Unit 4 Lecture 2: Pruning and cross-validating decision trees

November 1, 2022

Today, we will learn how to select the complexity of decision trees based on cost complexity pruning and cross-validation, as implemented in the `rpart` package.

First, let's load some libraries:

```
library(rpart)
library(rpart.plot)
library(tidyverse)
```

Regression trees

Like last time, we will be using the `hitters` data, splitting into training and testing:

```
hitters_data <- read_csv("hitters-data.csv")
set.seed(1) # set seed for reproducibility
train_samples <- sample(1:nrow(hitters_data), round(0.8 * nrow(hitters_data)))
hitters_train <- hitters_data %>% filter(row_number() %in% train_samples)
hitters_test <- hitters_data %>% filter(!(row_number() %in% train_samples))
```

As before, we fit a regression tree by calling `rpart`:

```
tree_fit <- rpart(Salary ~ ., data = hitters_train)
```

Tree pruning and cross validation

It turns out that in addition to growing the tree, behind the scenes `rpart` has already:

- used cost complexity pruning to get the nested sequence of trees
- applied 10-fold cross-validation to compute the CV estimates and standard errors for each value of α

All we need to do is call the `printcp` function to get a summary of all this information:

```
printcp(tree_fit)
```

```
##
## Regression tree:
## rpart(formula = Salary ~ ., data = hitters_train)
##
## Variables actually used in tree construction:
## [1] AtBat   CAtBat  CHits   CRBI    Errors  PutOuts Walks
##
## Root node error: 160.25/210 = 0.76309
##
## n= 210
##
##         CP nsplit rel error  xerror     xstd
## 1 0.567669      0   1.00000 1.00411 0.072613
## 2 0.063293      1   0.43233 0.47843 0.062225
## 3 0.060590      2   0.36904 0.45832 0.066787
## 4 0.033764      3   0.30845 0.36500 0.063361
## 5 0.029146      4   0.27468 0.38646 0.071271
## 6 0.015175      5   0.24554 0.37791 0.072805
## 7 0.011737      6   0.23036 0.35152 0.068380
## 8 0.010248      7   0.21863 0.35856 0.068482
## 9 0.010000      8   0.20838 0.36327 0.068681
```

Let's focus on the table at the bottom of this output. Each row corresponds to a tree in the sequence obtained by pruning. Let's discuss each column in turn:

- The `CP` column is the "complexity parameter". It is related to, but not exactly the same as, the α parameter from the slides. Be careful! The terminology "complexity parameter" is a bit misleading because higher complexity parameters correspond to less complex models (just like lambda in penalized regression).
- `nsplit` is the number of splits in the tree. Note that `1+nsplit` is the number of terminal nodes in the tree.
- `rel error` is the RSS training error of the tree, normalized by the total variance of the response; equivalently, this is $1 - R^2$. The training error decreases as the complexity increases.
- `xerror` is the cross-validation error estimate.
- `xstd` is the cross-validation standard error.

The exact values of the complexity parameter are not so important; we might as well parameterize the trees based on the number of terminal nodes. Armed with all this information, we can produce a CV plot. The built-in function to produce the CV plot is not as nice as the one built into `cv.glmnet`, so we'll make our own using `ggplot`:

```
cp_table <- printcp(tree_fit) %>% as_tibble()
```

```
##
## Regression tree:
## rpart(formula = Salary ~ ., data = hitters_train)
##
## Variables actually used in tree construction:
## [1] AtBat   CAtBat  CHits   CRBI    Errors  PutOuts Walks
##
## Root node error: 160.25/210 = 0.76309
##
## n= 210
##
##          CP nsplit rel error  xerror     xstd
## 1 0.567669      0   1.00000 1.00411 0.072613
## 2 0.063293      1   0.43233 0.47843 0.062225
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## 5 0.029146      4   0.27468 0.38646 0.071271
## 6 0.015175      5   0.24554 0.37791 0.072805
## 7 0.011737      6   0.23036 0.35152 0.068380
## 8 0.010248      7   0.21863 0.35856 0.068482
## 9 0.010000      8   0.20838 0.36327 0.068681
```
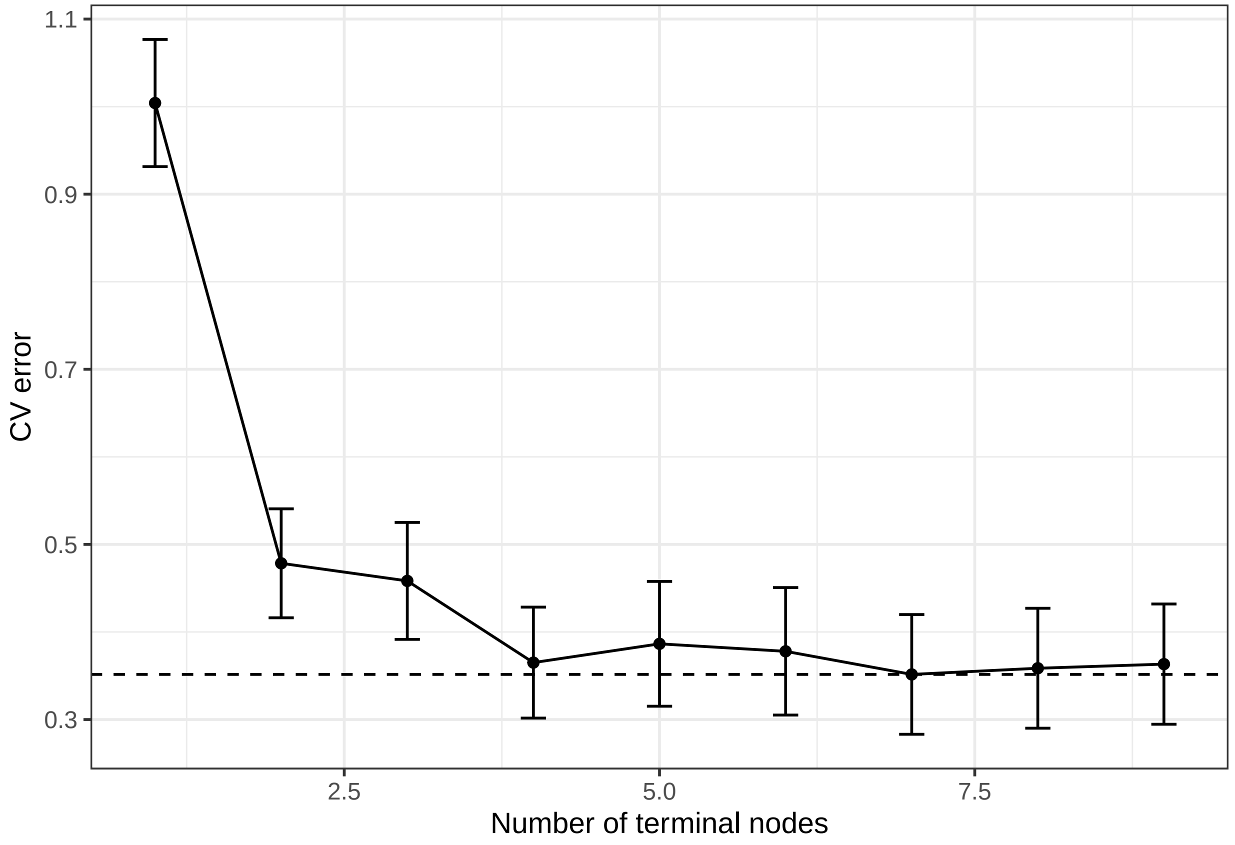

```
cp_table %>%
  ggplot(aes(
    x = nsplit + 1, y = xerror,
    ymin = xerror - xstd, ymax = xerror + xstd
  )) +
  geom_point() +
```

```r
  geom_line() +
  geom_errorbar(width = 0.2) +
  xlab("Number of terminal nodes") +
  ylab("CV error") +
  geom_hline(aes(yintercept = min(xerror)), linetype = "dashed") +
  theme_bw()
```



Audience participation: How many terminal nodes would we choose based on the one-standard-error rule?

Unfortunately, we don't have a convenient lambda.1se field of the output to directly extract the optimal complexity parameter based on the one standard error rule. Nevertheless, we can find it pretty simply using `dplyr`:

```r
optimal_tree_info <- cp_table %>%
  filter(xerror - xstd < min(xerror)) %>%
  arrange(nsplit) %>%
  head(1)
optimal_tree_info
```

```
## # A tibble: 1 x 5
##       CP nsplit `rel error` xerror   xstd
##    <dbl>  <dbl>       <dbl>  <dbl>  <dbl>
## 1 0.0338      3       0.308  0.365 0.0634
```

Audience participation: What is the above code is doing? Why is `nsplit` two rather than three as suggested by the plot above?

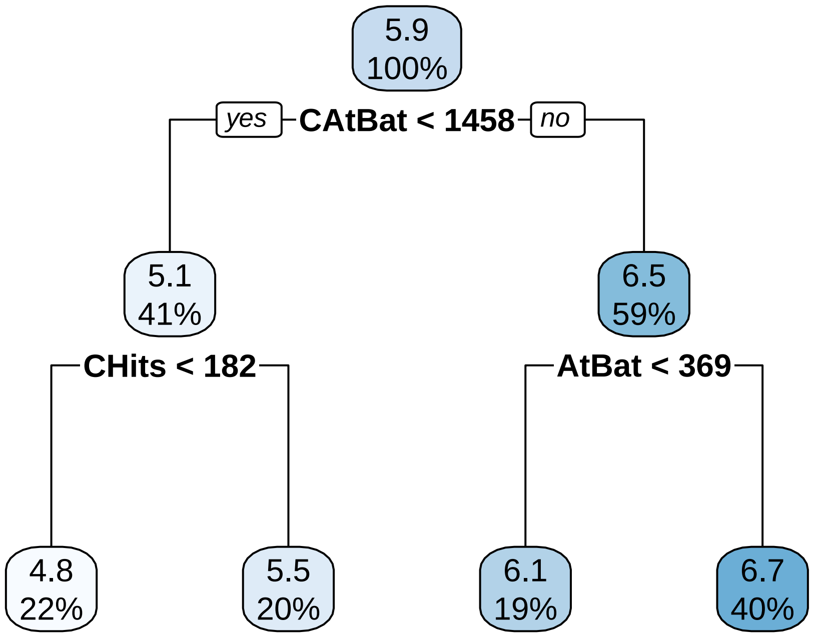
Extracting the pruned tree and making predictions

To actually get the optimal pruned tree, we need to use the function `prune`, specifying the complexity parameter

```
optimal_tree <- prune(tree_fit, cp = optimal_tree_info$CP)
```

As before, we can plot this tree using `rpart.plot`:

```
rpart.plot(optimal_tree)
```



That is a small tree! In the bias variance trade-off, sometimes less (complexity) is more (predictive performance).

Now we can make predictions on the test data and evaluate MSE using this tree:

```
pred <- predict(optimal_tree, newdata = hitters_test)
pred
```

```
##        1        2        3        4        5        6        7        8 
## 6.660241 4.810335 4.810335 4.810335 6.056463 4.810335 6.660241 6.660241 
##        9       10       11       12       13       14       15       16 
## 6.056463 6.660241 6.660241 5.494350 6.660241 6.660241 5.494350 6.660241 
##       17       18       19       20       21       22       23       24 
## 4.810335 6.660241 6.056463 6.056463 6.660241 5.494350 6.660241 6.056463 
##       25       26       27       28       29       30       31       32 
## 6.056463 6.660241 4.810335 6.660241 6.660241 5.494350 5.494350 6.660241 
##       33       34       35       36       37       38       39       40 
## 5.494350 4.810335 6.056463 6.056463 6.660241 6.660241 6.056463 6.660241 
##       41       42       43       44       45       46       47       48 
## 6.056463 6.660241 6.660241 4.810335 6.660241 6.660241 4.810335 6.660241 
##       49       50       51       52       53 
## 6.056463 5.494350 4.810335 6.660241 6.660241
```

```
mean((pred - hitters_test$Salary)^2)
```

```
## [1] 0.3088943
```

Exercise: Classification trees

Let's continue with the heart disease data from last time:

```r
heart_data <- read_csv("heart-data.csv")
set.seed(1) # set seed for reproducibility
train_samples <- sample(1:nrow(heart_data), round(0.8 * nrow(heart_data)))
heart_train <- heart_data %>% filter(row_number() %in% train_samples)
heart_test <- heart_data %>% filter(!(row_number() %in% train_samples))

# fit a classification tree
tree_fit <- rpart(AHD ~ .,
  method = "class",                # classification
  parms = list(split = "gini"),    # Gini index for splitting
  data = heart_train
)
```

Tree pruning and cross-validation

1. Produce the table of the trees in the sequence obtained from cost complexity pruning. How does `nsplit` vary with `CP`? Does this relationsihp make sense?
2. Produce the CV plot. How many terminal nodes would we choose based on the one-standard-error rule? Do we notice anything strange about the CV plot?
3. Extract and visualize the tree chosen by cross-validation. How many terminal nodes does the tree have?
4. What is the test misclassification error of this decision rule?