forbes2000$profits, where, length)
R> boxplot(Forbes2000$profits ~ where, varwidth = TRUE,
+         ylim = range(Forbes2000$profit) * 1.3,
+         pars = list(axes = FALSE),
+         ylab = "Profits in US dollars")
R> abline(h = 0, lty = 3)
R> axis(2)
R> text(1:length(n), max(Forbes2000$profit) * 1.2,
+       paste("n = ", n))

```



**Figure 8.2** Pruned regression tree for Forbes 2000 data with the distribution of the profit in each leaf depicted by a boxplot.

## 8.3.2 Glaucoma Diagnosis

```
R> data("GlaucomaM", package = "TH.data")
R> glaucoma_rpart <- rpart(Class ~ ., data = GlaucomaM,
+                          control = rpart.control(xval = 100))
R> glaucoma_rpart$cptable
```

	CP	nsplit	rel error	xerror	xstd
1	0.65306122	0	1.0000000	1.4387755	0.06418548
2	0.07142857	1	0.3469388	0.3877551	0.05647630
3	0.01360544	2	0.2755102	0.3877551	0.05647630
4	0.01000000	5	0.2346939	0.4897959	0.06143238

```
R> opt <- which.min(glaucoma_rpart$cptable[,"xerror"])
R> cp <- glaucoma_rpart$cptable[opt, "CP"]
R> glaucoma_prune <- prune(glaucoma_rpart, cp = cp)
```

As we discussed earlier, the choice of the appropriate sized tree is not a trivial problem. For the glaucoma data, the above choice of three leaves is very unstable across multiple runs of cross-validation. As an illustration of this problem we repeat the very same analysis as shown above and record the optimal number of splits as suggested by the cross-validation runs.

```
R> nsplitopt <- vector(mode = "integer", length = 25)
R> for (i in 1:length(nsplitopt)) {
+   cp <- rpart(Class ~ ., data = GlaucomaM)$cptable
+   nsplitopt[i] <- cp[which.min(cp[,"xerror"]), "nsplit"]
+ }
R> table(nsplitopt)
```

```
nsplitopt
 1  2  5
19  4  2
```

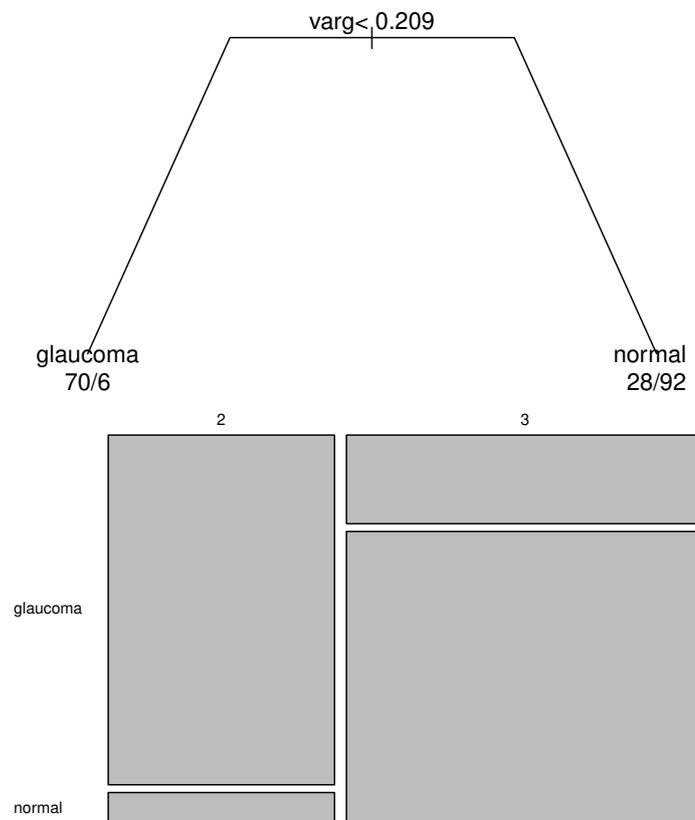
Although for 19 runs of cross-validation a simple tree with one split only is suggested, larger trees would have been favored in 6 of the cases. This short analysis shows that we should not trust the tree in Figure 8.3 too much.

One way out of this dilemma is the aggregation of multiple trees via *bagging*. In R, the bagging idea can be implemented by three or four lines of code. Case count or weight vectors representing the bootstrap samples can be drawn from the multinomial distribution with parameters  $n$  and  $p_1 = 1/n, \dots, p_n = 1/n$  via the `rmultinom` function. For each weight vector, one large tree is constructed without pruning and the *rpart* objects are stored in a list, here called `trees`:

```
R> trees <- vector(mode = "list", length = 25)
R> n <- nrow(GlaucomaM)
R> bootsamples <- rmultinom(length(trees), n, rep(1, n)/n)
R> mod <- rpart(Class ~ ., data = GlaucomaM,
+               control = rpart.control(xval = 0))
R> for (i in 1:length(trees))
+   trees[[i]] <- update(mod, weights = bootsamples[,i])
```

The `update` function re-evaluates the call of `mod`, however, with the weights

```
R> layout(matrix(1:2, nc = 1))
R> plot(glaucoma_prune, uniform = TRUE, margin = 0.1, branch = 0.5,
+       compress = TRUE)
R> text(glaucoma_prune, use.n = TRUE)
R> rn <- rownames(glaucoma_prune$frame)
R> lev <- rn[sort(unique(glaucoma_prune$where))]
R> where <- factor(rn[glaucoma_prune$where], levels = lev)
R> mosaicplot(table(where, GlaucomaM$Class), main = "", xlab = "",
+             las = 1)
```



**Figure 8.3** Pruned classification tree of the glaucoma data with class distribution in the leaves depicted by a mosaicplot.

being altered, i.e., fits a tree to a bootstrap sample specified by the weights. It is interesting to have a look at the structures of the multiple trees. For example, the variable selected for splitting in the root of the tree is not unique as can be seen by

```
R> table(sapply(trees, function(x) as.character(x$frame$var[1])))
      tmi varg vari vars
      1  15   7   2
```

Although `varg` is selected most of the time, other variables such as `vari` occur as well – a further indication that the tree in Figure 8.3 is questionable and that hard decisions are not appropriate for the glaucoma data.

In order to make use of the ensemble of trees in the list `trees` we estimate the conditional probability of suffering from glaucoma given the covariates for each observation in the original data set by

```
R> classprob <- matrix(0, nrow = n, ncol = length(trees))
R> for (i in 1:length(trees)) {
+   classprob[,i] <- predict(trees[[i]],
+                             newdata = GlaucomaM)[,1]
+   classprob[bootsamples[,i] > 0,i] <- NA
+ }
```

Thus, for each observation we get 25 estimates. However, each observation has been used for growing one of the trees with probability 0.632 and thus was not used with probability 0.368. Consequently, the estimate from a tree where an observation was not used for growing is better for judging the quality of the predictions and we label the other estimates with NA.

Now, we can average the estimates and we vote for glaucoma when the average of the estimates of the conditional glaucoma probability exceeds 0.5. The comparison between the observed and the predicted classes does not suffer from overfitting since the predictions are computed from those trees for which each single observation was *not* used for growing.

```
R> avg <- rowMeans(classprob, na.rm = TRUE)
R> predictions <- factor(ifelse(avg > 0.5, "glaucoma", "normal"))
R> predtab <- table(predictions, GlaucomaM$Class)
R> predtab
```

```
predictions glaucoma normal
 glaucoma      77      12
 normal       21      86
```

Thus, an honest estimate of the probability of a glaucoma prediction when the patient is actually suffering from glaucoma is

```
R> round(predtab[1,1] / colSums(predtab)[1] * 100)
 glaucoma
      79
```

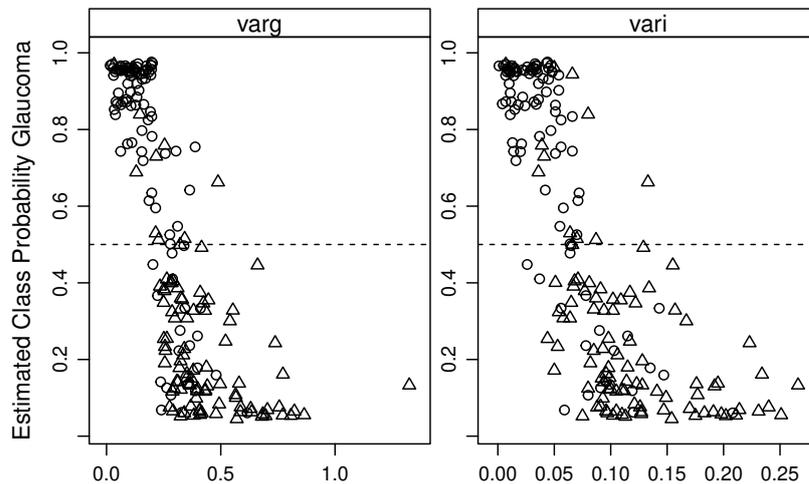
per cent. For

```
R> round(predtab[2,2] / colSums(predtab)[2] * 100)
 normal
      88
```

```

R> library("lattice")
R> gdata <- data.frame(avg = rep(avg, 2),
+   class = rep(as.numeric(GlaucomaM$Class), 2),
+   obs = c(GlaucomaM[["varg"]], GlaucomaM[["vari"]]),
+   var = factor(c(rep("varg", nrow(GlaucomaM)),
+     rep("vari", nrow(GlaucomaM))))))
R> panelf <- function(x, y) {
+   panel.xyplot(x, y, pch = gdata$class)
+   panel.abline(h = 0.5, lty = 2)
+ }
R> print(xyplot(avg ~ obs | var, data = gdata,
+   panel = panelf,
+   scales = "free", xlab = "",
+   ylab = "Estimated Class Probability Glaucoma"))

```

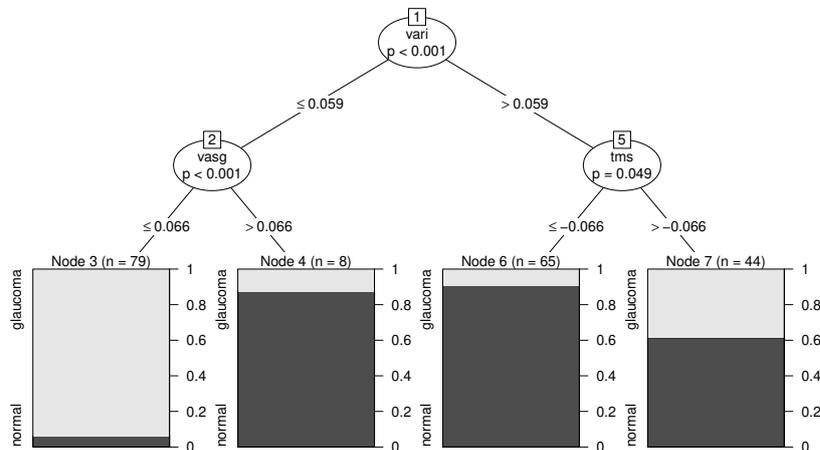


**Figure 8.4** Glaucoma data: Estimated class probabilities depending on two important variables. The 0.5 cut-off for the estimated glaucoma probability is depicted as horizontal line. Glaucomatous eyes are plotted as circles and normal eyes are triangles.

per cent of normal eyes, the ensemble does not predict a glaucomatous damage.

The *bagging* procedure is a special case of a more general approach called *random forest* (Breiman, 2001). The package *randomForest* (Breiman et al., 2006) can be used to compute such ensembles via

```
R> plot(glaucoma_ctree)
```



**Figure 8.5** Glaucoma data: Conditional inference tree with the distribution of glaucomatous eyes shown for each terminal leaf.

```
R> library("randomForest")
R> rf <- randomForest(Class ~ ., data = GlaucomaM)
and we obtain out-of-bag estimates for the prediction error via
R> table(predict(rf), GlaucomaM$Class)
```

	glaucoma	normal
glaucoma	79	12
normal	19	86

For the glaucoma data, such a *conditional inference tree* can be computed using the `ctree` function

```
R> library("party")
R> glaucoma_ctree <- ctree(Class ~ ., data = GlaucomaM)
```

and a graphical representation is depicted in Figure 8.5 showing both the cutpoints and the  $p$ -values of the associated independence tests for each node. The first split is performed using a cutpoint defined with respect to the volume of the optic nerve above some reference plane, but in the inferior part of the eye only (`vari`).

---

## Bibliography

---

- Breiman, L. (2001), "Random forests," *Machine Learning*, 45, 5–32.
- Breiman, L., Cutler, A., Liaw, A., and Wiener, M. (2006), *randomForest: Breiman and Cutler's Random Forests for Classification and Regression*, URL <http://stat-www.berkeley.edu/users/breiman/RandomForests>, R package version 4.5-18.