

Regression and Classification Trees

Nate Wells

Math 243: Stat Learning

November 4th, 2020

Outline

In today's class, we will...

- Investigate pruning algorithms for improving accuracy of regression trees
- Discuss classification trees for classification problems.

Section 1

Improving Regression Trees

Trees on Trees

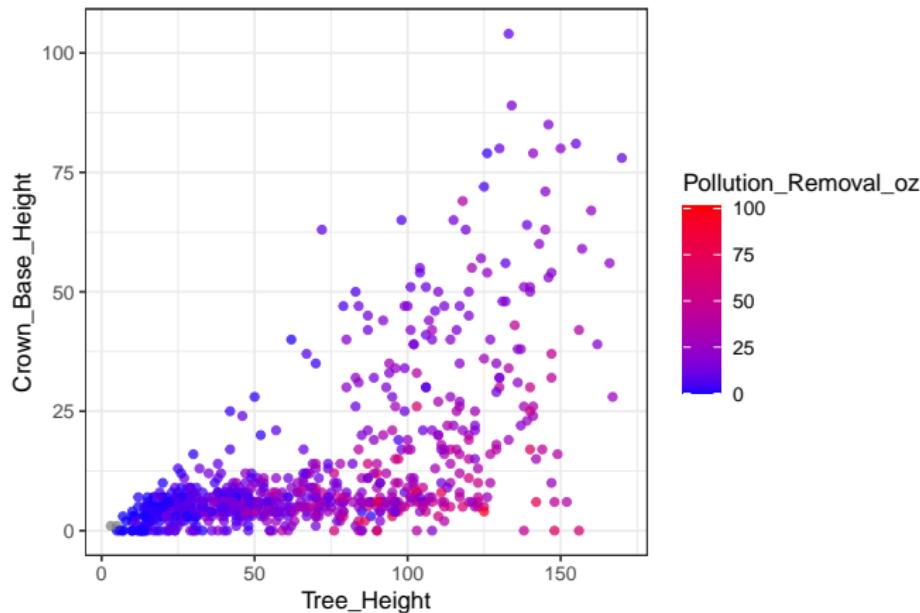
We use a subset of the pdxTrees dataset from the pdxTrees repo (maintained by K. McConville, I. Caldwell, and N. Horton)

Trees on Trees

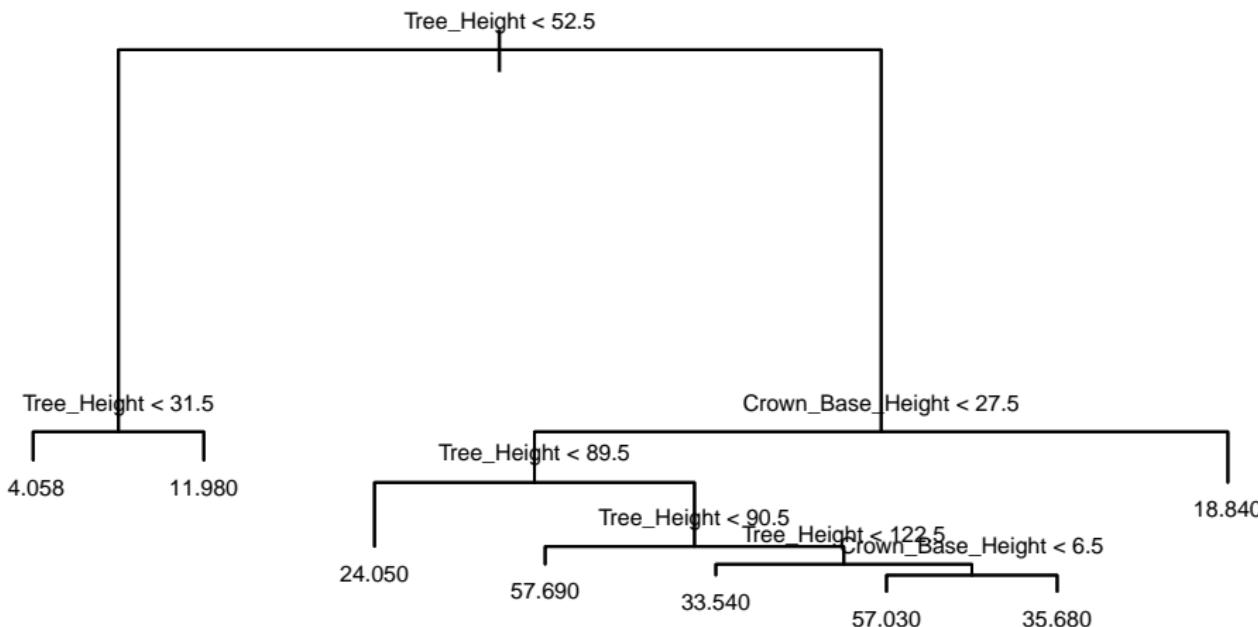
We use a subset of the pdxTrees dataset from the pdxTrees repo (maintained by K. McConville, I. Caldwell, and N. Horton)

```
## Rows: 1,000
## Columns: 10
## $ Species          <fct> PSME, CAJA, QUMU, CADE, PSME, CPSP, PRAV, PSME...
## $ Condition        <fct> Fair, Fair, Fair, Fair, Fair, Poor, Fair...
## $ Tree_Height      <int> 102, 23, 18, 78, 123, 85, 11, 145, 16, 72, 88, ...
## $ Crown_Width_NS   <int> 52, 36, 6, 17, 52, 36, 9, 36, 10, 86, 25, 12, ...
## $ Crown_Width_EW   <int> 43, 40, 6, 18, 38, 52, 11, 35, 10, 86, 10, 16, ...
## $ Crown_Base_Height <int> 63, 5, 5, 6, 13, 5, 6, 9, 5, 8, 6, 4, 4, 3, 2, ...
## $ Structural_Value <dbl> 6694.04, 2444.75, 71.28, 4162.43, 6159.02, 113...
## $ Carbon_Storage_lb <dbl> 1992.9, 917.5, 5.3, 1428.7, 1901.4, 11071.6, 2...
## $ Stormwater_ft    <dbl> 78.9, 43.9, 1.0, 19.8, 117.6, 52.0, 4.1, 80.1, ...
## $ Pollution_Removal_oz <dbl> 21.2, 11.8, 0.3, 5.3, 31.6, 14.0, 1.1, 21.5, 1...
```

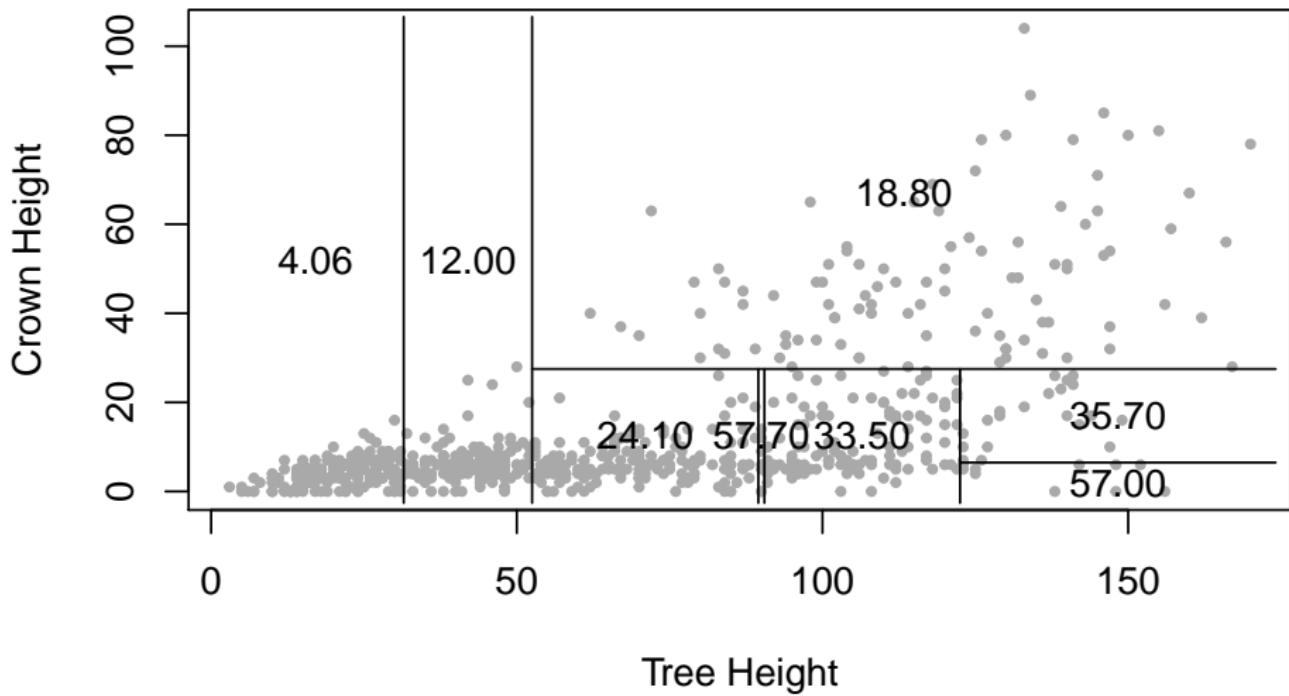
Pollution Removal



Regression Tree



Another Visualization



Tree Accuracy

Let's check MSE on a test set:

$$\text{MSE} = \frac{1}{n} \sum_{i=1}^n (y_i - \hat{y}_i)^2$$

```
##     Tree_MSE
## 1 169.0145
```

Tree Accuracy

Let's check MSE on a test set:

$$\text{MSE} = \frac{1}{n} \sum_{i=1}^n (y_i - \hat{y}_i)^2$$

```
##     Tree_MSE  
## 1 169.0145
```

And compared to the linear model:

```
##     lm_MSE  
## 1 412.3758
```

Tree Accuracy

Let's check MSE on a test set:

$$\text{MSE} = \frac{1}{n} \sum_{i=1}^n (y_i - \hat{y}_i)^2$$

```
## Tree_MSE  
## 1 169.0145
```

And compared to the linear model:

```
## lm_MSE  
## 1 412.3758
```

Why did the tree model outperform the linear model?

Tree Accuracy

Let's check MSE on a test set:

$$\text{MSE} = \frac{1}{n} \sum_{i=1}^n (y_i - \hat{y}_i)^2$$

```
## Tree_MSE  
## 1 169.0145
```

And compared to the linear model:

```
## lm_MSE  
## 1 412.3758
```

Why did the tree model outperform the linear model?

Nevertheless, what are some downsides to the tree model?

The general tree 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 squared error:

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

The general tree 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 squared error:

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

- ② Repeat step one on both S_1 and S_2 .

The general tree 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 squared error:

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

- ② Repeat step one on both S_1 and S_2 .
- ③ Repeat on the new regions.

The general tree 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 squared error:

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

- ② Repeat step one on both S_1 and S_2 .
- ③ Repeat on the new regions.
- ④ . . .

The general tree 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 squared error:

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

- ② Repeat step one on both S_1 and S_2 .
- ③ Repeat on the new regions.
- ④ ...
- ⑤ Stop?

The general tree 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 squared error:

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

- ② Repeat step one on both S_1 and S_2 .
- ③ Repeat on the new regions.
- ④ ...
- ⑤ Stop?

How do we decide when to abort algorithm?

The general tree 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 squared error:

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

- ② Repeat step one on both S_1 and S_2 .
- ③ Repeat on the new regions.
- ④ ...
- ⑤ Stop?

How do we decide when to abort algorithm?

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

Subtrees

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

Subtrees

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.

Subtrees

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 test RSS by exhaustively searching all subtrees for the best performing model.

Subtrees

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 test RSS by exhaustively searching all subtrees for the best performing model.

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

Subtrees

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 test 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

Pruning Algorithm

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

Pruning Algorithm

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.

Pruning Algorithm

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 .

Pruning Algorithm

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

$$\text{RSS} + \alpha|T|$$

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

Pruning Algorithm

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

$$\text{RSS} + \alpha|T|$$

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.

Pruning Algorithm

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

$$\text{RSS} + \alpha|T|$$

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.

Pruning Algorithm

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

$$\text{RSS} + \alpha|T|$$

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

Pruning Algorithm

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

$$\text{RSS} + \alpha|T|$$

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.

Pruning Algorithm

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

$$\text{RSS} + \alpha|T|$$

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.

Pruning Algorithm

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

$$\text{RSS} + \alpha|T|$$

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

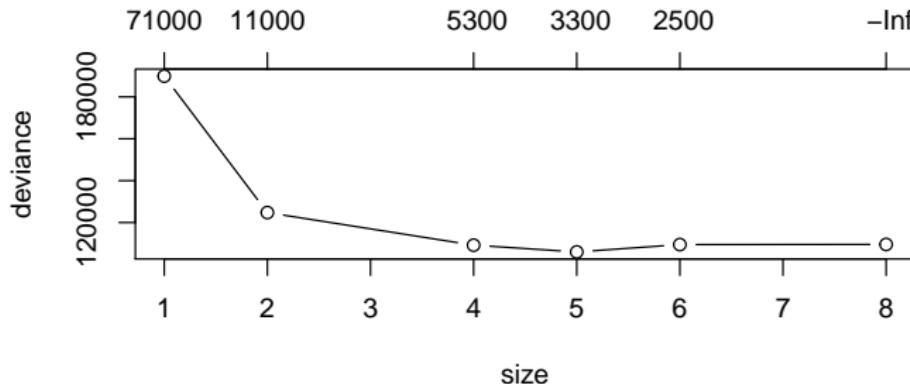
- That is, α penalizes a tree based on its number of terminal nodes.
- As α increases from 0 (i.e. the full tree), branches get pruned in a predictable way, making for relatively quick computation.
- We can find the optimal value of α using cross-validation

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

- ① Choose the tree with smallest MSE.
- ② Choose the *smallest* tree with MSE within 1 standard deviation of smallest MSE

Pruning Example

How does MSE vary as tree size changes?

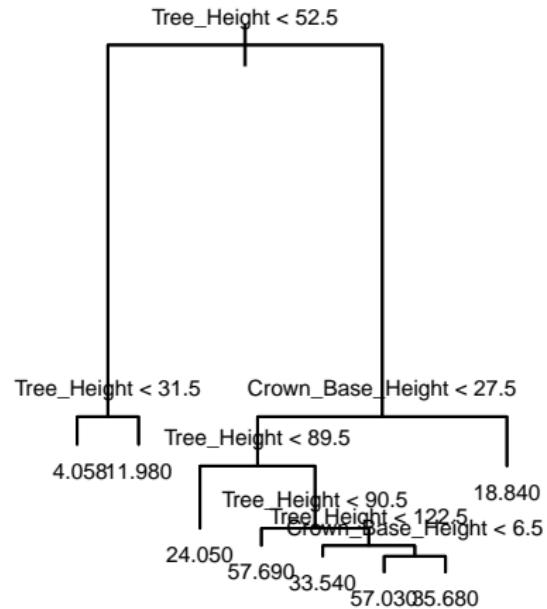
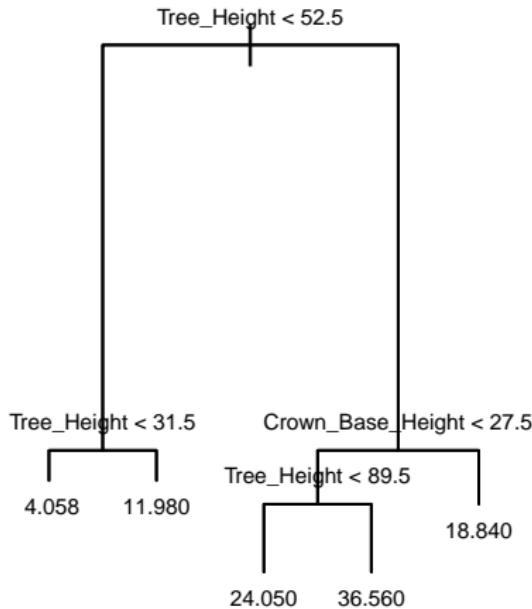


What are the test MSEs for the full tree and the subtree with 5 terminal nodes?

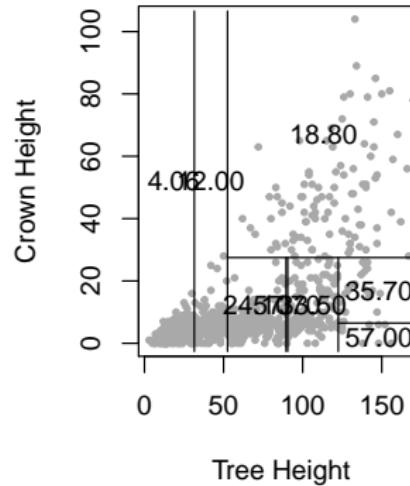
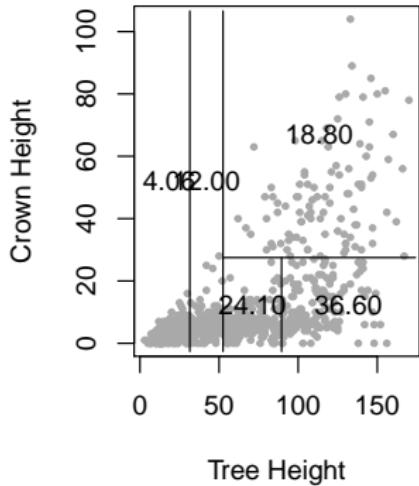
```
## Full_Tree_MSE
## 1       169.0145

## small_Tree_MSE
## 1       152.5175
```

Comparison



Comparison 2



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 its plots are ugly. ISLR uses `tree`.

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 its plots are ugly. ISLR uses `tree`.
- The `rpart` package is newer, computationally faster, and has more options. It also can be combined with the `partykit` and `ggparty` packages for **much** nicer plots. Applied Predictive Modeling uses `rpart` along with `caret` for cv.

Trees using tree

To fit a tree:

```
library(tree)
tree_model<-tree(Pollution_Removal_oz ~ ., data = small_pdxTrees)
```

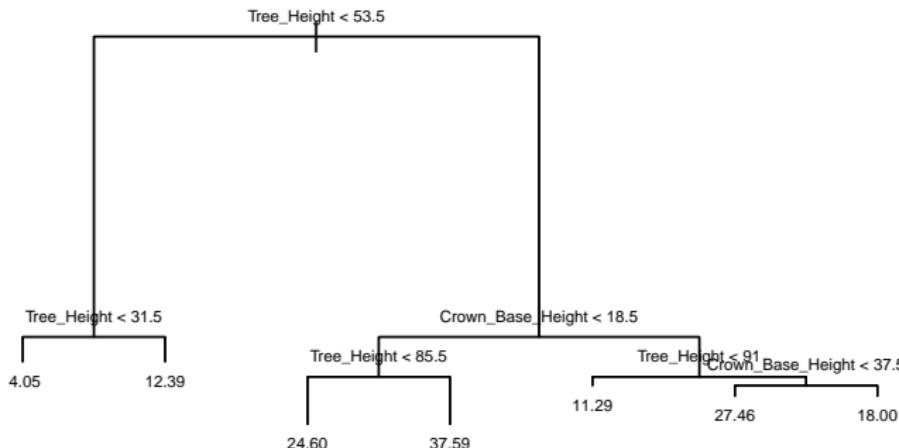
Trees using tree

To fit a tree:

```
library(tree)
tree_model<-tree(Pollution_Removal_oz ~ ., data = small_pdxTrees)
```

To view:

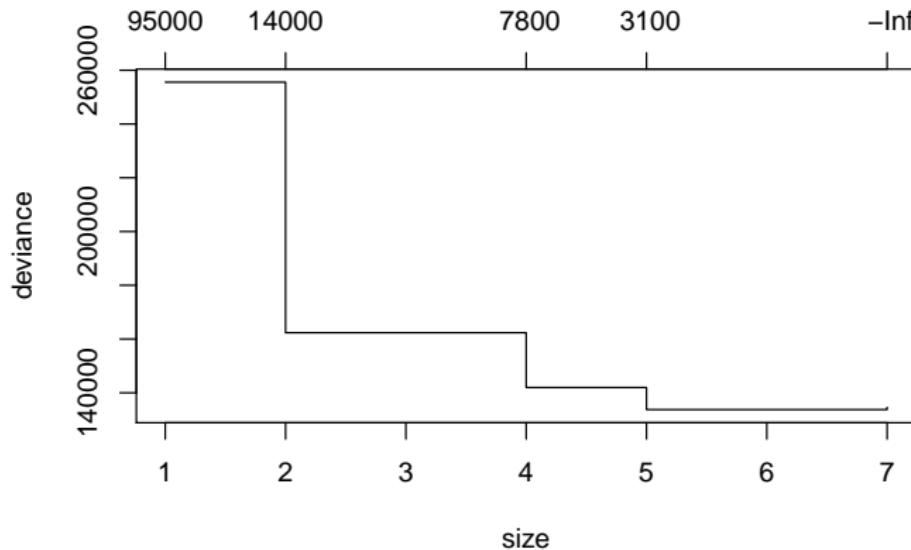
```
plot(tree_model)
text(tree_model, pretty = 0, cex = .5)
```



Trees in R via tree cont'd

To perform cost-complexity pruning:

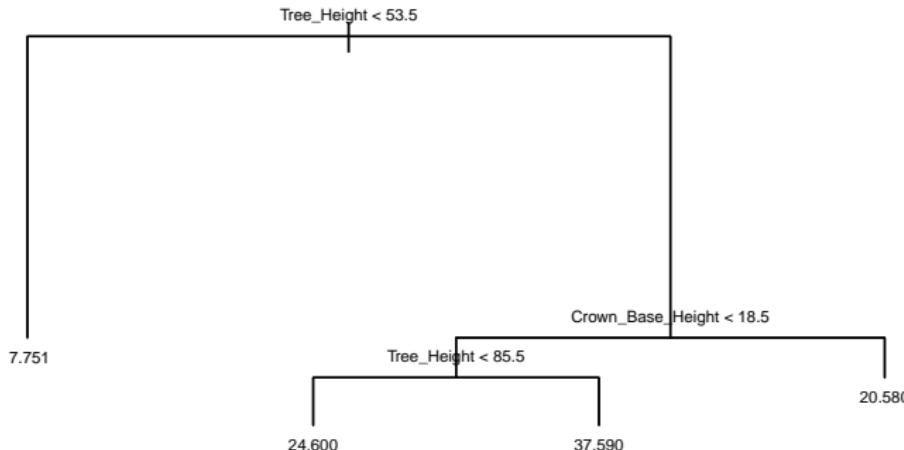
```
tree_model_cv<-cv.tree(tree_model)  
plot(tree_model_cv)
```



Trees in R via `tree` cont'd

And to get a pruned tree:

```
pruned_tree<-prune.tree(tree_model, best = 4)
plot(pruned_tree)
text(pruned_tree, pretty = 0, cex = .5)
```



Section 2

Classification Trees

Trees for Classification Problems

Can we predict the winner of a presidential election based on demographics, state polling, economic conditions, and other features?

Trees for Classification Problems

Can we predict the winner of a presidential election based on demographics, state polling, economic conditions, and other features?

- No. Too stressful.



Trees for Classification Problems

Can we predict the winner of a presidential election based on demographics, state polling, economic conditions, and other features?

- No. Too stressful.



Trees for Classification Problems

Can we predict the species of a Portland tree based on its crown height and overall height?

Trees for Classification Problems

Can we predict the species of a Portland tree based on its crown height and overall height?

- YES!



Classification Trees

Classification trees are very similar to regression trees, except the terminal nodes predict levels of a categorical variable, rather than values of a quantitative variable

Classification Trees

Classification trees are very similar to regression trees, except the terminal nodes predict levels of a categorical variable, rather than values of a quantitative variable

- But to *grow* a classification tree, we need to make cuts based on a metric other than RSS (why?)

Classification Trees

Classification trees are very similar to regression trees, except the terminal nodes predict levels of a categorical variable, rather than values of a quantitative variable

- But to *grow* a classification tree, we need to make cuts based on a metric other than RSS (why?)

Some options for decision metric:

Classification Trees

Classification trees are very similar to regression trees, except the terminal nodes predict levels of a categorical variable, rather than values of a quantitative variable

- But to *grow* a classification tree, we need to make cuts based on a metric other than RSS (why?)

Some options for decision metric:

- *Classification error rate* (i.e. prop. obs. in region not in most common class)

Classification Trees

Classification trees are very similar to regression trees, except the terminal nodes predict levels of a categorical variable, rather than values of a quantitative variable

- But to *grow* a classification tree, we need to make cuts based on a metric other than RSS (why?)

Some options for decision metric:

- *Classification error rate* (i.e. prop. obs. in region not in most common class)
 - But because of the greedy algorithm used to split trees, CER tends to overfit to noise

Classification Trees

Classification trees are very similar to regression trees, except the terminal nodes predict levels of a categorical variable, rather than values of a quantitative variable

- But to *grow* a classification tree, we need to make cuts based on a metric other than RSS (why?)

Some options for decision metric:

- *Classification error rate* (i.e. prop. obs. in region not in most common class)
 - But because of the greedy algorithm used to split trees, CER tends to overfit to noise
- The *Gini index* as a measure of total variance across all K classes:

$$G = \sum_{i=1}^K \hat{p}_{mk}(1 - \hat{p}_{mk}) \quad \text{where } \hat{p}_{mk} = \text{prop. obs. in region m in class k}$$

Classification Trees

Classification trees are very similar to regression trees, except the terminal nodes predict levels of a categorical variable, rather than values of a quantitative variable

- But to *grow* a classification tree, we need to make cuts based on a metric other than RSS (why?)

Some options for decision metric:

- *Classification error rate* (i.e. prop. obs. in region not in most common class)
 - But because of the greedy algorithm used to split trees, CER tends to overfit to noise
- The *Gini index* as a measure of total variance across all K classes:

$$G = \sum_{i=1}^K \hat{p}_{mk}(1 - \hat{p}_{mk}) \quad \text{where } \hat{p}_{mk} = \text{prop. obs. in region m in class k}$$

- The Gini index is small if all \hat{p}_{mk} are close to 0 or 1.