RECURSIVE PARTITIONING

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INTRODUCTION

INTRODUCTION

A particular kind of nonlinear predictive model: **prediction trees**.

2 varieties:

- *regression trees*
- *classification trees*

Then we'll look at ways to combine multiple trees

PREDICTION TREES

PREDICTION TREES

Tree-based methods aim at predicting y from a feature vector $x \in \mathbb{R}^p$

1. Divide up the feature space into rectangles
2. Fit a very simple model in each rectangle

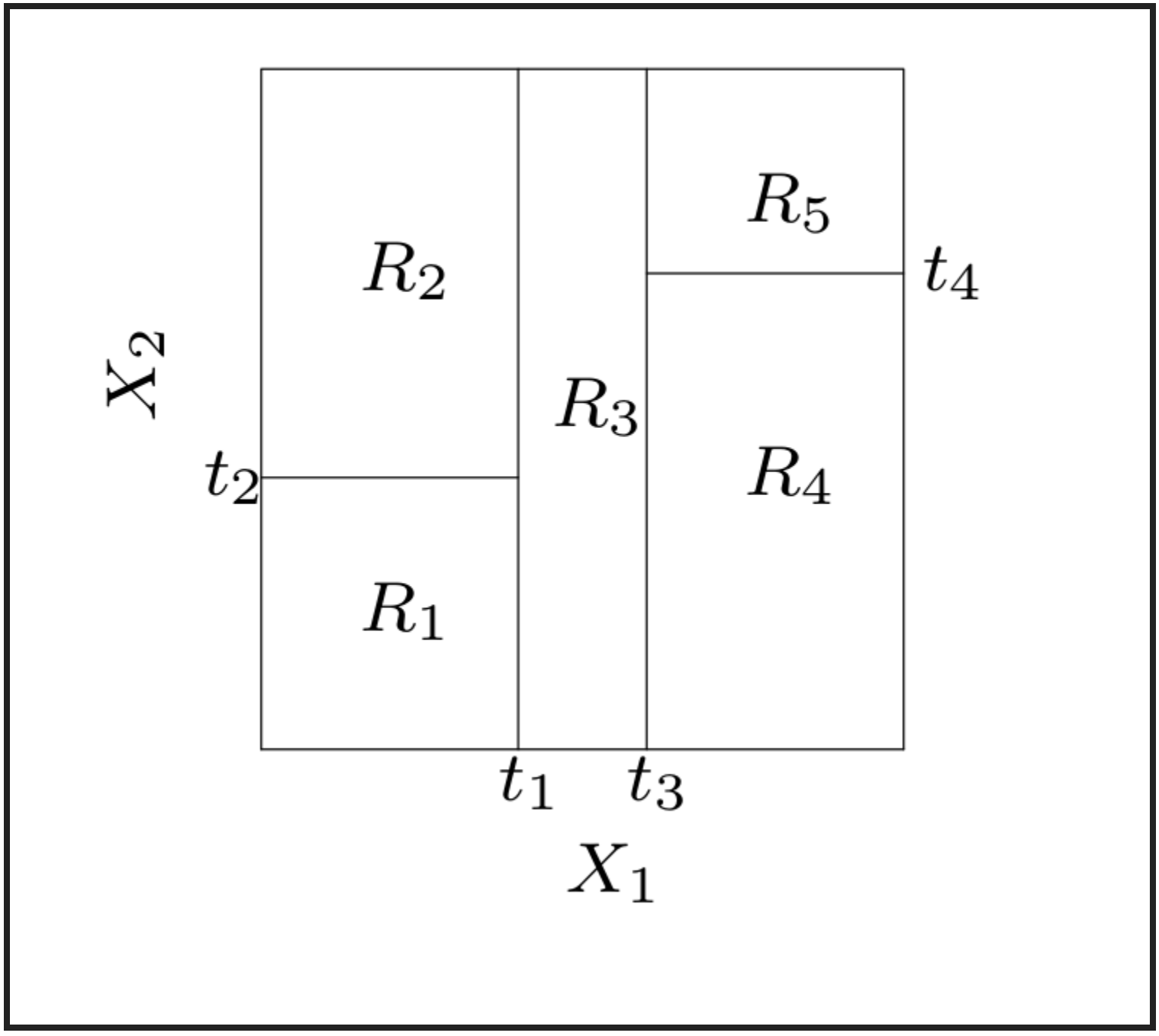
This works both when y is discrete and continuous, i.e., both for *classification* and *regression*

PREDICTION TREES

Consider a regression problem with a continuous response Y and explanatory variables X_1 and X_2.

1. Split the space into 2 regions
2. Model the response by the mean of Y in each region. We choose the variable (X_1 or X_2) and split-point that achieve the best fit
3. One or both of these regions are split into two more regions
4. Continue until some stopping rule is applied

PREDICTION TREES


R_5
R_2
t_4
X_2
R_3
R_4
t_2
R_1
t_1
t_3
X_1

PREDICTION TREES

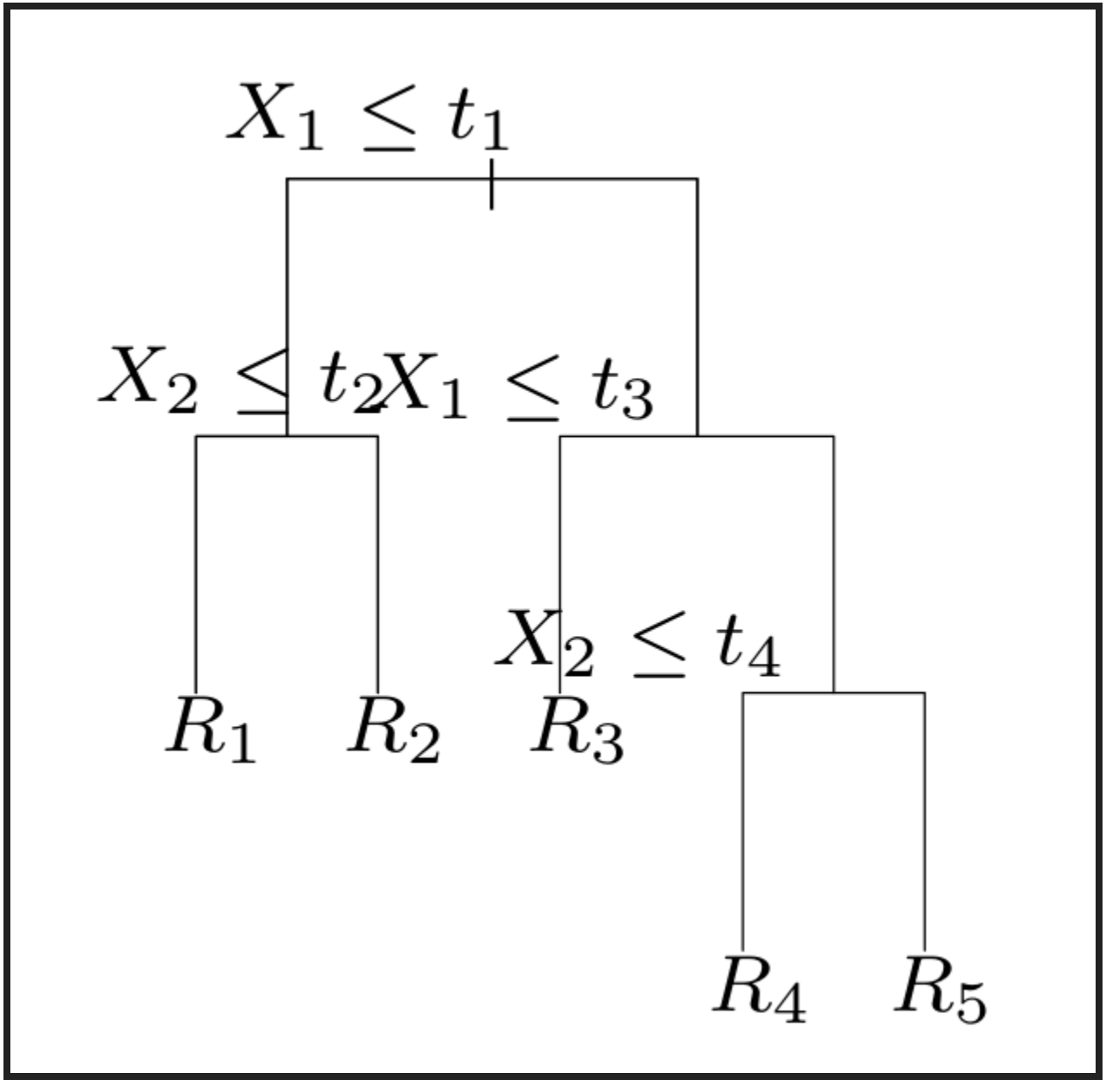
The result of this process is a partition into regions $R_1, R_2, \ldots, R_5$.

The corresponding regression model predicts Y with a constant c_m in Region R_m,

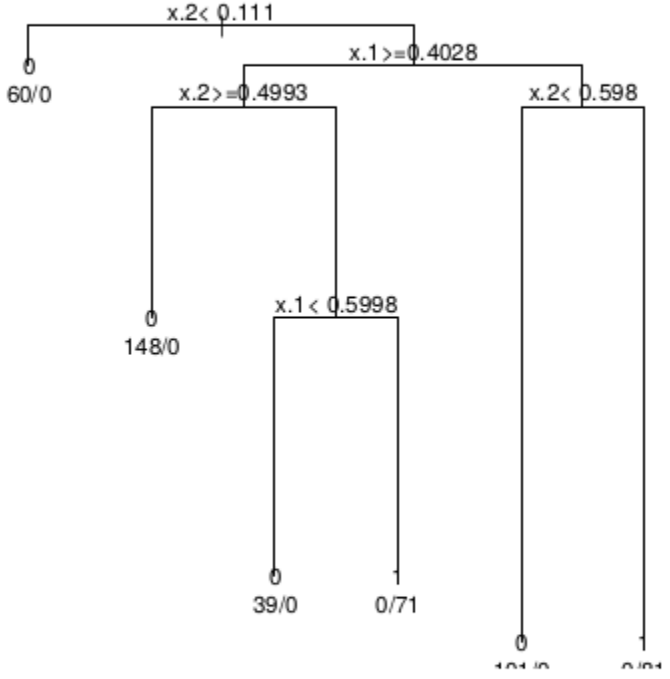
$\hat{f}(X) = \sum_{i=1}^{5} c_m \mathbf{I}\{(X_1, X_2) \in R_m\}$

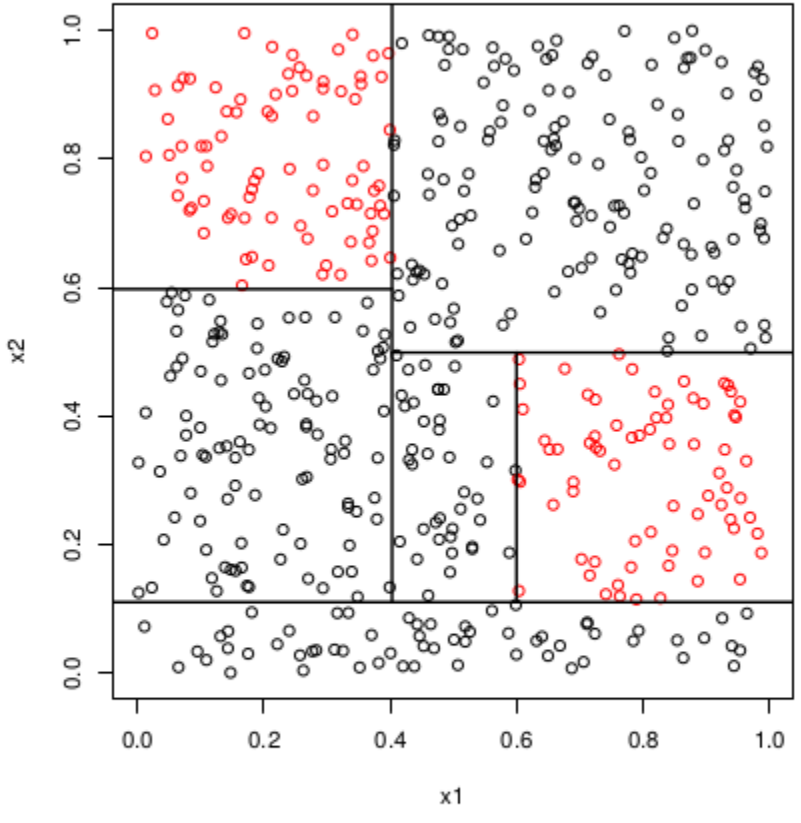
This model can be represented by a binary tree

PREDICTION TREES



PREDICTION TREES





REGRESSION TREES

The data consist of p explanatory variables and an outcome for n individuals

- (x_i, y_i) for $i = 1, \ldots, n$
- $x_i = (x_{i1}, \ldots, x_{ip})$

The algorithm needs to automatically decide on the splitting variables and split points.

Suppose that we have a partition into M regions $R_1, R_2, \ldots, R_M$, and we model the response as a constant c_m in each region

$$f(x) = \sum_{m=1}^{M} c_m \mathbf{I}(x \in R_m)$$

REGRESSION TREES

Using the *sum of squares*

$$\sum (y_i - f(x_i))^2$$

as minimisation criterion, the best $\hat{c}_m$ is the average of y_i in region R_m

$$\hat{c}_m = \frac{1}{n_m} \sum_{x_i \in R_m} y_i$$

But finding the best binary partition in terms of minimum sum of squares is generally computationally infeasible.

REGRESSION TREES

Instead we use a *greedy algorithm*:

Starting with all the data, consider a splitting variable j and split point s, and define the pair of half-planes

$$R_1(j,s) = \{X|X_j \leq s\} \quad \text{and} \quad R_2(j,s) = \{X|X_j > s\}$$

Then seek the splitting variable j and split point s that solve

$$\min_{j,s} \left[\min_{c_1} \sum_{x_i \in R_1(j,s)} (y_i - c_1)^2 + \min_{c_2} \sum_{x_i \in R_2(j,s)} (y_i - c_2)^2 \right]$$

For any choice j and s, the inner minimisation is solved by

$$\hat{c}_1 = \frac{1}{n_1} \sum_{x_i \in R_1} y_i \quad \text{and} \quad \hat{c}_2 = \frac{1}{n_2} \sum_{x_i \in R_2} y_i$$

Having found the best split, we partition the data into the two resulting regions and repeat the process in each of the two regions ...

REGRESSION TREES

How large should the tree be?

Too large, we may overfit the data (e.g., 1 data point per region is useless).

Too small, we might miss some important structure in the data

→ Tree size is a tuning parameter governing the model's complexity, and the optimal tree size should be chosen from the data

- One possibility would be to split the data only if a further split decreases the sum of squares more than a prespecified threshold
- Too short sighted: a seemingly worthless split might lead to a very good split below it

REGRESSION TREES

Pruning

1. Grow a large tree T_0, stopping the splitting process only when some minimum node size is reached
2. *Prune* this large tree using *cost-complexity pruning*

Define a subtree $T \subset T_0$ that can be obtained by pruning T_0

Let m be the index of the terminal nodes, with node m representing region R_m.

Let $|T|$ denote the number of terminal nodes in T

REGRESSION TREES

Let

$$N_m = \#\{x_i \in R_m\},$$
$$\hat{c}_m = \frac{1}{n_m} \sum_{x_i \in R_m} y_i,$$
$$Q_m(T) = \frac{1}{n_m} \sum_{x_i \in R_m} (y_i - \hat{c}_m)^2$$

The cost complexity criterion is defined as

$$C_\alpha(T) = \sum_{m=1}^{|T|} N_m Q_m(T) + \alpha|T|$$

The tuning parameter $\alpha \geq 0$ governs the trade-off between tree-size and goodness-of-fit.

α chosen via a validation set or **cross-validation**

k-FOLD CROSS-VALIDATION

Cross-validation is a widely used method for estimating prediction error

- Randomly divide the set of observations into k groups or *folds* of approximately equal size
- The first fold is treated as validation set while the tree is fitted on the remaining $k-1$ folds
- Compute the prediction error in the held-out fold using (in our case)

$$L(Y^{-k}, \hat{f}^{-k}(X)) = (y^{-k} - \hat{f}^{-k}(x))^2$$

- The procedure is repeated k-times resulting in k estimates of the test error
- The k-fold CV estimate is then

$$CV_{(k)} = \frac{1}{k} \sum_{j=1}^{k} L(Y^{-j}, \hat{f}^{-j}(X))$$

k is typically set to 5 or 10.

BUILDING A REGRESSION TREE

1. Use recursive binary splitting to grow a large tree on the training data, stopping only when each terminal node has fewer than some minimum number of observations
2. Apply cost complexity pruning to the large tree in order to obtain a sequence of best subtrees as a function of α
3. Use k-fold cross-validation to chose α, i.e., divide the data into K folds. For each $k = 1, \ldots, K$
    1. Repeat 1. and 2. on all but the k-th fold
    2. Evaluate the MSE in the left-out fold as a function of α.

    Average the results for each value of α, and pick α to minimise the average error
4. Return the subtree from Step 2 that corresponds to the chosen value of α

CLASSIFICATION TREES

Now the target is a classification outcome taking values $1, 2, 3, \ldots, K$

The only changes needed in the algorithm is in the splitting criterion and how to prune the tree

Let

$$\hat{p}_{mk} = \frac{1}{n_m} \sum_{x_i \in R_m} \mathbf{I}(y_i = k)$$

the proportion of class k observations in node m.

We classify the observations in node m to class

$$k(m) = \arg\max_k \hat{p}_{mk}$$

CLASSIFICATION TREES

Different measures of node impurity can be defined

- *Missclassification error:* $\frac{1}{n_m} \sum_{i \in R_m} \mathbf{I}(y_i \neq k(m)) = 1 - \hat{p}_{mk}$
- *Gini index:* $\sum_{k \neq k'} \hat{p}_{mk} \hat{p}_{mk'} = \sum_{k=1}^{K} \hat{p}_{mk}(1 - \hat{p}_{mk})$
- *Cross-entropy or deviance:* $-\sum_{k=1}^{K} \hat{p}_{mk} \log \hat{p}_{mk}$

The latter 2 have the advantage that they are differentiable, hence more amenable to numerical optimisation

ILLUSTRATION

Forbes2000

The `Forbes2000` contains the list of the world's biggest industrial companies. Here, our interest is to construct a model explaining the profit of a company based on assets, sales and the market value.

```
data("Forbes2000", package = "HSAUR3")
head(Forbes2000)
```

```
  rank                name        country             category  sales
1    1           Citigroup  United States              Banking  94.71
2    2    General Electric  United States        Conglomerates 134.19
3    3 American Intl Group  United States            Insurance  76.66
4    4           ExxonMobil  United States Oil & gas operations 222.88
5    5                   BP United Kingdom Oil & gas operations 232.57
6    6     Bank of America  United States              Banking  49.01
  profits  assets marketvalue
1   17.85 1264.03      255.30
2   15.59  626.93      328.54
3    6.46  647.66      194.87
4   20.96  166.99      277.02
5   10.27  177.57      173.54
6   10.81  736.45      117.55
```

ILLUSTRATION — FORBES

```
library("rpart", quietly = TRUE)
Forbes2000 <- subset(Forbes2000, !is.na(profits))
fm <- profits ~ assets + marketvalue + sales
forbes_rpart <- rpart(fm, data = Forbes2000)
```

ILLUSTRATION — FORBES

- Plot tree

```
library(partykit, quietly = TRUE)
plot(as.party(forbes_rpart))
```

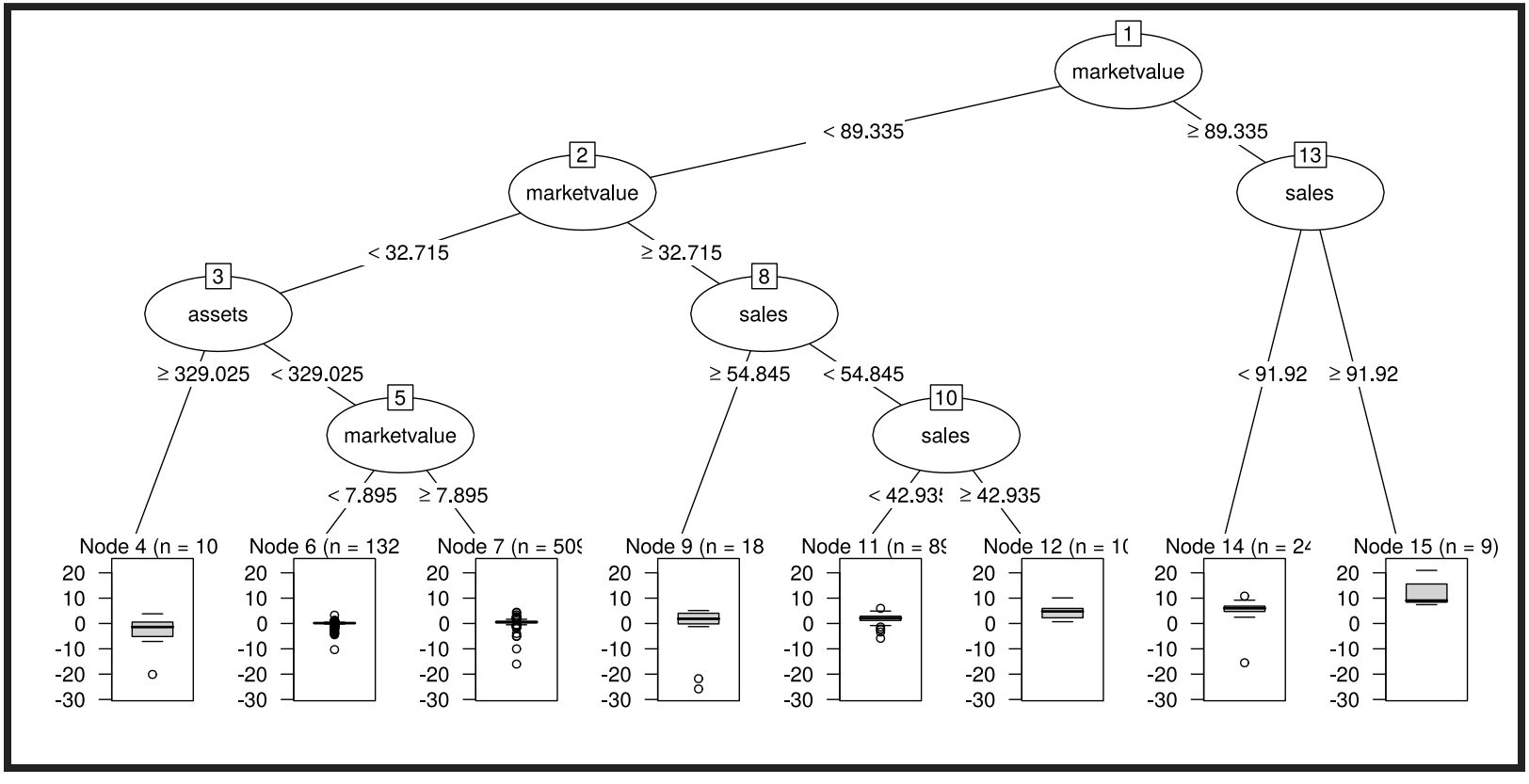


ILLUSTRATION — FORBES

- Complexity parameter

```
print(forbes_rpart$cptable)
```

```
          CP nsplit rel error    xerror      xstd
1 0.23748446      0 1.0000000 1.0008635 0.1947505
2 0.04600397      1 0.7625155 0.7934546 0.1885664
3 0.04258786      2 0.7165116 0.8145116 0.2052389
4 0.02030891      3 0.6739237 0.7568222 0.1985484
5 0.01854336      4 0.6536148 0.7756804 0.1998008
6 0.01102304      5 0.6350714 0.7649640 0.2000350
7 0.01076006      6 0.6240484 0.7732730 0.2057003
8 0.01000000      7 0.6132883 0.7667107 0.2056990
```

```
plotcp(forbes_rpart)
```

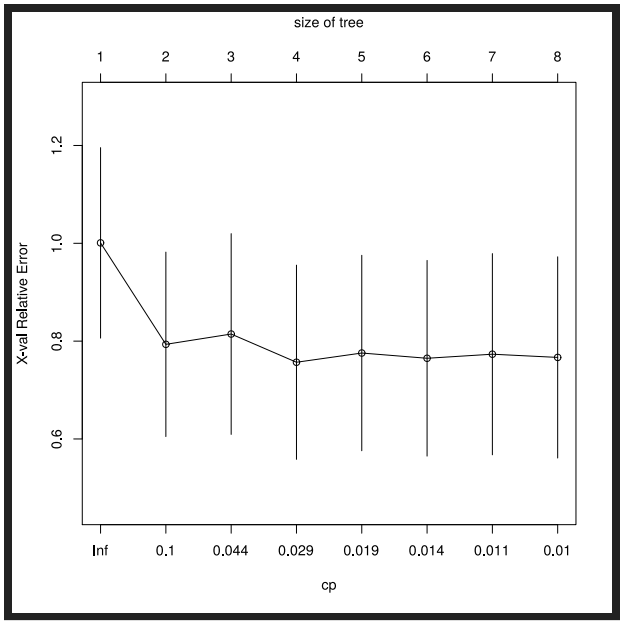

size of tree
1
2
3
4
5
6
7
8
X-val Relative Error
0.6
0.8
1.0
1.2
Inf
0.1
0.044
0.029
0.019
0.014
0.011
0.01
cp

ILLUSTRATION — FORBES

```
opt <- which.min(forbes_rpart$cptable[,"xerror"])
cp <- forbes_rpart$cptable[opt, "CP"]
forbes_prune <- prune(forbes_rpart, cp = cp)
plot(as.party(forbes_prune))
```

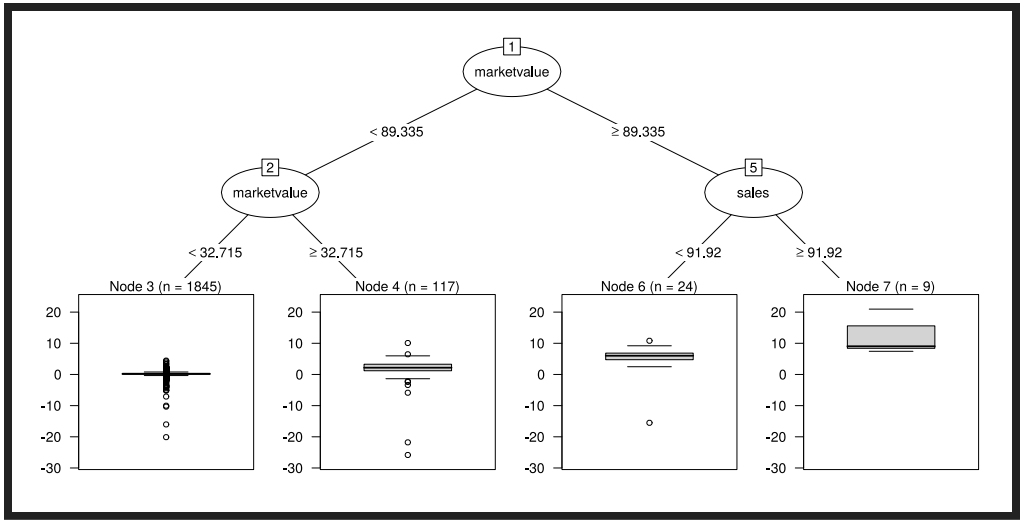


ILLUSTRATION — GLAUCOMA

For 196 people, 98 patients suffering glaucoma and 98 controls which have been matched by age and sex, 62 numeric variables derived from the laser scanning images are available.

The variables describe the morphology of the optic nerve head, i.e., measures of volumes and areas in certain regions of the eye background. Those regions have been manually outlined by a physician. Our aim is to construct a prediction model which is able to decide whether an eye is affected by glaucomateous changes based on the laser image data.

Here, we are primarily interested in the construction of a predictor. The relationship between the 62 covariates and the glaucoma status itself is not very interesting. We start with a large initial tree and prune back branches according to the cross-validation criterion.

ILLUSTRATION — GLAUCOMA

```
data("GlaucomaM", package = "TH.data")
set.seed(290875)
glaucoma_rpart <- rpart(Class ~ ., data = GlaucomaM,
             control = rpart.control(minsplit = 2, xval = 100))
glaucoma_rpart$cptable
```

```
          CP nsplit  rel error    xerror       xstd
1 0.65306122      0 1.00000000 1.5306122 0.06054391
2 0.07142857      1 0.34693878 0.3877551 0.05647630
3 0.04081633      2 0.27551020 0.3571429 0.05471329
4 0.03061224      3 0.23469388 0.4081633 0.05757556
5 0.02551020      4 0.20408163 0.4489796 0.05960655
6 0.02040816      6 0.15306122 0.4591837 0.06008148
7 0.01020408      9 0.09183673 0.4897959 0.06143238
8 0.01000000     16 0.02040816 0.5510204 0.06382443
```

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

ILLUSTRATION — GLAUCOMA

```
plot(as.party(glaucoma_prune))
```

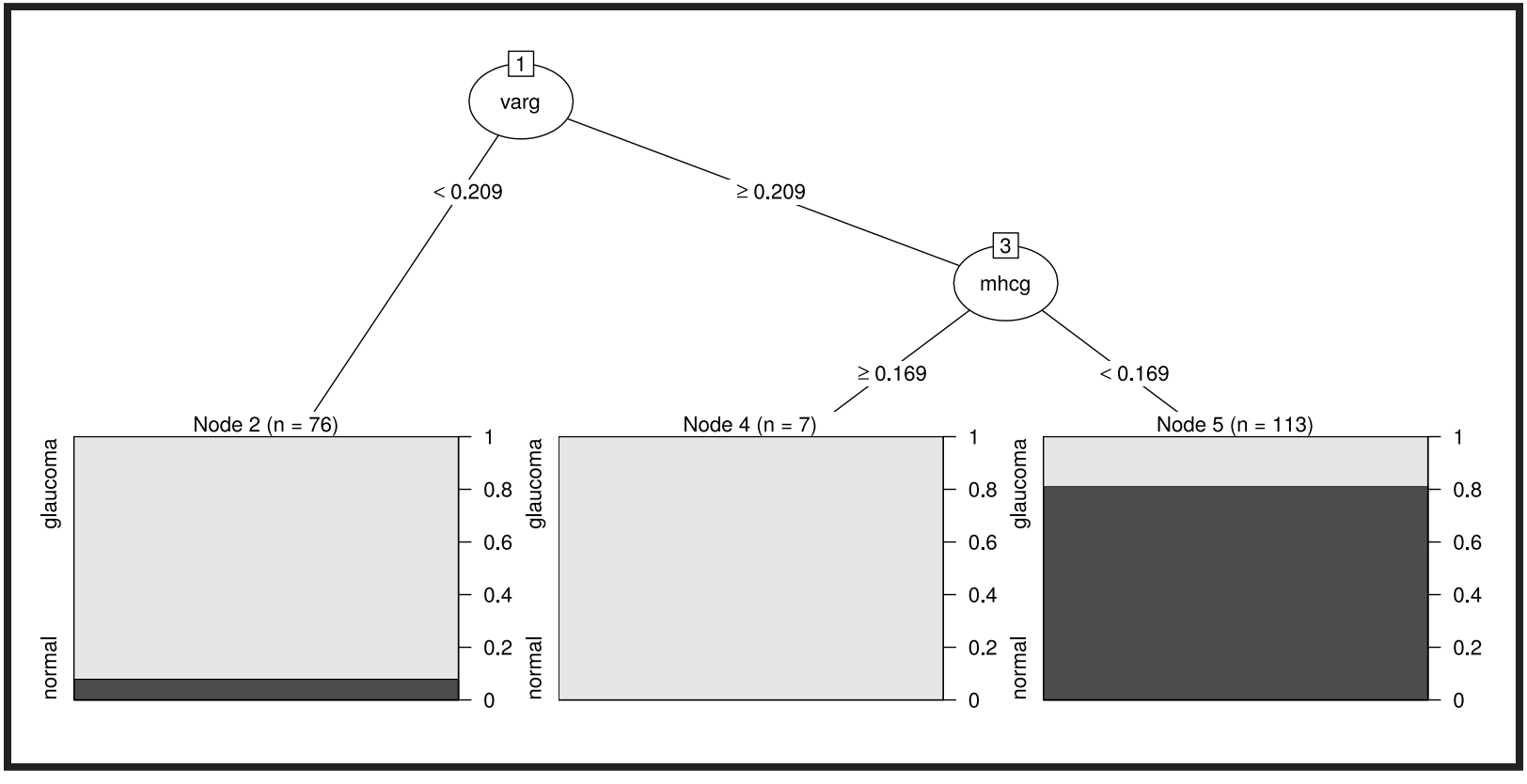


ILLUSTRATION — GLAUCOMA

Instability of trees

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

```
nsplitopt
 1  2  5
14  7  4
```

SUMMARY

Trees are easy to interpret

but have a high variance

BAGGING

BOOTSTRAP

The *bootstrap* is a widely applicable and extremely powerful statistical tool that can be used to quantify the uncertainty associated with a given estimator or statistical learning method.

Suppose that a r.v Y comes from a c.d.f $F(y) = \Pr(Y \leq y)$ and that we have a sample of size n coming from this unknown distribution.

As F is unknown we can't do any derivation analytically → Simulate! But we don't know F

F can be estimated from the empirical c.d.f

$$F_n(y) = \frac{1}{n} \sum_{i=1}^{n} \mathbf{I}(Y_i \leq y).$$

Now pretend that $F_n(y)$ is the original population distribution $F(y)$.

Sampling from F_n is equivalent to sampling with replacement from the observed data $Y_1, Y_2, \ldots, Y_n$

BOOTSTRAP

- Take B samples of size n with replacement
  - With B chosen such that the summary measure of the individual statistics is nearly as good as taking $B = \infty$
- Compute your statistic T_b on each *bootstrapped sample*
- Summarise, e.g.,

$$\widehat{\text{var}}(T) = \frac{1}{B-1} \sum_{b=1}^{B} (T_b - \bar{T})^2$$

with $\bar{T} = 1/B \sum_b T_b$

BAGGING

Consider we fit a model to the training data $\mathbf{Z} = \{(x_1, y_1), \ldots, (x_n, y_n)\}$ and obtain the prediction $\hat{f}(x)$ for input x.

Bootstrap aggregation or *bagging* averages this prediction over a collection of bootstrap samples

→ Reduction in variance

BAGGING

For each bootstrap sample $\mathbf{Z}^{*b}$, $b = 1, 2, \ldots, B$, fit the model and obtain prediction $\hat{f}^{*b}$.

The bagging estimate is defined as

$$\hat{f}_{\text{bag}}(x) = \frac{1}{B} \sum_{b=1}^{B} \hat{f}^{*b}$$

RANDOM FOREST

MOTIVATION

The idea of bagging was to average many noisy but unbiased models, and thus reduce the variance

Each tree generated in bagging is i.d.

- The bias of bagged trees is the same as that of the individual trees
- The variance of the average (with positive pairwise correlation ρ) is

$$\rho\sigma^2 + \frac{1-\rho}{B}\sigma^2$$

As B increases, the second term disappears but the correlation of bagged trees limits the benefits of averaging.

→ The idea of *random forest* is to "de-correlate" the trees through random selection of the input variables

RANDOM FOREST ALGORITHM

1. For $b = 1$ to B:
    1. Draw a bootstrap sample $\mathbf{Z}^*$ of size n from the data
    2. Grow a random-forest tree T_b to the bootstrapped data until the minimum node size $n_{\min}$ is reached by repeating the following steps
        1. Select m variables at random from the p variables
        2. Pick the best variable/split-point among the m
        3. Split the node into two daughter nodes
2. Output the ensemble of trees $\{T_b\}_1^B$

To make a prediction at a new point x:

- *regression:* $\hat{f}_{\mathrm{rf}}^B(x) = \frac{1}{B}\sum_{b=1}^B T_b(x)$
- *classification:* Let $\hat{C}_b(x)$ be the class prediction of the b-th random-forest tree. Then $\hat{C}_{\mathrm{rf}}^B(x) =$ *majority vote* $\{\hat{C}_{\mathrm{rf}}^B(x)\}_1^B$

CHOICE OF m

The inventors of random forest make the following recommendations

- For classification, the default value for m is $\lfloor \sqrt{p} \rfloor$ and the minimum node size is one
- For regression, the default value for m is $\lfloor p/3 \rfloor$ and the minimum node size is five

In practice, m should be treated as a tuning parameter

OUT-OF-BAG SAMPLES

An important feature of random forests is its use of *out-of-bag* (OOB) samples:

- On average, each bootstrapped tree makes use of around two-third of the observations. The remaining 1/3 of the observations not used to fit a given tree are called *out-of-bag* observations
- For each observation $z_i = (x_i, y_i)$, construct its random forest predictor by averaging **only** those trees corresponding to bootstrap samples in which z_i **did not** appear

An OOB error estimate is almost the same as that obtained by K-fold cross-validation.

No need for separate test data

INTERPRETATION

Simple trees are easy to interpret. The entire model can be represented by a single graphic

Random forest and bagging loose this important feature and must be interpreted in different ways

VARIABLE IMPORTANCE

For a single decision tree, the following measure can be used to compute a relative importance of a predictor X_l

$$\mathcal{I}_l^2(T) = \sum_{j=1}^{J-1} \hat{i}_t^2 \mathbf{I}(v(t) = l),$$

- the sum is over the $J-1$ internal nodes of the tree
- At each node t, one of the input variable $X_{v(t)}$ is used to partition the region
- The particular variable chosen is the one that gives maximal estimated improvement $\hat{i}_t^2$ in squared error risk (or Gini index, ...)

The squared relative importance of variable X_l is the sum of such squared improvements over all internal nodes for which it was chosen as the splitting variable

For bagging and random forests, this measure is averaged over the trees

$$\mathcal{I}_l^2 = \frac{1}{B} \sum^{B} \mathcal{I}_l^2(T_b)$$

$$\hat{f}_{\text{bag}}(x) = \frac{1}{B}\sum_{b=1}$$

ILLUSTRATION — GLAUCOMA

- Bagging. It's a random forest without random selection of the predictors

```
(glau_bag <- randomForest(Class ~ ., GlaucomaM, mtry = ncol(GlaucomaM) - 1, importance = TRUE))
```

```
Call:
 randomForest(formula = Class ~ ., data = GlaucomaM, mtry = ncol(GlaucomaM) -      1, importance
               Type of random forest: classification
                     Number of trees: 500
No. of variables tried at each split: 62

        OOB estimate of  error rate: 15.82%
Confusion matrix:
         glaucoma normal class.error
glaucoma       78     20   0.2040816
normal         11     87   0.1122449
```

ILLUSTRATION — GLAUCOMA

- Random forest

```
(glau_rf <- randomForest(Class ~ ., GlaucomaM, mtry = floor(sqrt(ncol(GlaucomaM) - 1)), importar
```

```
Call:
 randomForest(formula = Class ~ ., data = GlaucomaM, mtry = floor(sqrt(ncol(GlaucomaM) -      1)
               Type of random forest: classification
                     Number of trees: 500
No. of variables tried at each split: 7

        OOB estimate of  error rate: 13.78%
Confusion matrix:
         glaucoma normal class.error
glaucoma       82     16   0.1632653
normal         11     87   0.1122449
```

ILLUSTRATION — GLAUCOMA

Find $mtry$ through cross-validation

```
set.seed(434)
mtry_find_glau <- rfcv(GlaucomaM[, -ncol(GlaucomaM)], GlaucomaM[, ncol(GlaucomaM)],
                       mtry = function(p) max(p/2, 1), step = 0.7)

plot(mtry_find_glau$n.var, mtry_find_glau$error.cv, type = "p", cex = 2)
lines(mtry_find_glau$n.var, mtry_find_glau$error.cv)
```

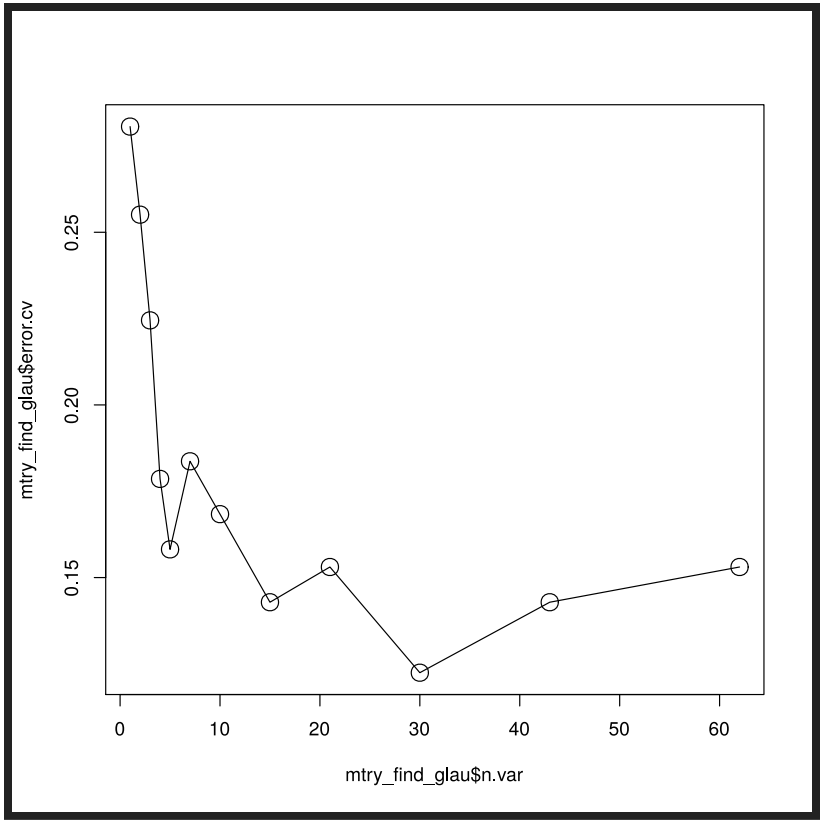

mtry_find_glau$error.cv
0.15
0.20
0.25
0
10
20
30
40
50
60
mtry_find_glau$n.var

ILLUSTRATION — GLAUCOMA

```
rf_glau_ <- randomForest(Class ~ ., GlaucomaM,
                         mtry = mtry_find_glau$n.var[which.min(mtry_find_glau$error.cv)],
                         importance = TRUE)

varImpPlot(rf_glau_, type = 2)
```