Classification and Regression Trees

Nate Wells

Math 243: Stat Learning

November 8th, 2021

Outline

In today's class, we will...

- Investigate pruning algorithms for improving accuracy of trees
- Create and prune decision trees in R

Section 1

Pruning

Begin with the entire data set S and search every value of every predictor to cut S into two groups S₁ and S₂ that minimizes sum of squred error:

$$\mathrm{SSE} = \sum_{i \in S_1} (y_i - \bar{y}_1)^2 + \sum_{i \in S_2} (y_i - \bar{y}_2)^2$$

Begin with the entire data set S and search every value of every predictor to cut S into two groups S₁ and S₂ that minimizes sum of squred error:

$$ext{SSE} = \sum_{i \in S_1} (y_i - \bar{y}_1)^2 + \sum_{i \in S_2} (y_i - \bar{y}_2)^2$$

2 Repeat step one on both S_1 and S_2 .

1 Begin with the entire data set S and search every value of every predictor to cut S into two groups S_1 and S_2 that minimizes sum of squred error:

$$ext{SSE} = \sum_{i \in S_1} (y_i - \bar{y}_1)^2 + \sum_{i \in S_2} (y_i - \bar{y}_2)^2$$

- **2** Repeat step one on both S_1 and S_2 .
- **8** Repeat on the new regions.

1 Begin with the entire data set S and search every value of every predictor to cut S into two groups S_1 and S_2 that minimizes sum of squred error:

$$ext{SSE} = \sum_{i \in S_1} (y_i - \bar{y}_1)^2 + \sum_{i \in S_2} (y_i - \bar{y}_2)^2$$

- **2** Repeat step one on both S_1 and S_2 .
- 8 Repeat on the new regions.

4 . . .

1 Begin with the entire data set S and search every value of every predictor to cut S into two groups S_1 and S_2 that minimizes sum of squred error:

$$ext{SSE} = \sum_{i \in S_1} (y_i - \bar{y}_1)^2 + \sum_{i \in S_2} (y_i - \bar{y}_2)^2$$

- **2** Repeat step one on both S_1 and S_2 .
- **8** Repeat on the new regions.
- 4 . . .
- Stop?

1 Begin with the entire data set S and search every value of every predictor to cut S into two groups S_1 and S_2 that minimizes sum of squred error:

$$ext{SSE} = \sum_{i \in S_1} (y_i - \bar{y}_1)^2 + \sum_{i \in S_2} (y_i - \bar{y}_2)^2$$

- **2** Repeat step one on both S_1 and S_2 .
- **8** Repeat on the new regions.
- 4 . . .
- Stop?

How do we decide when to abort the algorithm?

1 Begin with the entire data set S and search every value of every predictor to cut S into two groups S_1 and S_2 that minimizes sum of squred error:

$$ext{SSE} = \sum_{i \in S_1} (y_i - \bar{y}_1)^2 + \sum_{i \in S_2} (y_i - \bar{y}_2)^2$$

- **2** Repeat step one on both S_1 and S_2 .
- **8** Repeat on the new regions.
- 4 . . .
- Stop?

How do we decide when to abort the algorithm?

Consider the RSS of a big tree. How might training and test RSS compare?

A **subtree** is a regression tree obtained by removing some of the branches and nodes from the full regression tree.

A **subtree** is a regression tree obtained by removing some of the branches and nodes from the full regression tree.

• Compare test and training RSS between full tree and a subtree.

A **subtree** is a regression tree obtained by removing some of the branches and nodes from the full regression tree.

• Compare test and training RSS between full tree and a subtree.

Like the best subset selection algorithm for linear models, we can improve training RSS by exhaustively searching all subtrees for the best performing model.

A **subtree** is a regression tree obtained by removing some of the branches and nodes from the full regression tree.

• Compare test and training RSS between full tree and a subtree.

Like the best subset selection algorithm for linear models, we can improve training RSS by exhaustively searching all subtrees for the best performing model.

• But this search is actually even more computationally expensive than best subset!

A ${\bf subtree}$ is a regression tree obtained by removing some of the branches and nodes from the full regression tree.

• Compare test and training RSS between full tree and a subtree.

Like the best subset selection algorithm for linear models, we can improve training RSS by exhaustively searching all subtrees for the best performing model.

- But this search is actually even more computationally expensive than best subset!
- So we instead restrict our attention to those subtrees most likely to improve RSS

Once a tree is fully grown, we prune it using cost-complexity tuning

Once a tree is fully grown, we prune it using cost-complexity tuning

• The goal is to find a tree of optimal size with the smallest error rate.

Once a tree is fully grown, we prune it using cost-complexity tuning

- The goal is to find a tree of optimal size with the smallest error rate.
- We consider a sequence of trees indexed by a tuning parameter α .

Once a tree is fully grown, we prune it using cost-complexity tuning

- The goal is to find a tree of optimal size with the smallest error rate.
- We consider a sequence of trees indexed by a tuning parameter α .

For each value of α , there exists a unique subtree T of the full tree T_0 that minimizes

 $RSS + \alpha |T|$ where |T| is the number of terminal nodes of the tree T.

Once a tree is fully grown, we prune it using cost-complexity tuning

- The goal is to find a tree of optimal size with the smallest error rate.
- We consider a sequence of trees indexed by a tuning parameter α .

For each value of α , there exists a unique subtree T of the full tree T₀ that minimizes

 $RSS + \alpha |T|$

where |T| is the number of terminal nodes of the tree T.

• That is, α penalizes a tree based on its number of terminal nodes.

Once a tree is fully grown, we prune it using cost-complexity tuning

- The goal is to find a tree of optimal size with the smallest error rate.
- We consider a sequence of trees indexed by a tuning parameter α .

For each value of α , there exists a unique subtree T of the full tree T_0 that minimizes

 $RSS + \alpha |T|$

where |T| is the number of terminal nodes of the tree T.

- That is, α penalizes a tree based on its number of terminal nodes.
- As α increases from 0 (i.e. the full tree), branches get pruned in a predictable way, making for relatively quick computation.

Once a tree is fully grown, we prune it using cost-complexity tuning

- The goal is to find a tree of optimal size with the smallest error rate.
- We consider a sequence of trees indexed by a tuning parameter α .

For each value of α , there exists a unique subtree T of the full tree T_0 that minimizes

 $RSS + \alpha |T|$

where |T| is the number of terminal nodes of the tree T.

- That is, α penalizes a tree based on its number of terminal nodes.
- As α increases from 0 (i.e. the full tree), branches get pruned in a predictable way, making for relatively quick computation.
- We can find the optimal value of α using cross-validation

Once a tree is fully grown, we prune it using cost-complexity tuning

- The goal is to find a tree of optimal size with the smallest error rate.
- We consider a sequence of trees indexed by a tuning parameter α .

For each value of α , there exists a unique subtree T of the full tree T_0 that minimizes

 $RSS + \alpha |T|$

where |T| is the number of terminal nodes of the tree T.

- That is, α penalizes a tree based on its number of terminal nodes.
- As α increases from 0 (i.e. the full tree), branches get pruned in a predictable way, making for relatively quick computation.
- We can find the optimal value of α using cross-validation

There are two ways to select the **best** subtree.

Once a tree is fully grown, we prune it using cost-complexity tuning

- The goal is to find a tree of optimal size with the smallest error rate.
- We consider a sequence of trees indexed by a tuning parameter α .

For each value of α , there exists a unique subtree T of the full tree T_0 that minimizes

 $RSS + \alpha |T|$

where |T| is the number of terminal nodes of the tree T.

- That is, α penalizes a tree based on its number of terminal nodes.
- As α increases from 0 (i.e. the full tree), branches get pruned in a predictable way, making for relatively quick computation.
- We can find the optimal value of α using cross-validation

There are two ways to select the **best** subtree.

1 Choose the tree with smallest MSE.

Once a tree is fully grown, we prune it using cost-complexity tuning

- The goal is to find a tree of optimal size with the smallest error rate.
- We consider a sequence of trees indexed by a tuning parameter α .

For each value of α , there exists a unique subtree T of the full tree T_0 that minimizes

 $RSS + \alpha |T|$

where |T| is the number of terminal nodes of the tree T.

- That is, α penalizes a tree based on its number of terminal nodes.
- As α increases from 0 (i.e. the full tree), branches get pruned in a predictable way, making for relatively quick computation.
- We can find the optimal value of α using cross-validation

There are two ways to select the **best** subtree.

- 1 Choose the tree with smallest MSE.
- Ochoose the smallest tree with MSE within 1 standard deviation of smallest MSE

Trees on Trees

We use a subset of the pdxTrees dataset from the pdxTrees repo (maintained by K. McConville, I. Caldwell, and N. Horton)

To keep things manageable, we'll focus on trees in 3 parks nearby Reed.
 library(pdxTrees)
 my_pdxTrees <- get_pdxTrees_parks(park = c("Powel Park", "Woodstock Park", "Berkeley Park"))

Trees on Trees

We use a subset of the pdxTrees dataset from the pdxTrees repo (maintained by K. McConville, I. Caldwell, and N. Horton)

To keep things manageable, we'll focus on trees in 3 parks nearby Reed.
 library(pdxTrees)
 my_pdxTrees <- get_pdxTrees_parks(park = c("Powel Park", "Woodstock Park", "Berkeley Park"))

• And use trees from another park as a test set: my_pdxTrees_test <- get_pdxTrees_parks(park = c("Glenwood Park"))</pre>

Trees on Trees

We use a subset of the pdxTrees dataset from the pdxTrees repo (maintained by K. McConville, I. Caldwell, and N. Horton)

To keep things manageable, we'll focus on trees in 3 parks nearby Reed.
 library(pdxTrees)
 my_pdxTrees <- get_pdxTrees_parks(park = c("Powel Park", "Woodstock Park", "Berkeley Park"))

 And use trees from another park as a test set: my_pdxTrees_test <- get_pdxTrees_parks(park = c("Glenwood Park"))

• Can we predict carbon sequestration based on Tree_Height and Crown_Width_EW?

Pruning Example

How does MSE vary as tree size changes?



• What are the test MSEs for the full tree and the subtrees with 5 and 7 terminal nodes?

A tibble: 3 x 4 ## model .metric .estimator .estimate <chr>> <chr>> <chr> <dbl> ## ## 1 full standard 20.3 rmse ## 2 pruned standard 19.7 rmse ## 3 very pruned rmse standard 20.1

Comparison



Section 2

Trees in R

Nate Wells (Math 243: Stat Learning)

Creating Tree Models in R

There are two common packages for creating regression trees in R: tree and rpart.

Creating Tree Models in R

There are two common packages for creating regression trees in R: tree and rpart.

• The tree package is one of the oldest packages on CRAN. It is a (tiny) bit easier to use. But allows far less customization. ISLR uses tree. (Traditional)

Creating Tree Models in R

There are two common packages for creating regression trees in R: tree and rpart.

- The tree package is one of the oldest packages on CRAN. It is a (tiny) bit easier to use. But allows far less customization. ISLR uses tree. (Traditional)
- The rpart package is newer, computationally faster, and has more options. It also can be combined with other packages for **much** nicer plots. Applied Predictive Modeling uses rpart. (Recommended)

Trees using 'rpart"

 To fit a tree using variables Tree_Height, Crown_Width_EW, Crown_Width_NS, Crown_Base_Height:

Trees using 'rpart"

• To fit a tree using variables Tree_Height, Crown_Width_EW, Crown_Width_NS, Crown_Base_Height:

```
    We can change several features of the tree by adding a control argument:
set.seed(1)
tree_model2 <- rpart(Carbon_Sequestration_lb ~
Tree_Height + Crown_Width_EW + Crown_Width_NS + Crown_Base_Height,
control = rpart.control(minsplit = 30, xval = 10, maxdepth = 8),
data = my_pdxTrees)
```

Trees using 'rpart"

 To fit a tree using variables Tree_Height, Crown_Width_EW, Crown_Width_NS, Crown_Base_Height:

 We can change several features of the tree by adding a control argument: set.seed(1) tree_model2 <- rpart(Carbon_Sequestration_lb ~ Tree_Height + Crown_Width_EW + Crown_Width_NS + Crown_Base_Height, control = rpart.control(minsplit = 30, xval = 10, maxdepth = 8), data = my_pdxTrees)

- minsplit is the minimum number of observations in a node
- xval is the number of cross-validation folds used
- maxdepth is the maximum depth of any node in the final tree

Plots using plot

- There are several options for visualizing trees with varying ease-of-use and aesthetics.
 - The base R plot function quickly generates plots, but...

Plots using plot

- There are several options for visualizing trees with varying ease-of-use and aesthetics.
 - The base R plot function quickly generates plots, but...

```
plot(tree_model1)
text(tree_model1, pretty = 0, cex = .5)
```



Plots using rpart.plot

• An alternative to plot is the rpart.plot function from the package of the same name:

library(rpart.plot)
rpart.plot(tree_model1)



• Some further customization available (see ?rpart.plot)

Trees in R via rpart cont'd

• The rpart function automatically performs *k*-fold CV when choosing among potential splits.

Trees in R via rpart cont'd

• The rpart function automatically performs *k*-fold CV when choosing among potential splits.

• To access results, append \$cptable to the rpart model object: tree_model1\$cptable

##		CP	nsplit	rel error	xerror	xstd
##	1	0.31073097	0	1.0000000	1.0105895	0.09666964
##	2	0.07370105	1	0.6892690	0.7679112	0.07560215
##	3	0.04577064	2	0.6155680	0.7211540	0.07009241
##	4	0.04342290	4	0.5240267	0.6668256	0.06922100
##	5	0.03450324	5	0.4806038	0.6378779	0.06854061
##	6	0.01877027	7	0.4115973	0.6624756	0.08409966
##	7	0.01778685	9	0.3740568	0.7124886	0.09350971
##	8	0.0100000	11	0.3384831	0.7070176	0.09248091

Trees in R via rpart cont'd

• The rpart function automatically performs *k*-fold CV when choosing among potential splits.

• To access results, append \$cptable to the rpart model object: tree model1\$cptable

##		CP	nsplit	rel error	xerror	xstd
##	1	0.31073097	0	1.0000000	1.0105895	0.09666964
##	2	0.07370105	1	0.6892690	0.7679112	0.07560215
##	3	0.04577064	2	0.6155680	0.7211540	0.07009241
##	4	0.04342290	4	0.5240267	0.6668256	0.06922100
##	5	0.03450324	5	0.4806038	0.6378779	0.06854061
##	6	0.01877027	7	0.4115973	0.6624756	0.08409966
##	7	0.01778685	9	0.3740568	0.7124886	0.09350971
##	8	0.01000000	11	0.3384831	0.7070176	0.09248091

- CP is the value of the complexity parameter
- nsplit is number of splits
- rel error is $1 R^2$, using $R^2 = 1 \frac{RSS}{TSS}$
- xerror is cross-validated estimate of relative error
- xstd is the standard deviation in xerror based on CV

Analyze Results

• The printcp function displays key model information printcp(tree_model1)

##

```
## Regression tree:
## rpart(formula = Carbon Sequestration lb ~ Tree Height + Crown Width EW +
##
       Crown Width NS + Crown Base Height, data = my pdxTrees)
##
## Variables actually used in tree construction:
##
   [1] Crown Base Height Crown Width EW
                                          Crown Width NS
                                                            Tree Height
##
## Root node error: 406713/307 = 1324.8
##
## n= 307
##
##
           CP nsplit rel error xerror
                                           vstd
                  0 1.00000 1.01059 0.096670
## 1 0.310731
## 2 0.073701
                  1
                      0.68927 0.76791 0.075602
## 3 0.045771
                  2 0.61557 0.72115 0.070092
## 4 0.043423
                  4 0.52403 0.66683 0.069221
## 5 0.034503
                  5 0.48060 0.63788 0.068541
## 6 0.018770
                  7
                      0.41160 0.66248 0.084100
## 7 0.017787
                  9 0.37406 0.71249 0.093510
## 8 0.010000
                  11
                       0.33848 0.70702 0.092481
```

Analyze Results cont'd

• Detailed listing of model parts can be accessed via summary:

Analyze Results cont'd

• Detailed listing of model parts can be accessed via summary:

summary(tree_model1)

```
## Call:
## rpart(formula = Carbon_Sequestration_lb ~ Tree_Height + Crown_Width_EW +
      Crown_Width_NS + Crown_Base_Height, data = my_pdxTrees)
##
##
    n= 307
##
##
             CP nsplit rel error
                                    xerror
                                                  xstd
## 1 0.31073097
                     0 1.0000000 1.0105895 0.09666964
## 2 0.07370105
                     1 0.6892690 0.7679112 0.07560215
## 3 0.04577064
                     2 0.6155680 0.7211540 0.07009241
## 4 0.04342290
                     4 0.5240267 0.6668256 0.06922100
## 5 0.03450324
                     5 0.4806038 0.6378779 0.06854061
## 6 0.01877027
                     7 0.4115973 0.6624756 0.08409966
## 7 0.01778685
                     9 0.3740568 0.7124886 0.09350971
## 8 0.01000000
                    11 0.3384831 0.7070176 0.09248091
##
##
  Variable importance
##
      Crown Width EW
                                              Tree_Height Crown_Base_Height
                        Crown Width NS
##
                  38
                                    28
                                                       24
                                                                         10
##
## Node number 1: 307 observations.
                                       complexity param=0.310731
##
     mean=47.95081, MSE=1324.797
##
    left son=2 (137 obs) right son=3 (170 obs)
##
    Primary splits:
##
         Crown Width EW
                           < 43.5 to the left, improve=0.31073100, (0 missing)
##
         Crown Width NS
                           < 49.5 to the left, improve=0.28692940, (0 missing)
##
         Tree Height
                           < 78.5 to the left, improve=0.16233240, (0 missing)
##
         Crown Base Height < 4.5 to the left. improve=0.05039755, (0 missing)
##
     Surrogate splits:
##
         Crown_Width_NS
                           < 43.5 to the left,
                                                 agree=0.788, adj=0.526, (0 split)
##
         Tree_Height
                           < 45.5 to the left,
                                                 agree=0.739, adj=0.416, (0 split)
  Nate Wells (Math 243: Stat Learning)
                                                   Classification and Regression Trees
```

CV Plots

• We can plot the results of cross-validation using plotcp:

CV Plots

• We can plot the results of cross-validation using plotcp:

plotcp(tree_model1)



ср

• The horizontal line is 1 SE above minimum relative error

Pruning

- Based on the CV plot, 6 splits with CP = 0.039 gives the lowest error
 - While 5 splits with CP = 0.045 gives least splits within 1 SE of best.

Pruning

- Based on the CV plot, 6 splits with CP = 0.039 gives the lowest error
 - While 5 splits with CP = 0.045 gives least splits within 1 SE of best.
- We can prune our tree using the prune function with a given value of cp

Pruning

- Based on the CV plot, 6 splits with CP = 0.039 gives the lowest error
 - While 5 splits with CP = 0.045 gives least splits within 1 SE of best.

• We can prune our tree using the prune function with a given value of cp pruned_tree <- prune(tree_model1, cp = 0.039)



• How well do models do on the test data?

• How well do models do on the test data?

• How well do models do on the test data?

• And use rmse from yardstick to assess:

• How well do models do on the test data?

```
• And use rmse from yardstick to assess:
library(yardstick)
results %>% group_by(model) %>% rmse(truth = obs, estimate = preds)
## # 4 tibble: 2 x 4
```

				-	
##		model	.metric	.estimator	.estimate
##		<chr></chr>	<chr></chr>	<chr></chr>	<dbl></dbl>
##	1	full	rmse	standard	21.1
##	2	pruned	rmse	standard	19.2