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Big Data Analytics

Session 6

Decision Trees

Where were we last week

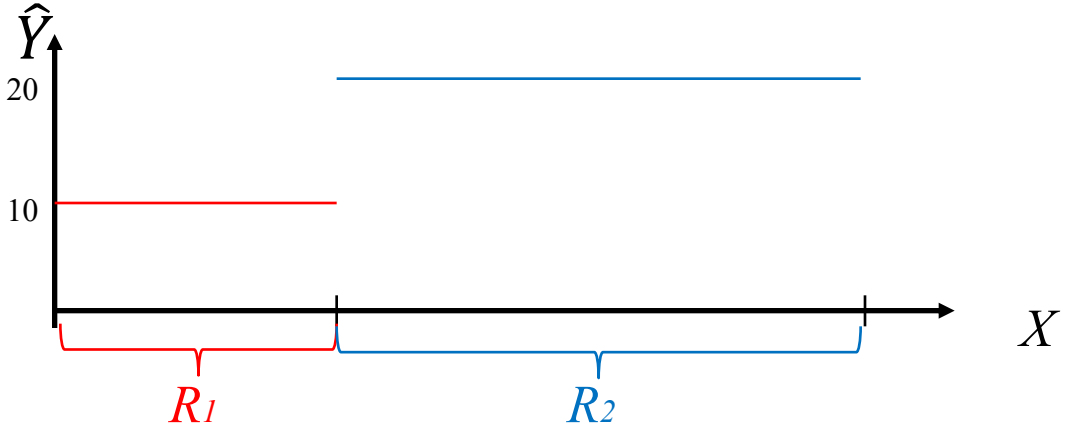
- To assess the model accuracy, the measure of fit is
  - Test MSE for regression
  - Test error rate for classification
- Bias and Variance tradeoff
  - Generally,
    - The more flexible a method is, the less bias it will generally have.
    - The more flexible a method is, the more variance it has.
- Cross Validation
  - Estimate the test MSE/error rate in the absence of the designated test data
  - Compare different models and select the best one
    - Validation set approach, LOOCV and k-fold CV
  - Once the best model is selected
    - Use the whole dataset to train a model
    - Make prediction using this model

Outline

- The Basics of Decision Trees
  - Regression Trees
  - Classification Trees
  - Pruning Trees
  - Trees vs. Linear Models
  - Advantages and Disadvantages of Trees

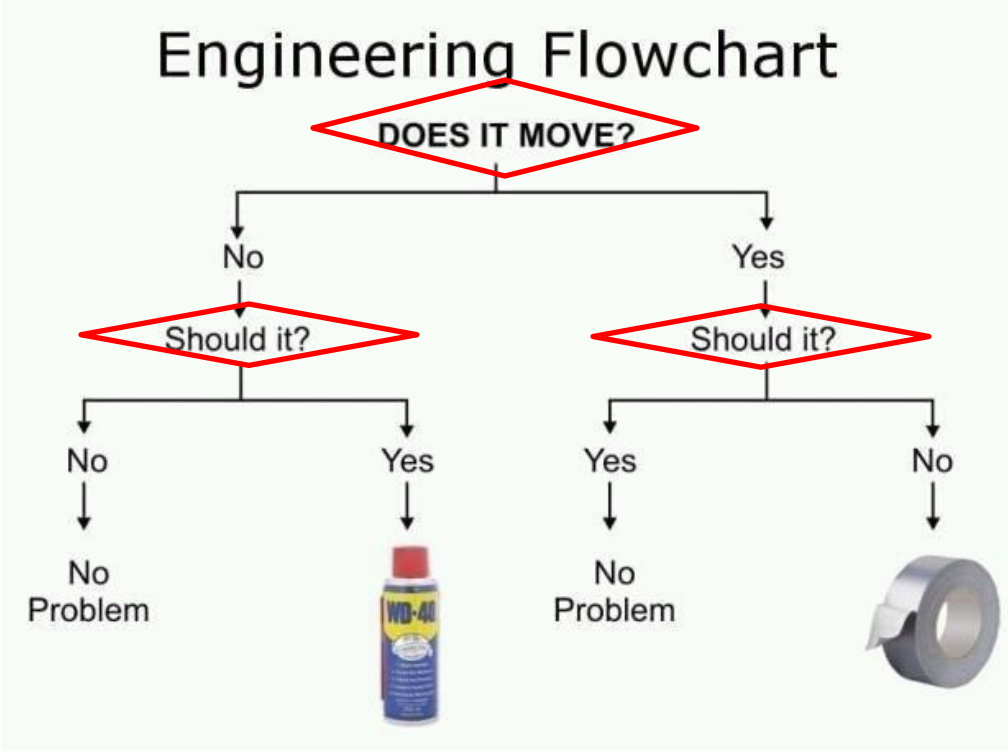
Partitioning Up the Predictor Space

- One way to make predictions in a regression problem is to divide the predictor space (i.e. all the possible values for $X_1,X_2,\ldots,X_p$) into distinct regions, say $R_1,R_2,\ldots,R_k$
  - Suppose for example we have two regions R_1 and R_2 with $\hat{Y}_1 = 10, \hat{Y}_2 = 20$
- Then for every X that falls in a particular region (say R_j) we make the same prediction.
  - Then for any value of X such that $X \in R_1$ we would predict 10, otherwise if $X \in R_2$ we would predict 20.



Decision Tree

- Decision tree
  - A flow-chart-like tree structure
  - Internal node denotes a test on an attribute
  - Branch represents an outcome of the test
  - Leaf nodes represent class labels or class distribution



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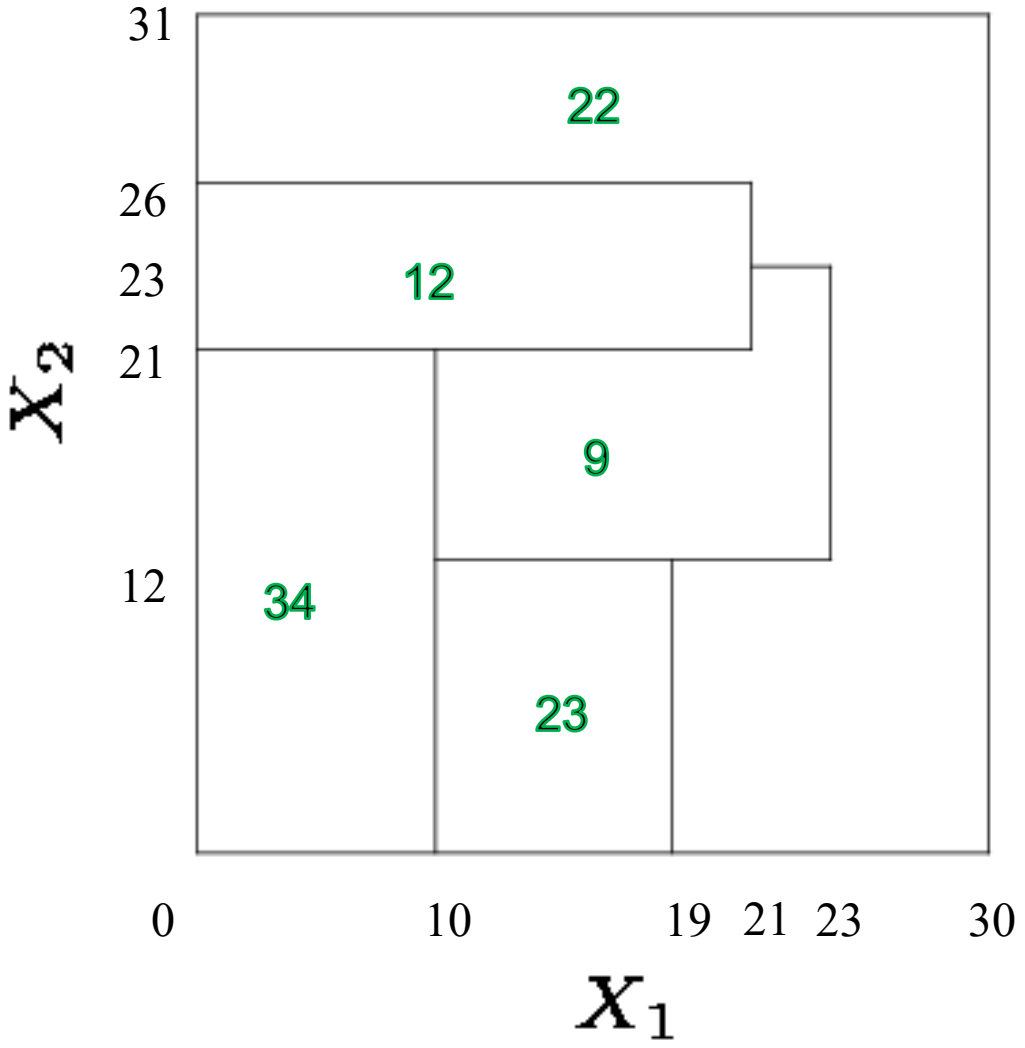
Regression Trees

Predicting a quantitative response

e.g., predicting baseball players' salary

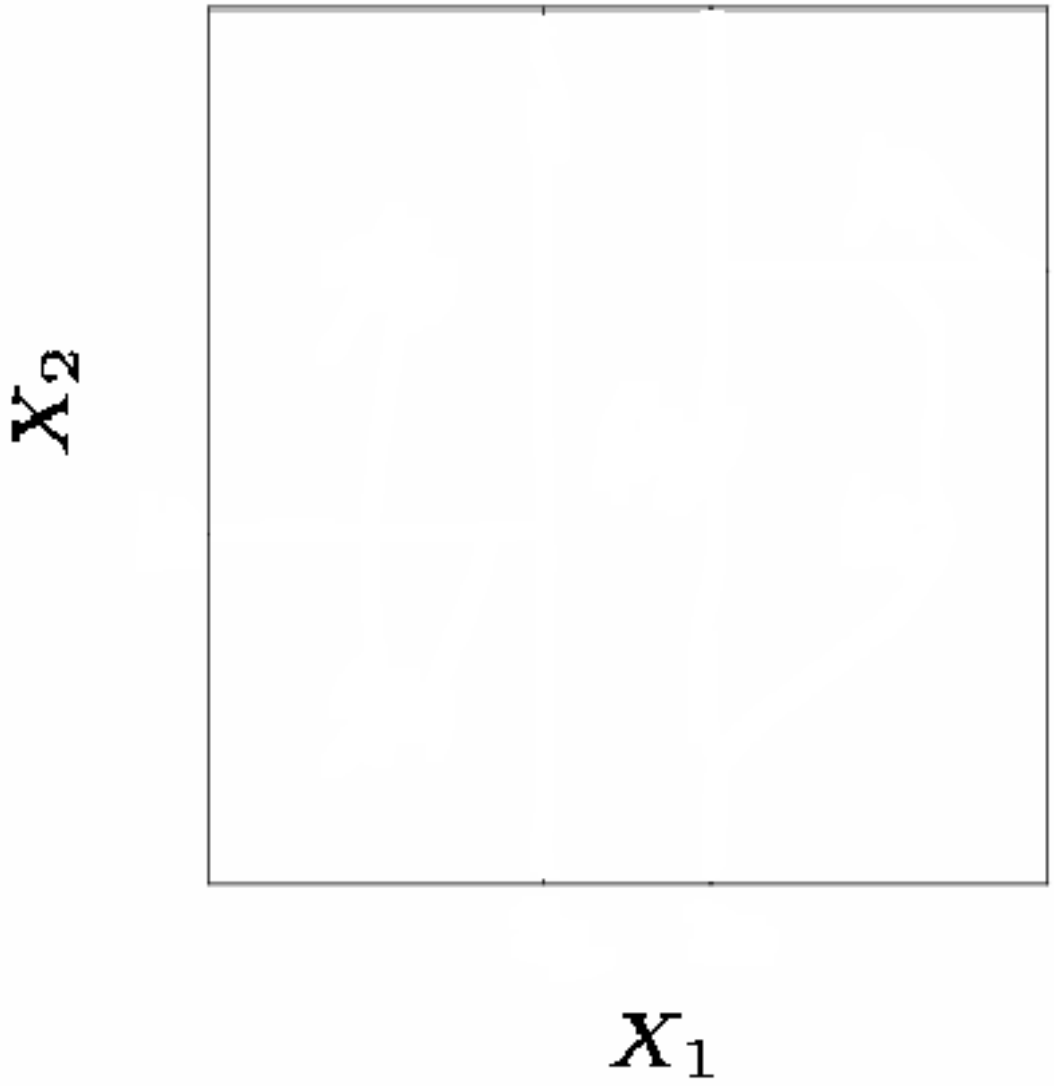
The General View

- Here we have two predictors and five distinct regions
- Depending on which region our new X comes from we would make one of five possible predictions for Y
- Predict Y based on
  - $X_1 = 15, X_2 = 15$
  - $X_1 = 28, X_2 = 24$
  - $X_1 = 5, X_2 = 29$
  - $X_1 = 22, X_2 = 25$



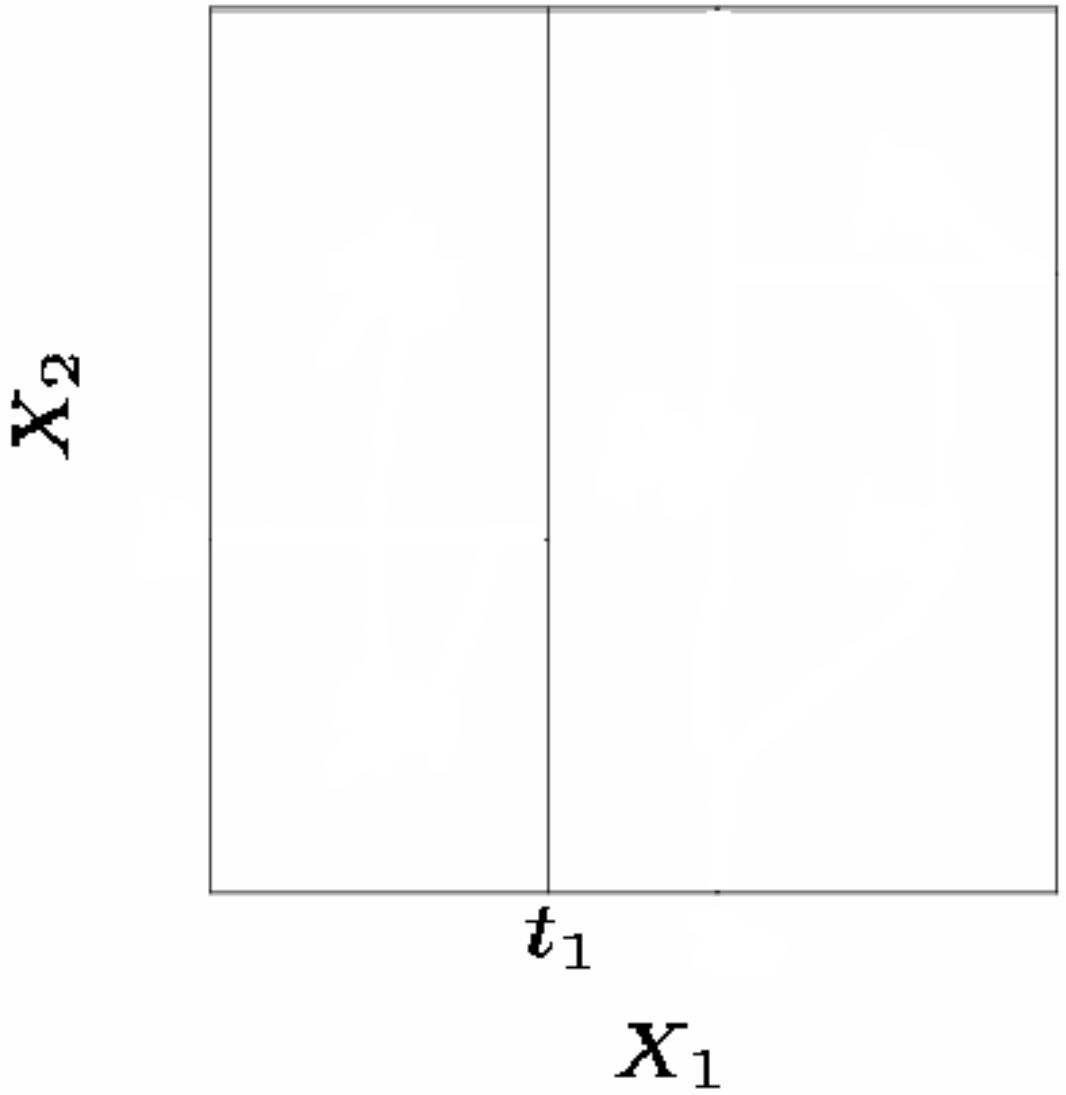
Splitting the X Variables

- Generally we create the partitions by iteratively splitting one of the X variables into two regions



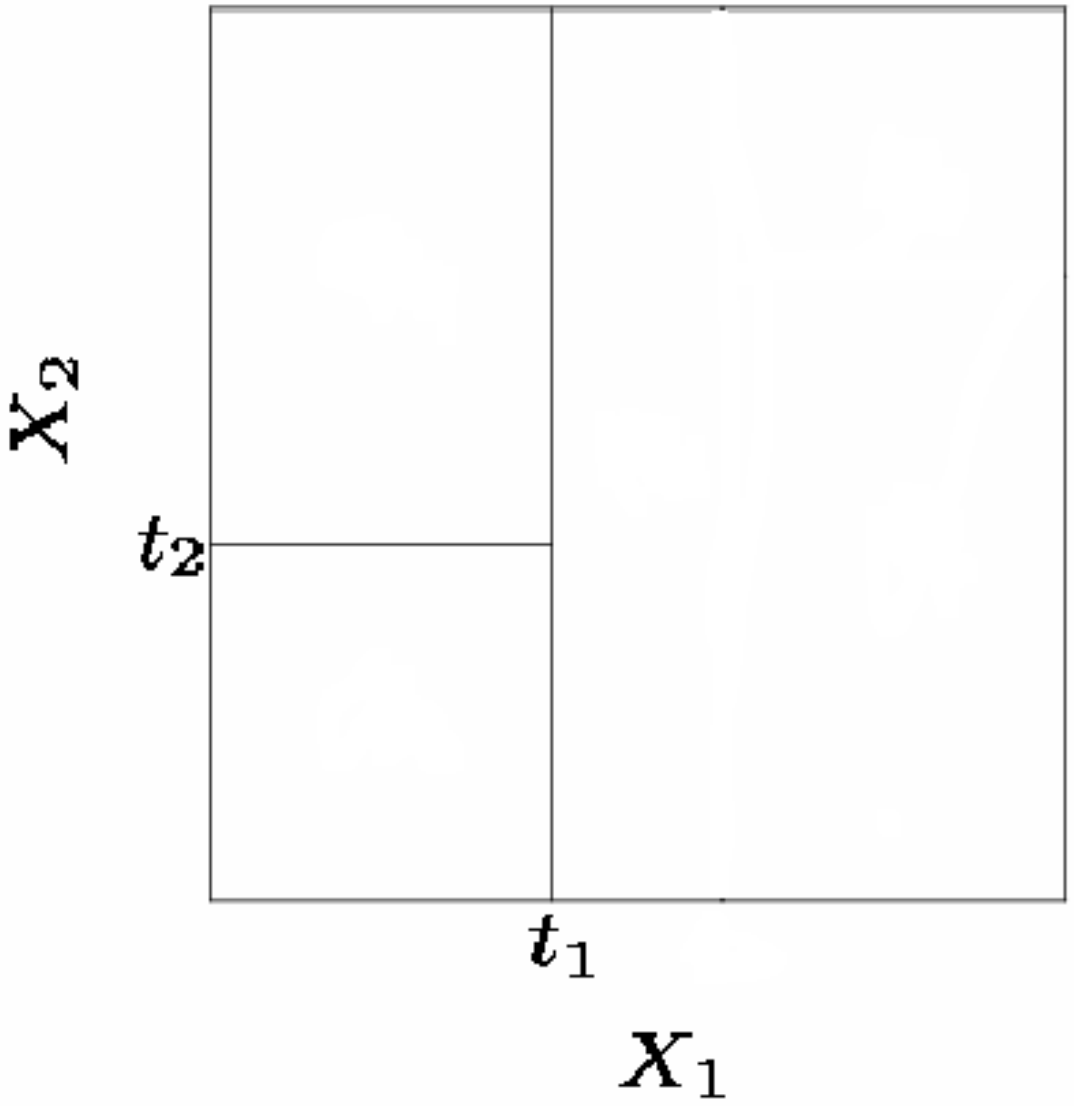
Splitting the X Variable

1. First split on $X_1 = t_1$



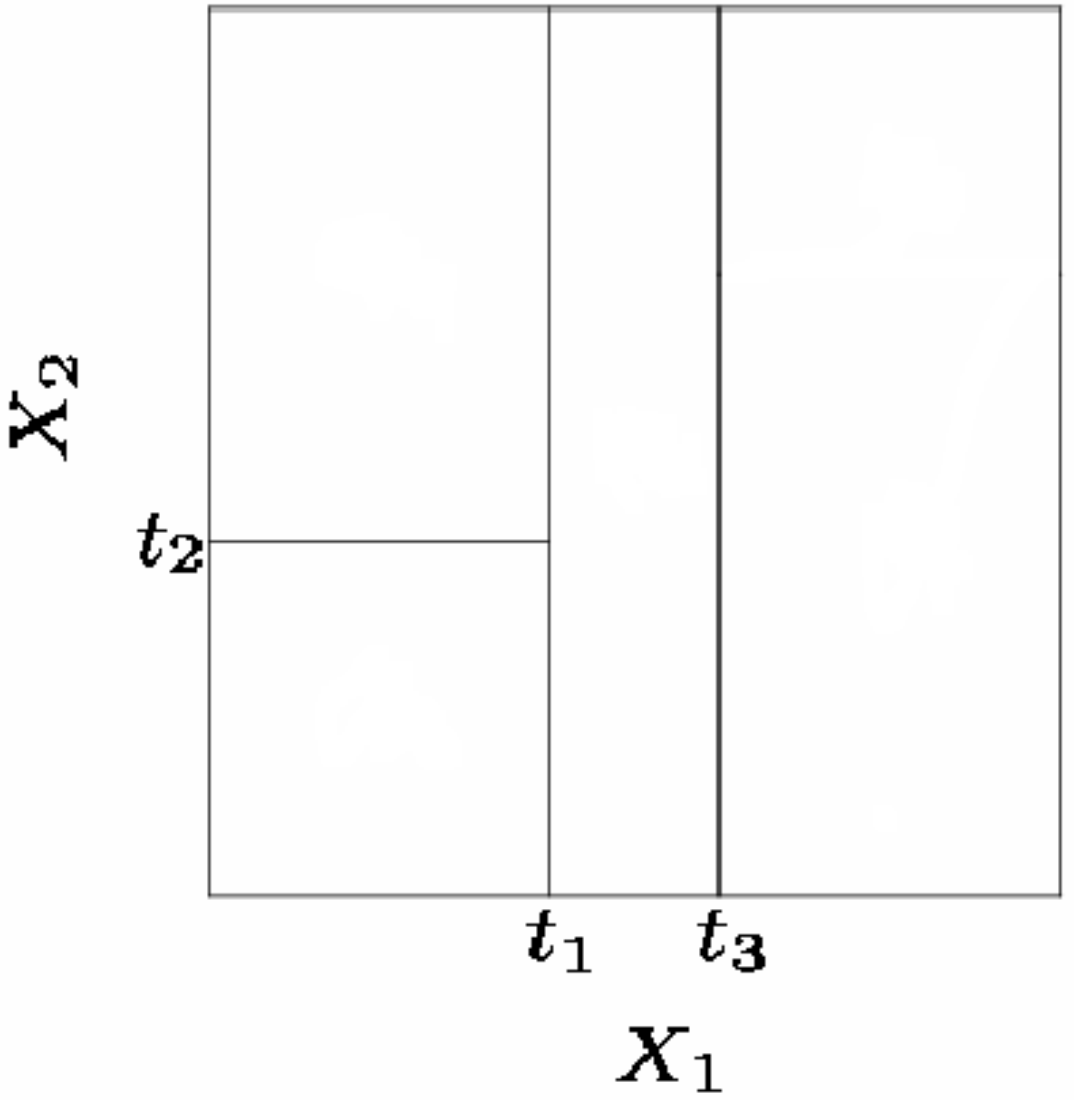
Splitting the X Variable

1. First split on $X_1 = t_1$
2. If $X_1 < t_1$, split on $X_2 = t_2$



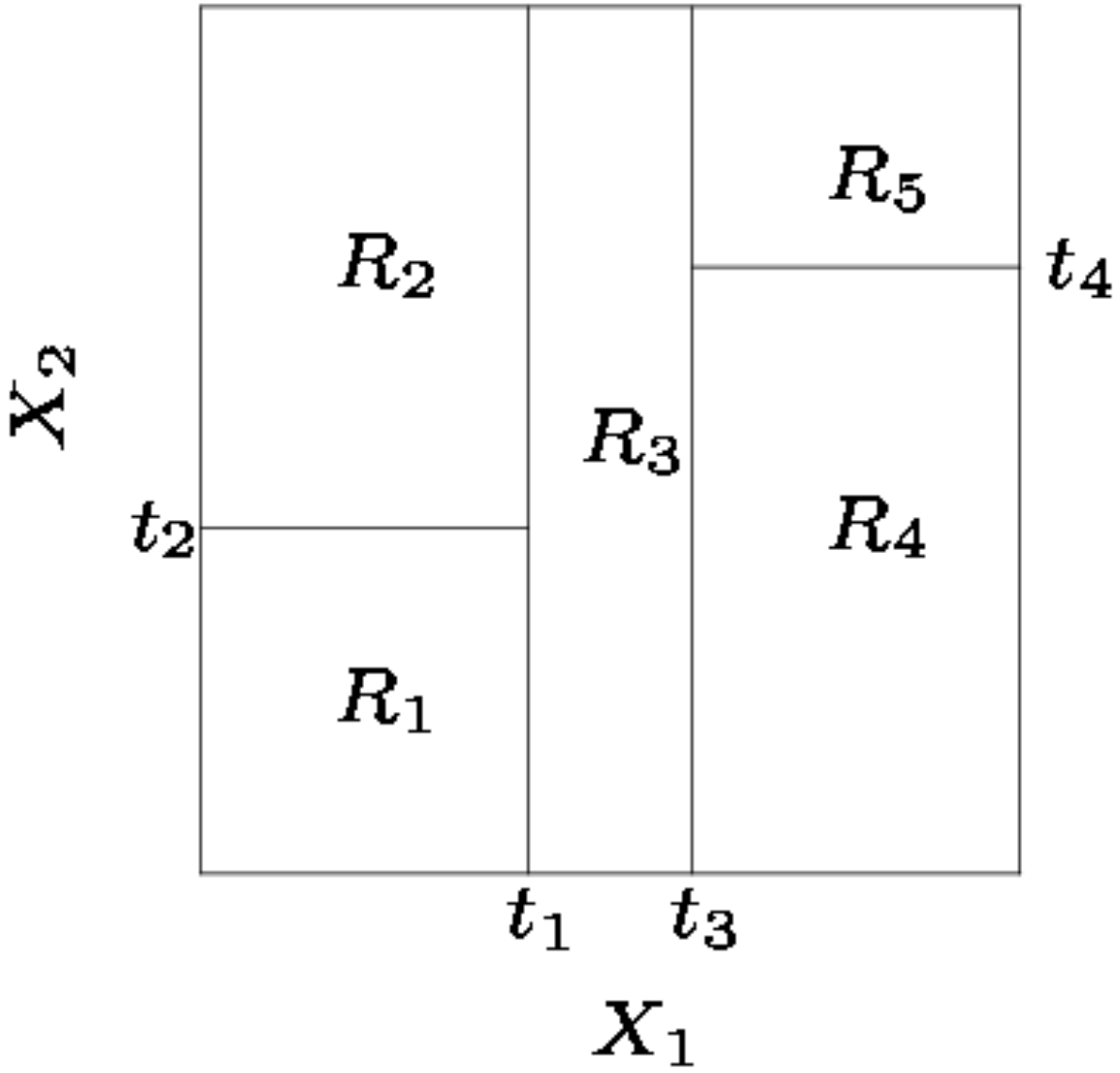
Splitting the X Variable

1. First split on $X_1 = t_1$
2. If $X_1 < t_1$, split on $X_2 = t_2$
3. If $X_1 > t_1$, split on $X_1 = t_3$

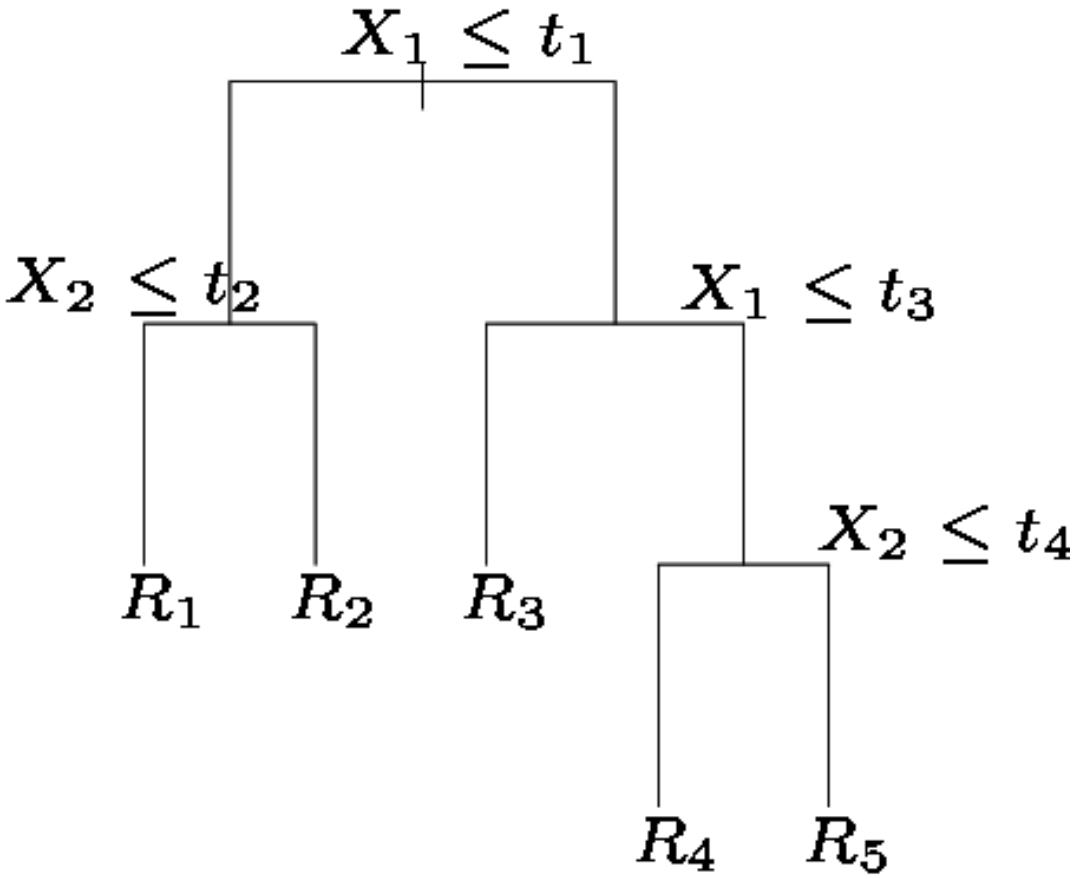


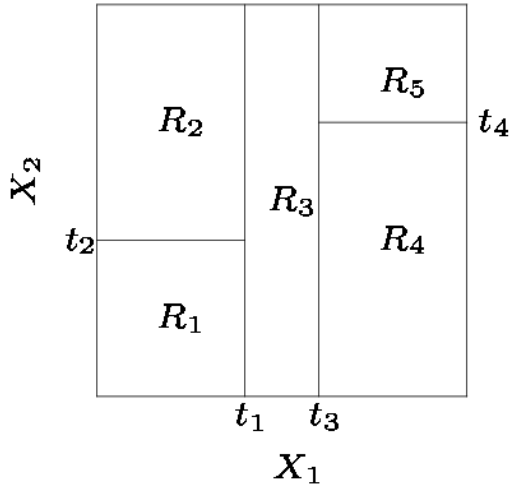
Splitting the X Variable

1. First split on $X_1 = t_1$
2. If $X_1 < t_1$, split on $X_2 = t_2$
3. If $X_1 > t_1$, split on $X_1 = t_3$
4. If $X_1 > t_3$, split on $X_2 = t_4$



Splitting the X Variable





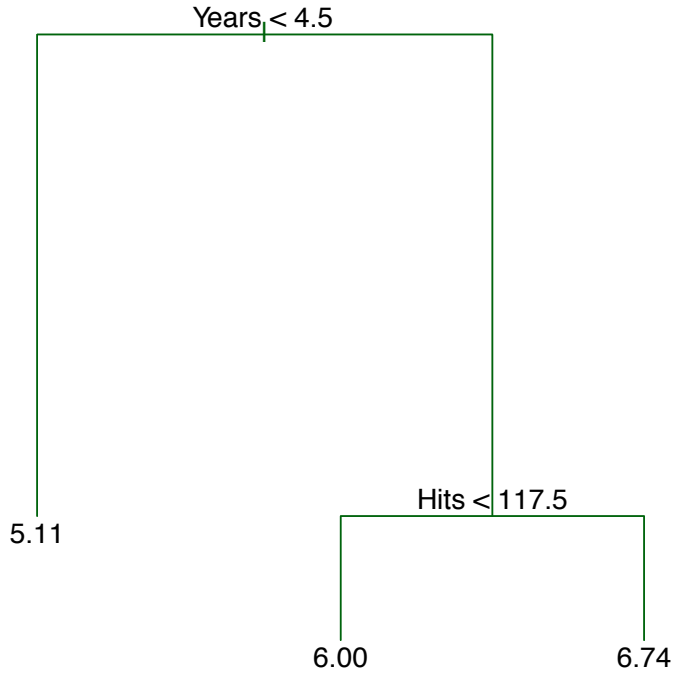
- When we create partitions this way we can always represent them using a tree structure.
- This provides a very simple way to explain the model to a non-expert e.g. your boss!

Example: Baseball Players' Salaries

- To predict baseball player's salaries by regression tree based on
  - Years
  - Hits
- Note that in the dataset, Salary is measured in 1000s. Here, Salary is then log-transformed (Why?)
- The predicted salary for a player who played in the league for more than 4.5 years and had less than 117.5 hits last year is

$$\$1000 \times e^{6.00} = \$402,834$$

Hitters is a dataset in the ISLR



- Can you 1) build a regression tree using Years and Hits and 2) make the prediction for a player with Years = 5 and Hits = 100 using R?

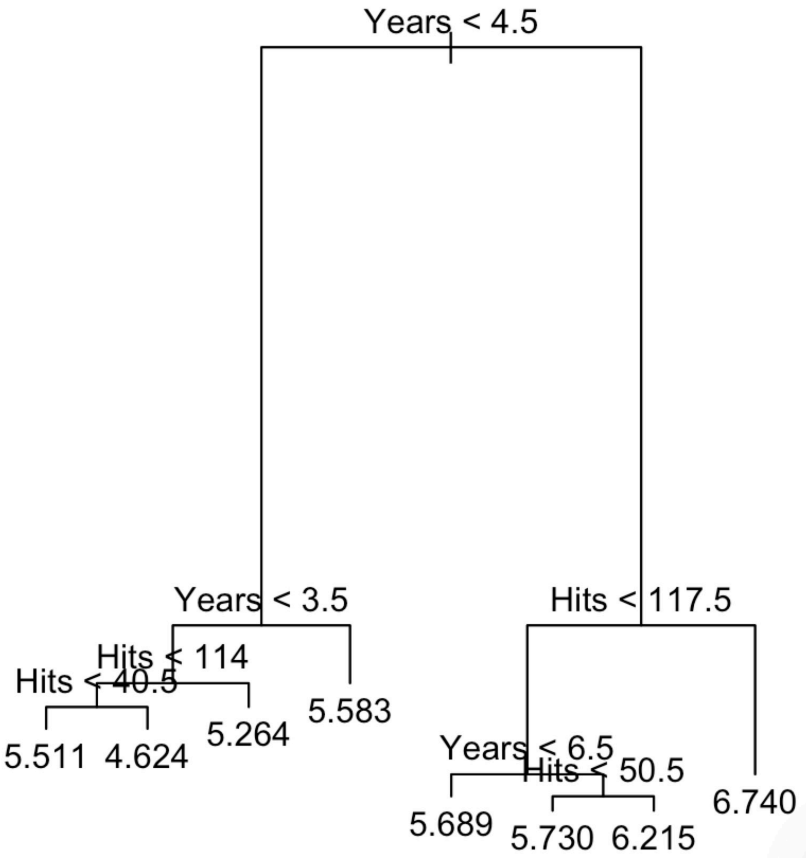
Example: Baseball Players' Salaries

- Step 1: Building the tree:

```
library(tree)
nrow(Hitters)
[1] 322

Hitters <- na.omit(Hitters)   #remove rows with missing observations
nrow(Hitters)
[1] 263

tree.hitters <- tree(log(Hitters$Salary)~Years+Hits, Hitters)
# type in tree.hitters or summary(tree.hitters) to see more details

plot(tree.hitters)                    #Why is this tree different from the one before?
text(tree.hitters,pretty=0)
```

Example: Baseball Players' Salaries

```
> tree.hitters
node), split, n, deviance, yval
      * denotes terminal node

 1) root 263 207.200 5.927
   2) Years < 4.5 90  42.350 5.107
     4) Years < 3.5 62  23.010 4.892
       8) Hits < 114 43  17.150 4.727
        16) Hits < 40.5 5  10.400 5.511 *
        17) Hits > 40.5 38  3.280 4.624 *
       9) Hits > 114 19  2.069 5.264 *
     5) Years > 3.5 28  10.130 5.583 *
   3) Years > 4.5 173  72.710 6.354
     6) Hits < 117.5 90  28.090 5.998
      12) Years < 6.5 26  7.238 5.689 *
      13) Years > 6.5 64  17.350 6.124
        26) Hits < 50.5 12  2.689 5.730 *
        27) Hits > 50.5 52  12.370 6.215 *
     7) Hits > 117.5 83  20.880 6.740 *
```



n: the number of observations in that branch

yval: the overall prediction for the branch

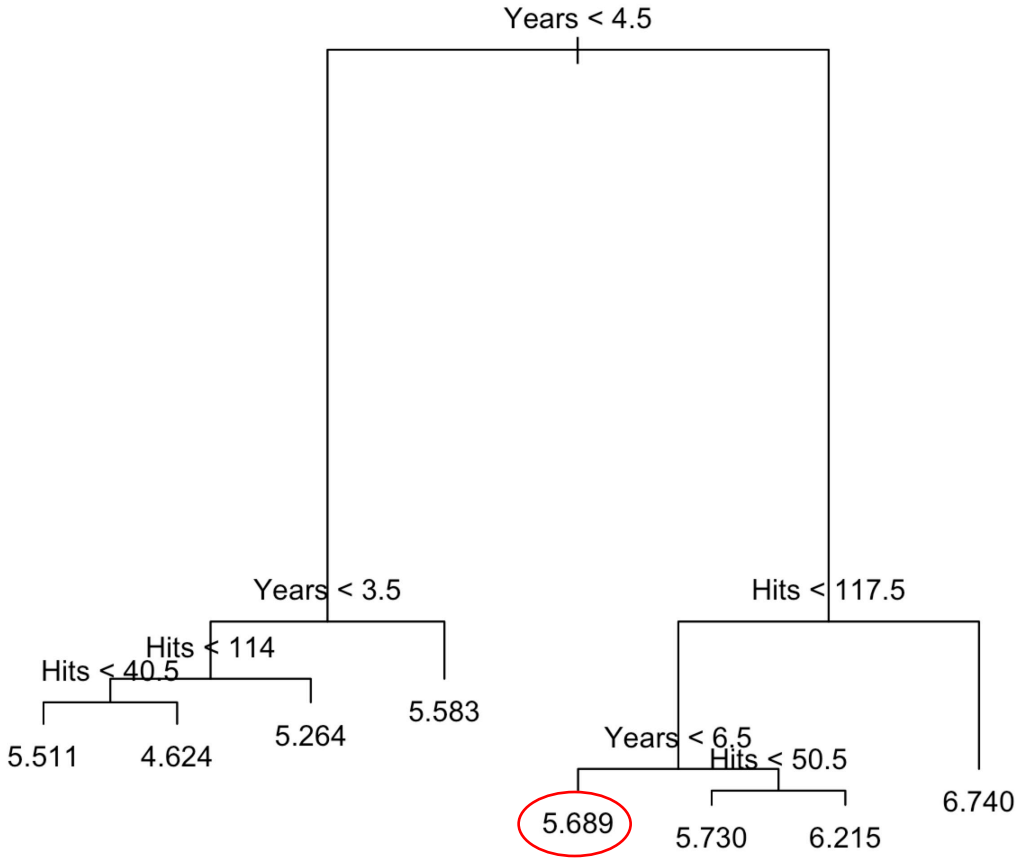
deviance: node residual sums of squares summed over the terminal nodes of the tree

Example: Baseball Players' Salaries

- Step 2: Making predictions

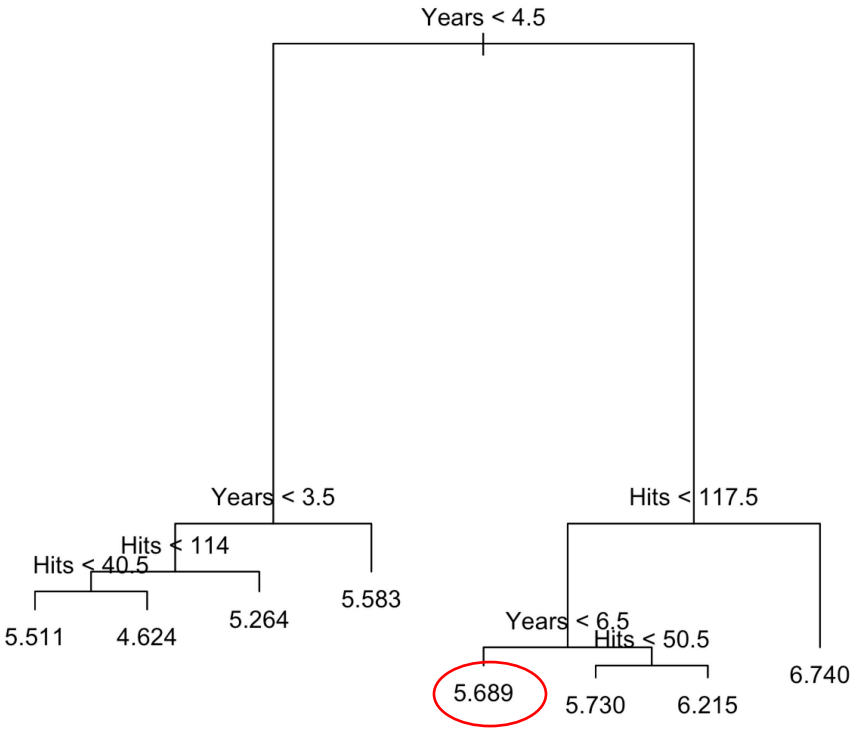
Given Years=5 and Hits=100, what is the prediction?

```
yhat <- predict(tree.hitters, newdata=list("Years"=5, "Hits"=100))
yhat
 1
5.688925
```



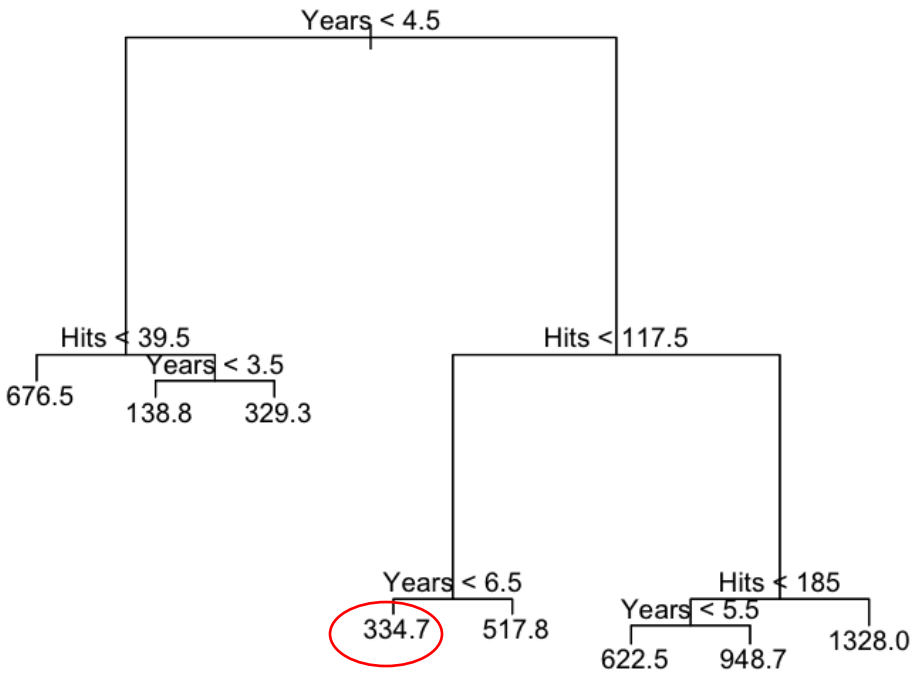
A Comparison

Given Years=5 and Hits=100, what is the prediction?



log-transformed

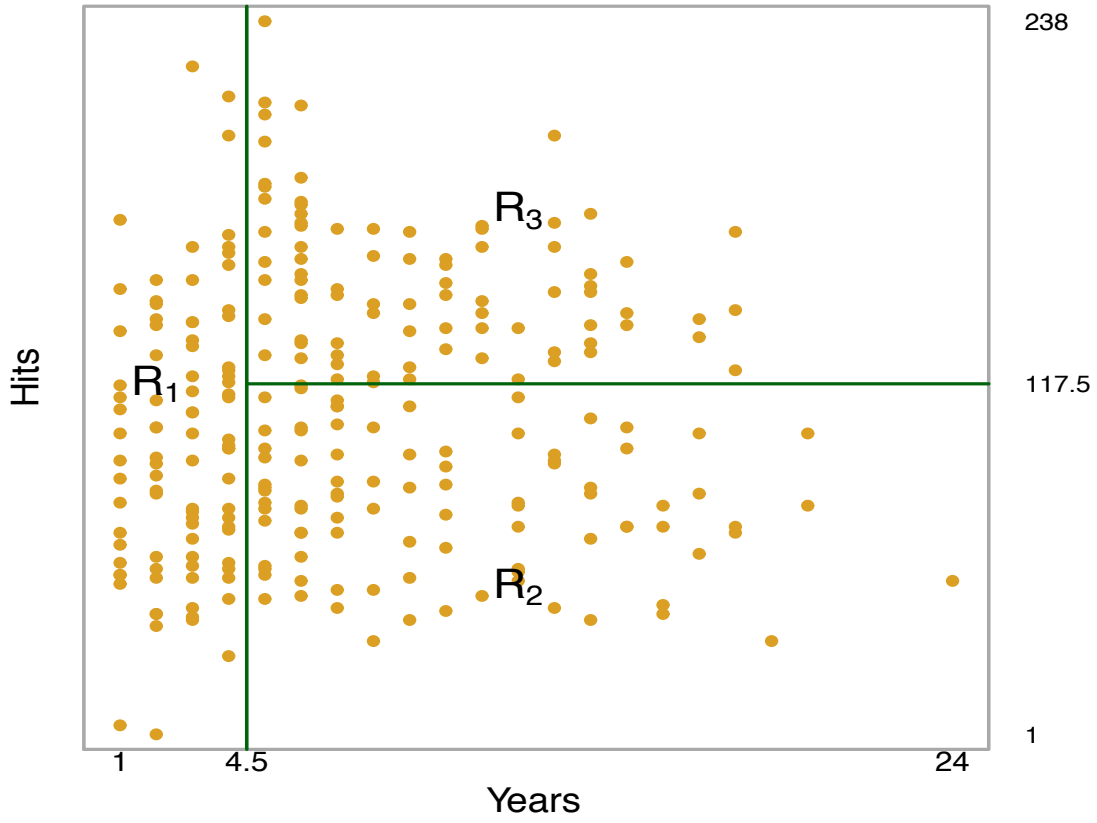
$e^{5.689} = 295.6$



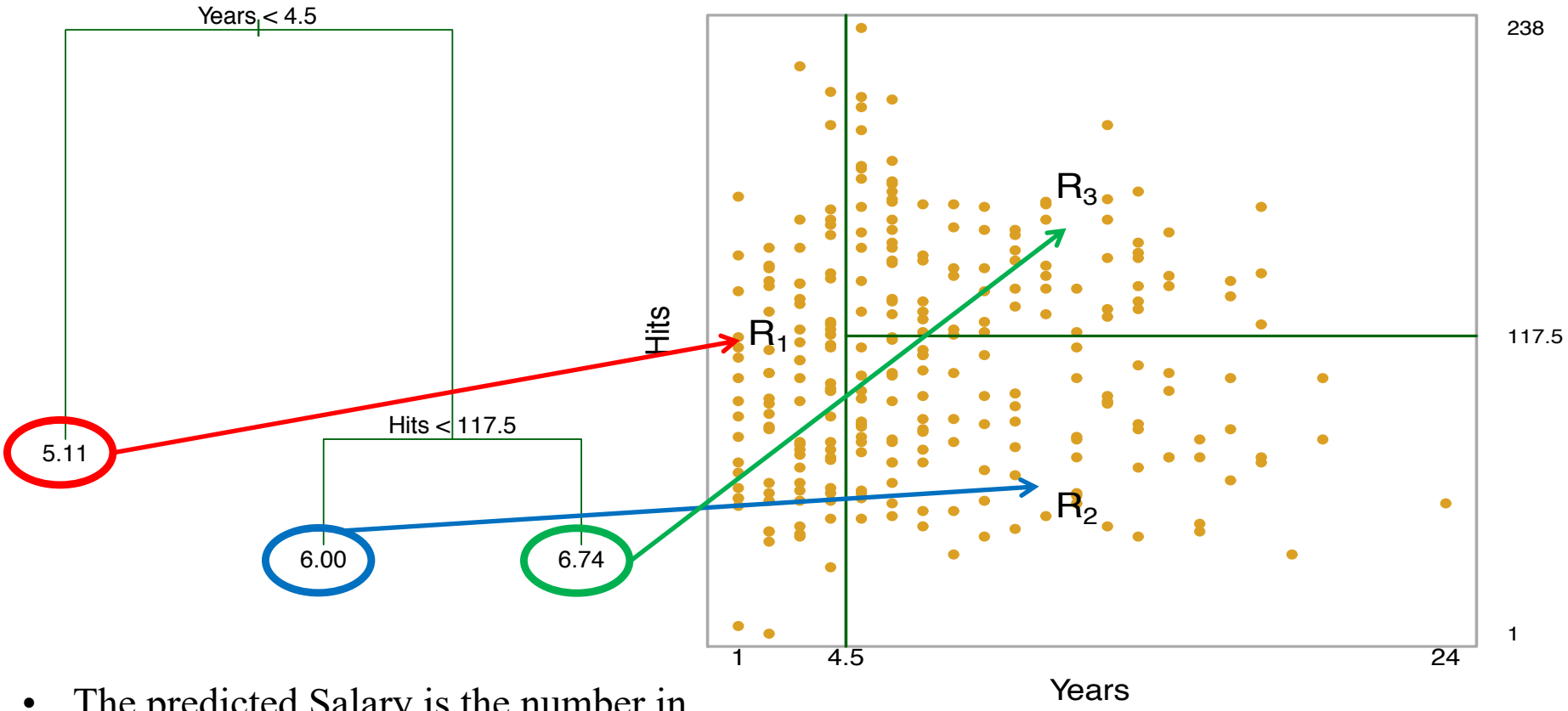
NOT log-transformed

334.7

Another way of visualising the decision tree



Linking two visualisations

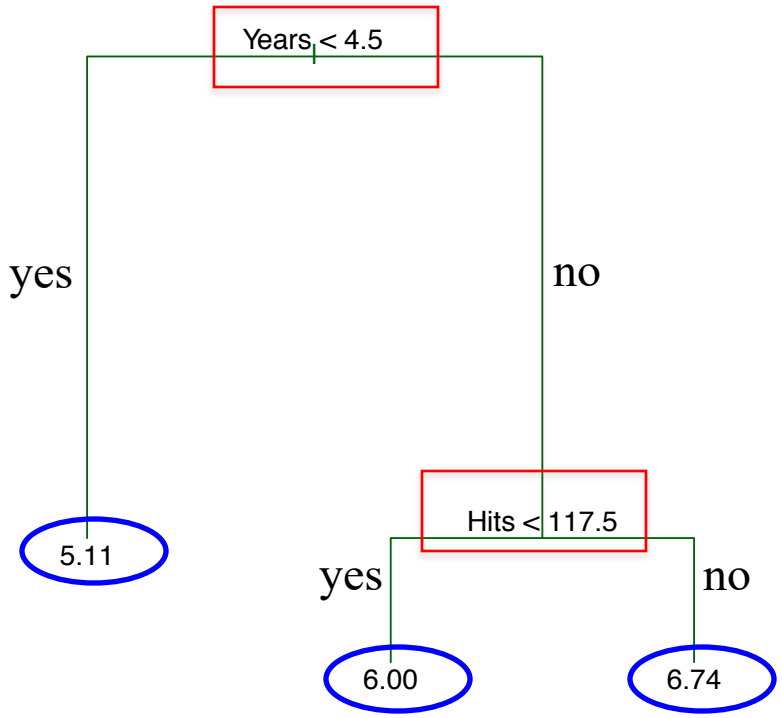


- The predicted Salary is the number in each leaf node.
- It is the <u>mean</u> of the response for the observations that fall there

5.11 is the mean salary in region R_1
6.00 is the mean salary in region R_2
6.74 is the mean salary in region R_3

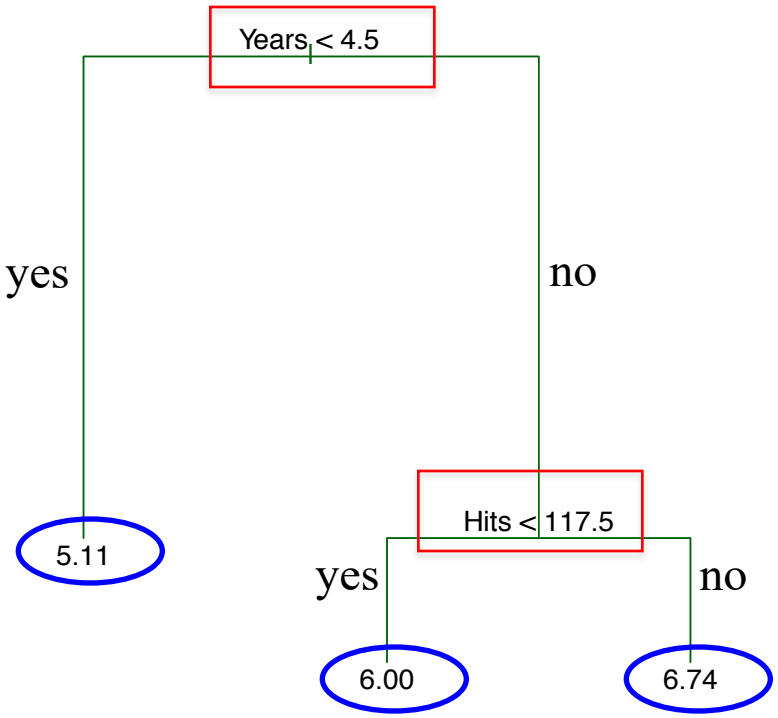
Terminology of Decision Tree

- Terminal nodes (leaves) of the tree
- Internal nodes
- Branches
  - The segments of the trees that connect the nodes
- Upside down



Interpreting the Decision Tree

- `Years` is the most important factor in determining `Salary`
  - Players with less experience tend to earn less
- For less experienced players
  - The number of hits plays little role in the salaries
- For experienced players
  - The more hits being made, the higher salary they tend to earn



Some Natural Questions

Q1. Where to split?

i.e., how do we decide on what regions to use i.e. $R_1, R_2, \ldots, R_k$?

or equivalently, what tree structure should we use?

Q2. What values should we use for $\hat{Y}_1, \hat{Y}_2, \ldots, \hat{Y}_k$?

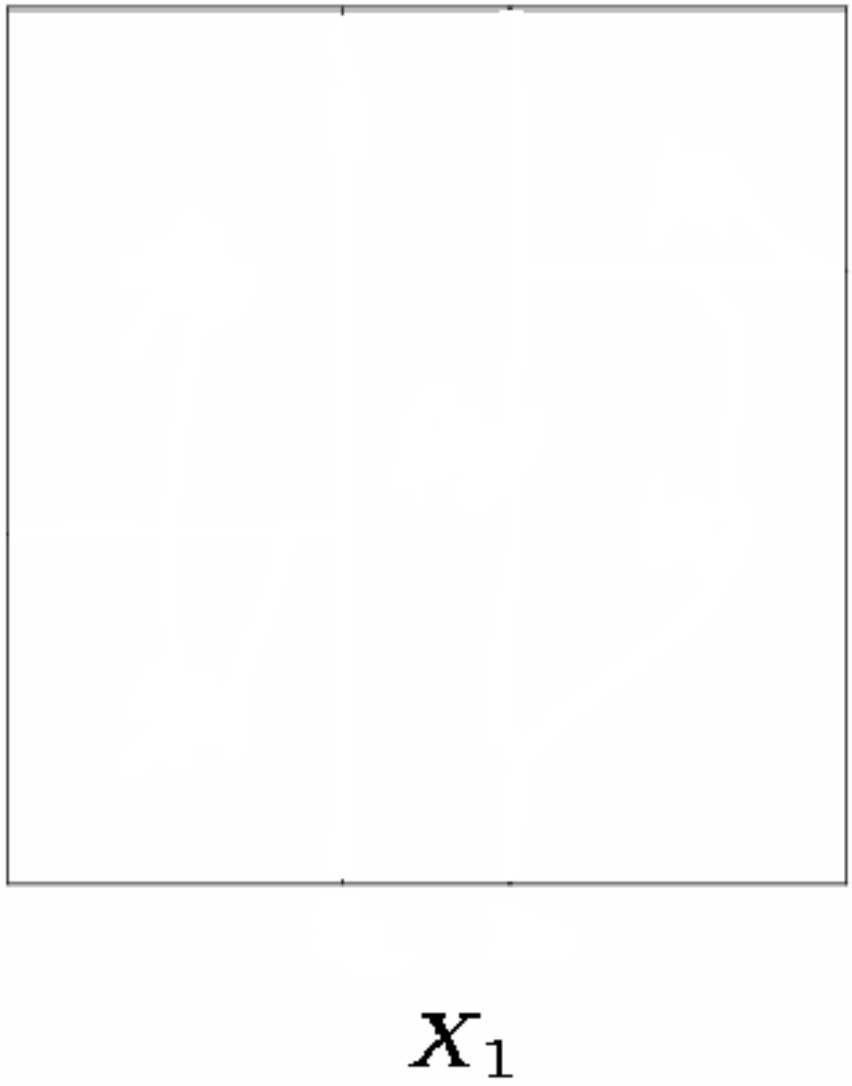
Q2. What values should we use for $\hat{Y}_1, \hat{Y}_2, \ldots, \hat{Y}_k$?

- Simple!

- For region R_j, the best prediction is simply the average of all the responses from our training data that fell in region R_j.

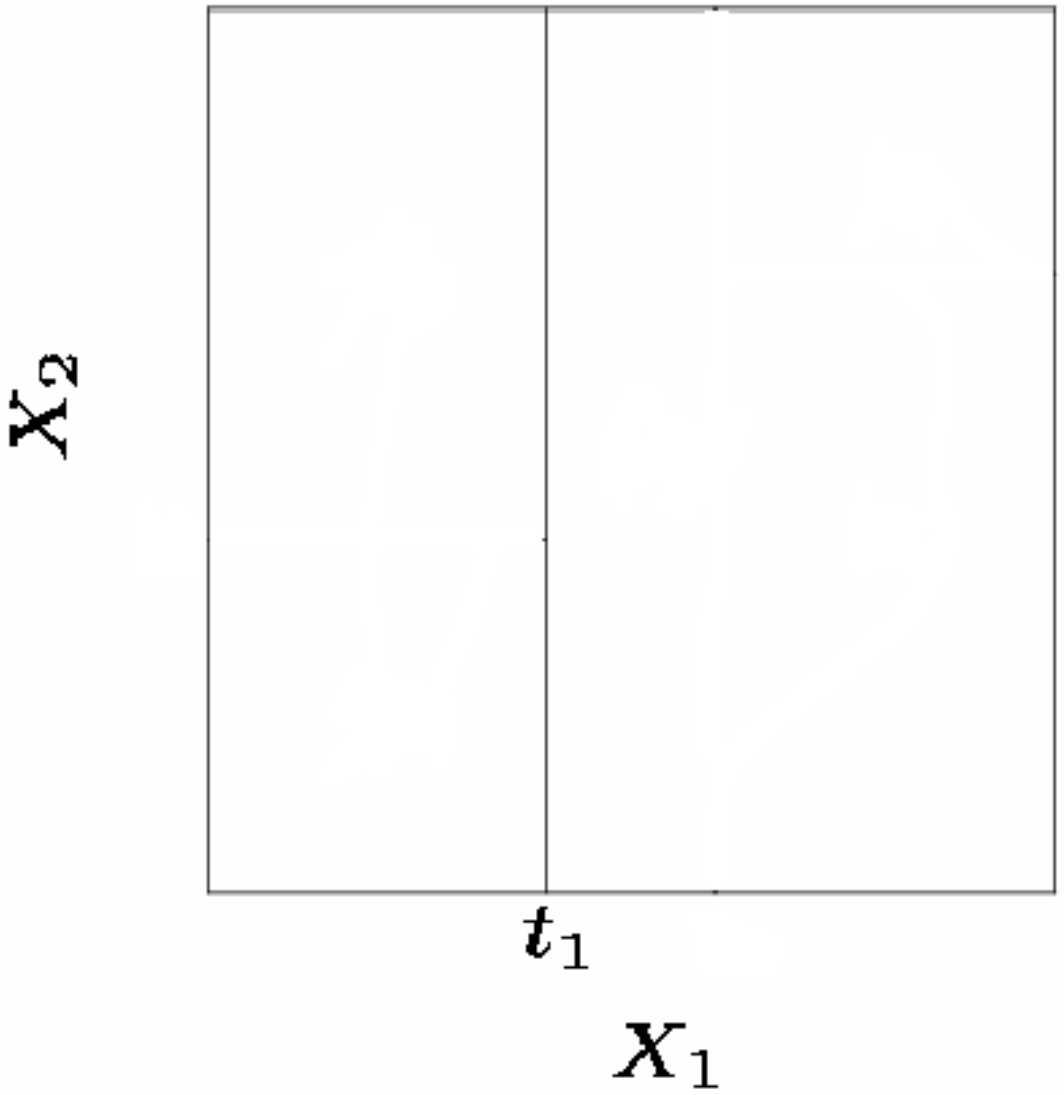
Q1. Where to Split?

- We consider splitting into two regions, $X_j > s$ and $X_j < s$ for all possible values of s and j.
- We then choose the s and j that results in the lowest MSE on the training data.
- X_1: Years
- X_2: Hits



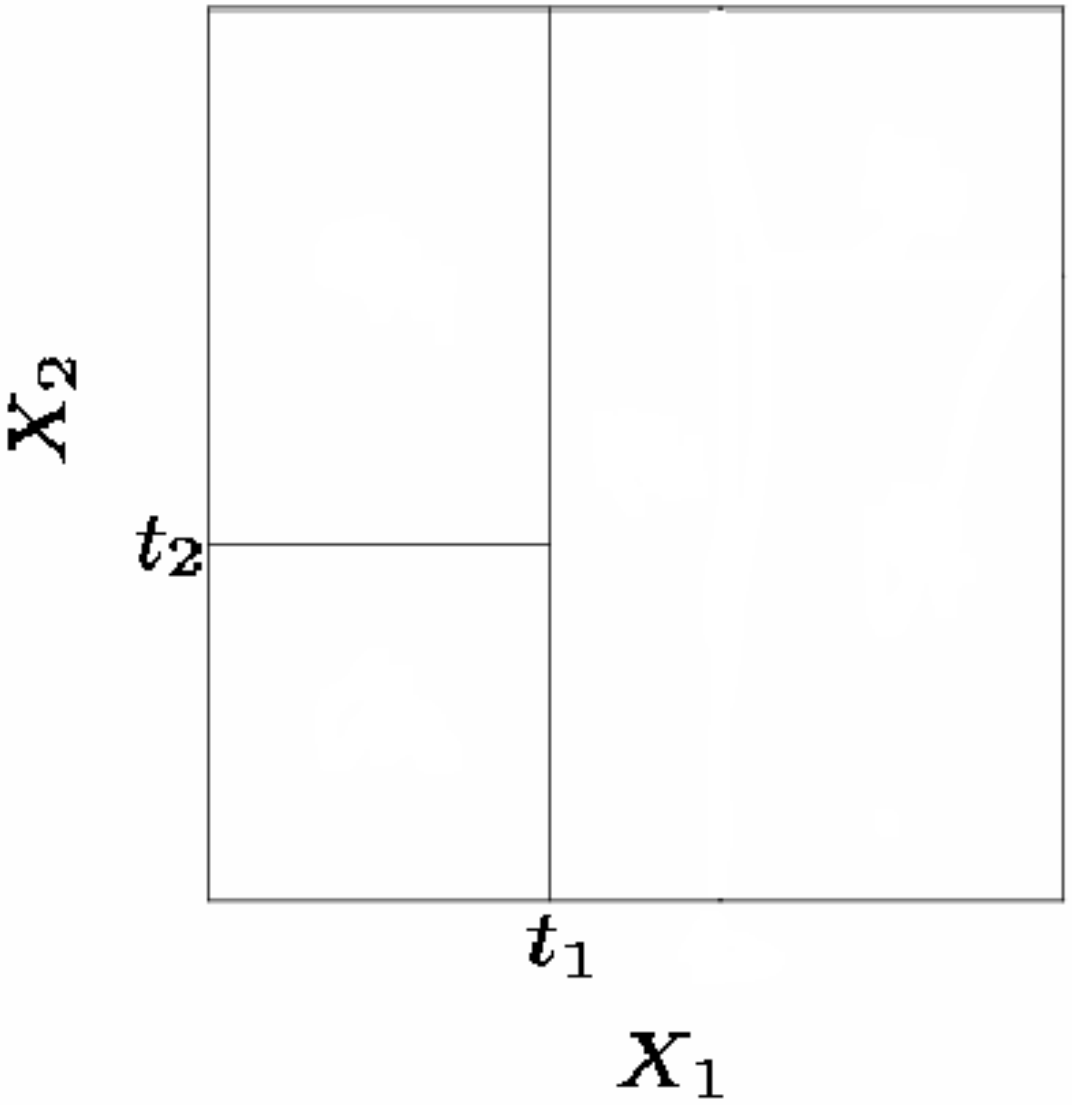
Q1. Where to Split?

- Here the optimal split was on X_1 at point t_1.
- Now we repeat the process looking for the next best split except that we must also consider whether to split the first region or the second region up.
- Again the criteria is smallest MSE.



Where to Split?

- Here the optimal split was the left region on X_2 at point t_2.
- [Stopping criteria] This process continues until our regions have too few observations to continue e.g. all regions have 5 or fewer points.



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Tree Pruning

Improving Tree Accuracy

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- A large tree (i.e. one with many terminal nodes) may tend to over fit the training data.
  - Large tree: lower bias, higher variance, worse interpretation
  - Small tree: higher bias, lower variance, better interpretation
- Generally, we can improve accuracy by "pruning" the tree i.e. cutting off some of the terminal nodes.
- How do we know how far back to prune the tree?
  - We use **cross validation** to see which tree has the lowest error rate.

Outline of the Decision Tree Approach

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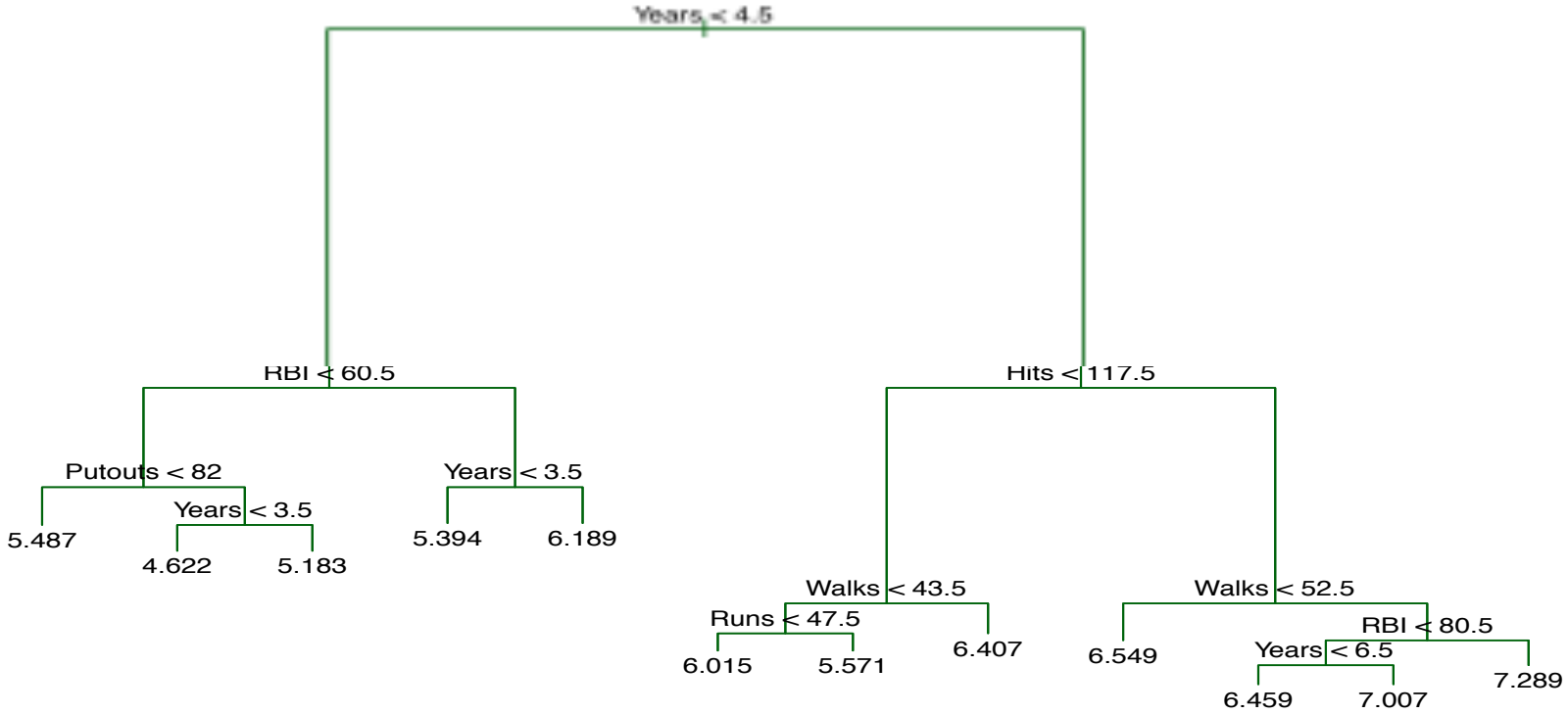
- Split the dataset `DS` into two subsets:
  - `DS.train` and `DS.test`
- Use `DS.train` to build a decision tree tree.train
- Use cross validation (`cv.tree()`) to see
  - whether pruning the tree will improve performance
  - If yes, how many leaves (`w`) the best tree will have
- Use `prune.tree(tree.train,best=w)` to prune the tree if necessary
- Make predictions on the test set `DS.test` and evaluate how well the model performs
  - Calculate the test MSE or test error rate

Example: Baseball Players' Salaries



Can anyone get the same tree as this one when building a regression tree of Salary on 9 predictors?

Y: salary

X: 9 predictors

Hits+Runs+RBI+Walks+Years+PutOuts+AtBat+Assists+Errors

Example: Baseball Players' Salaries

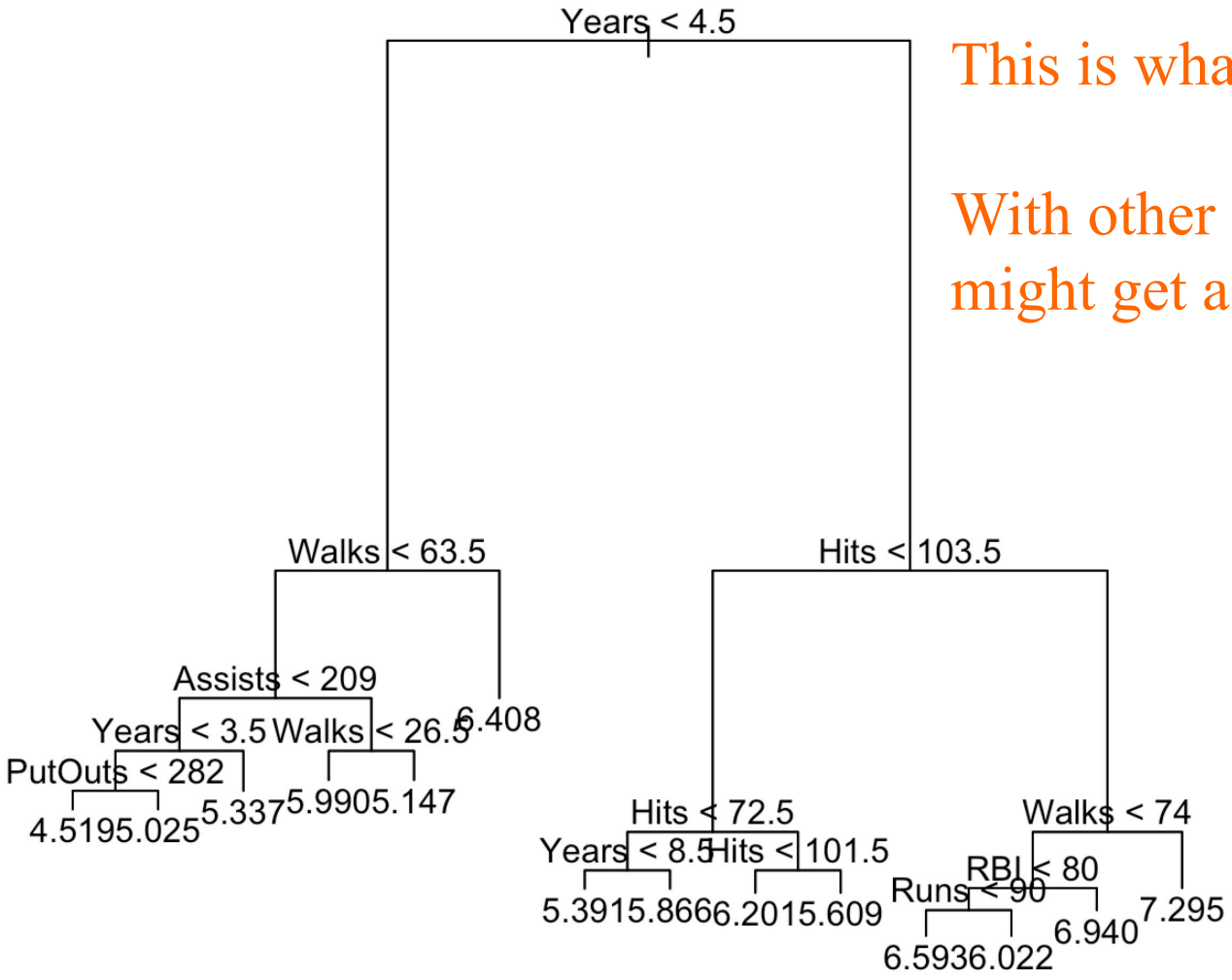
```
set.seed(1)   #choosing a different seed → a different tree
train <- sample(1:nrow(Hitters),132)

tree.hitters.train <- tree(log(Hitters$Salary)~ Hits+Runs+RBI+
                      Walks+Years+PutOuts+AtBat+Assists+Errors,
                      Hitters,subset=train)
plot(tree.hitters.train)
text(tree.hitters.train)
```

Use `summary(tree.hitters.train)` to see how many predictors actually contributed to the tree

```
Variables actually used in tree construction:
[1] "Years"   "Walks"   "Assists" "PutOuts" "Hits"    "RBI"
"Runs"
Number of terminal nodes:  14
```

Example: Baseball Players' Salaries



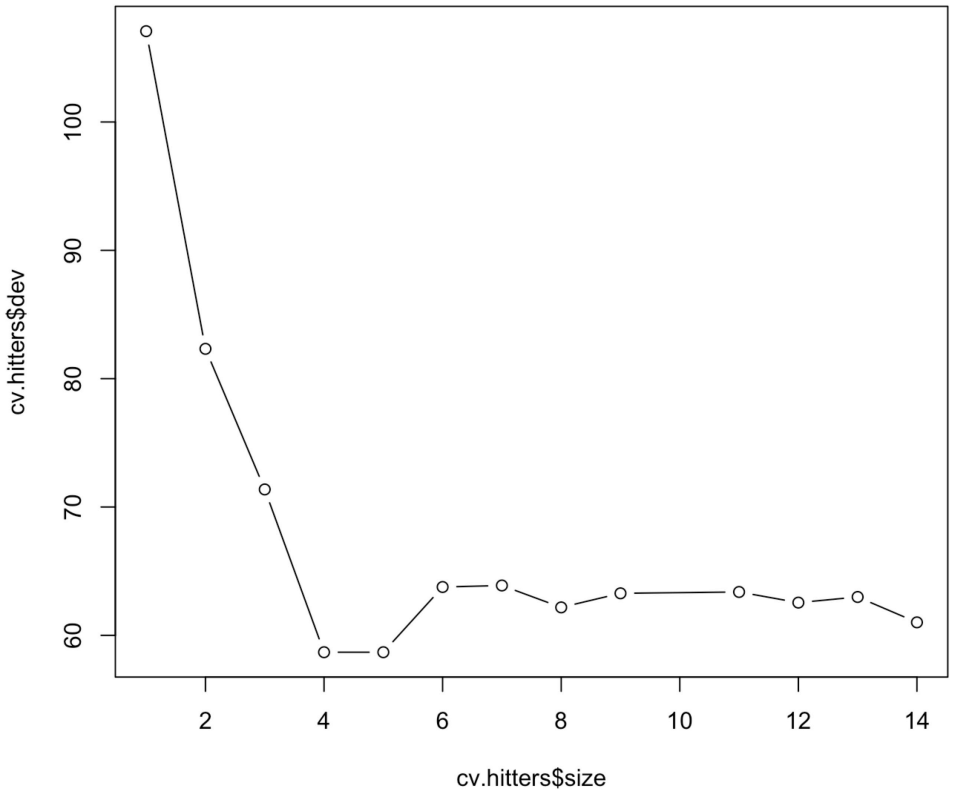
This is what I've got:

With other seeds, you might get a different tree

Example: Baseball Players' Salaries

Now we use cv.tree() function to see whether pruning the tree will improve performance.

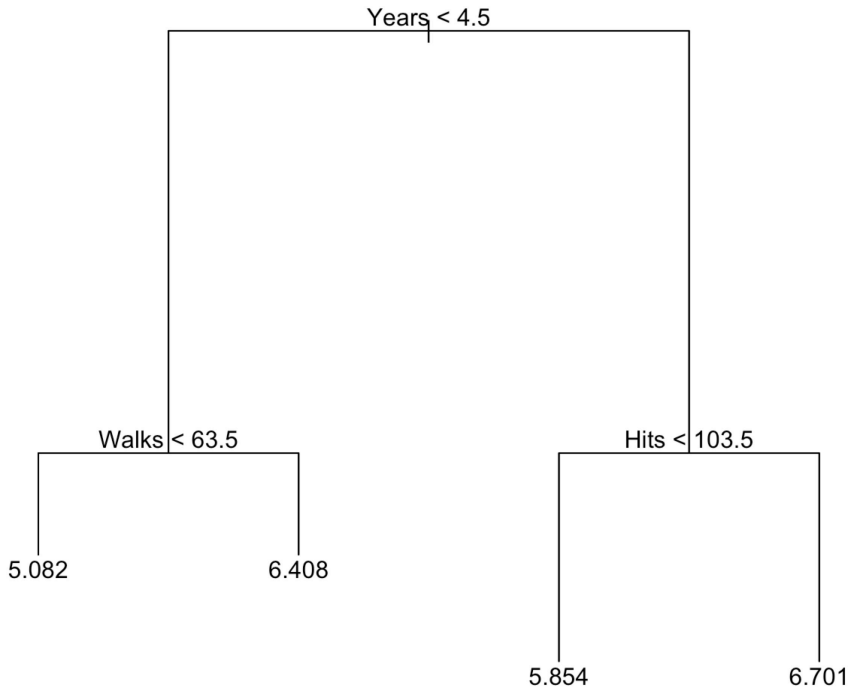
```
cv.hitters <- cv.tree(tree.hitters.train)
plot(cv.hitters$size,cv.hitters$dev,type='b')
```



Example: Baseball Players' Salaries

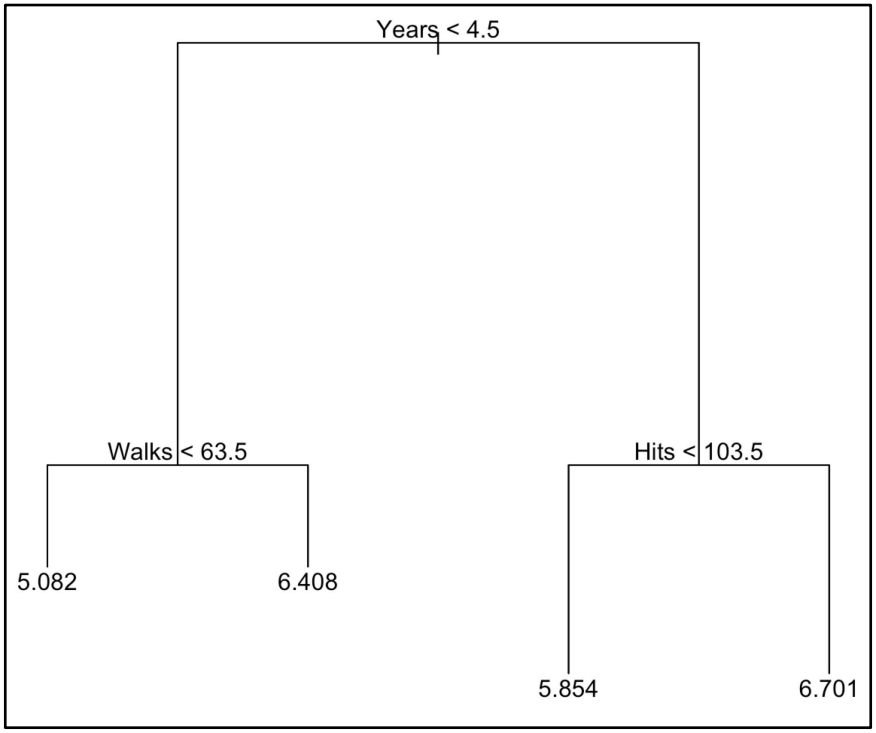
- Cross Validation indicated that the minimum MSE is when the tree size is 4 or 5 (i.e. the number of leaf nodes is 4 or 5)

- Now, we prune the tree to be of size 4:

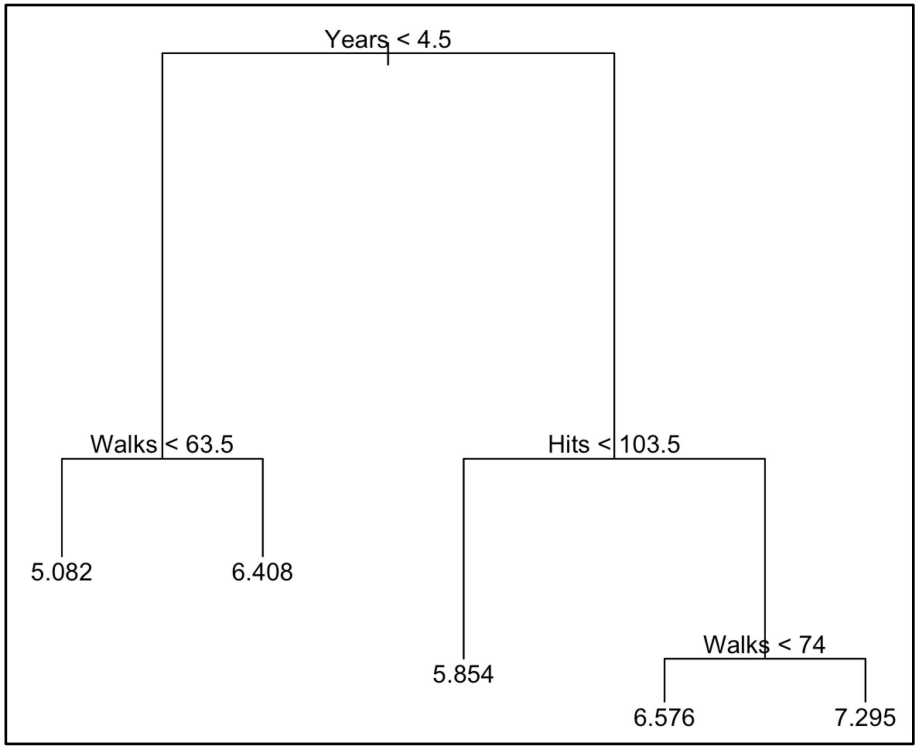



```
prune.hitters <- prune.tree(tree.hitters.train,best=4)
plot(prune.hitters)
text(prune.hitters,pretty=0)
# pretty=0 includes the category names for any qualitative predictors,
# rather than simply displaying a letter for each category
```

Example: Baseball Players' Salaries



Tree pruned to be of size 4



Tree pruned to be of size 5

```
prune.hitters <- prune.tree(tree.hitters.train, best=5)
plot(prune.hitters)
text(prune.hitters,pretty=0)
```

Making Predictions

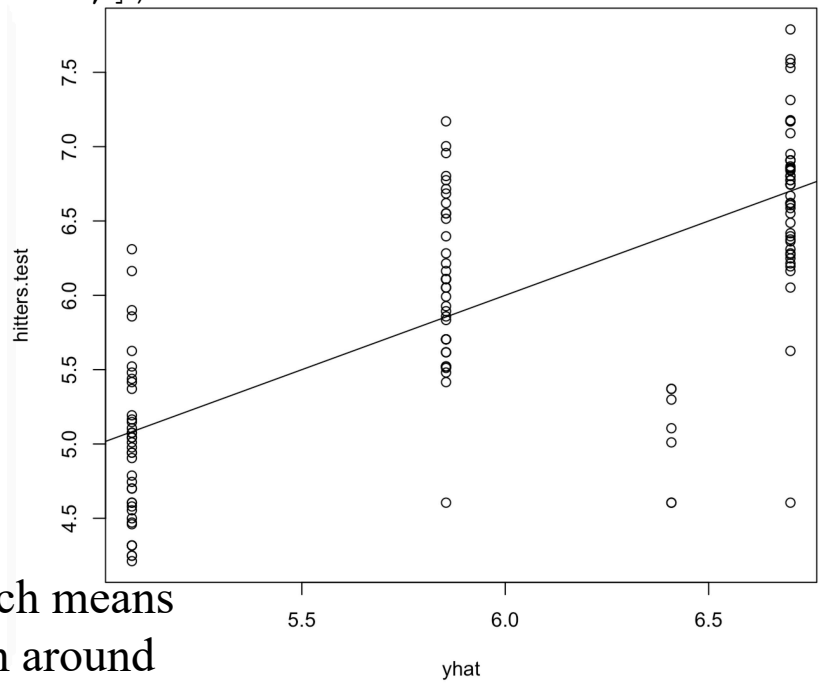
Use the pruned tree (size 4) to make predictions on the test set

```
yhat<-predict(prune.hitters,newdata=Hitters[-train,])
hitters.test <- log(Hitters[-train, "Salary"])

plot(yhat,hitters.test)
abline(0,1)

mean((yhat-hitters.test)^2)
[1] 0.3886456
```

← The test MSE associated with the regression tree




```
sqrt(0.3886456)
[1] 0.6234145
```

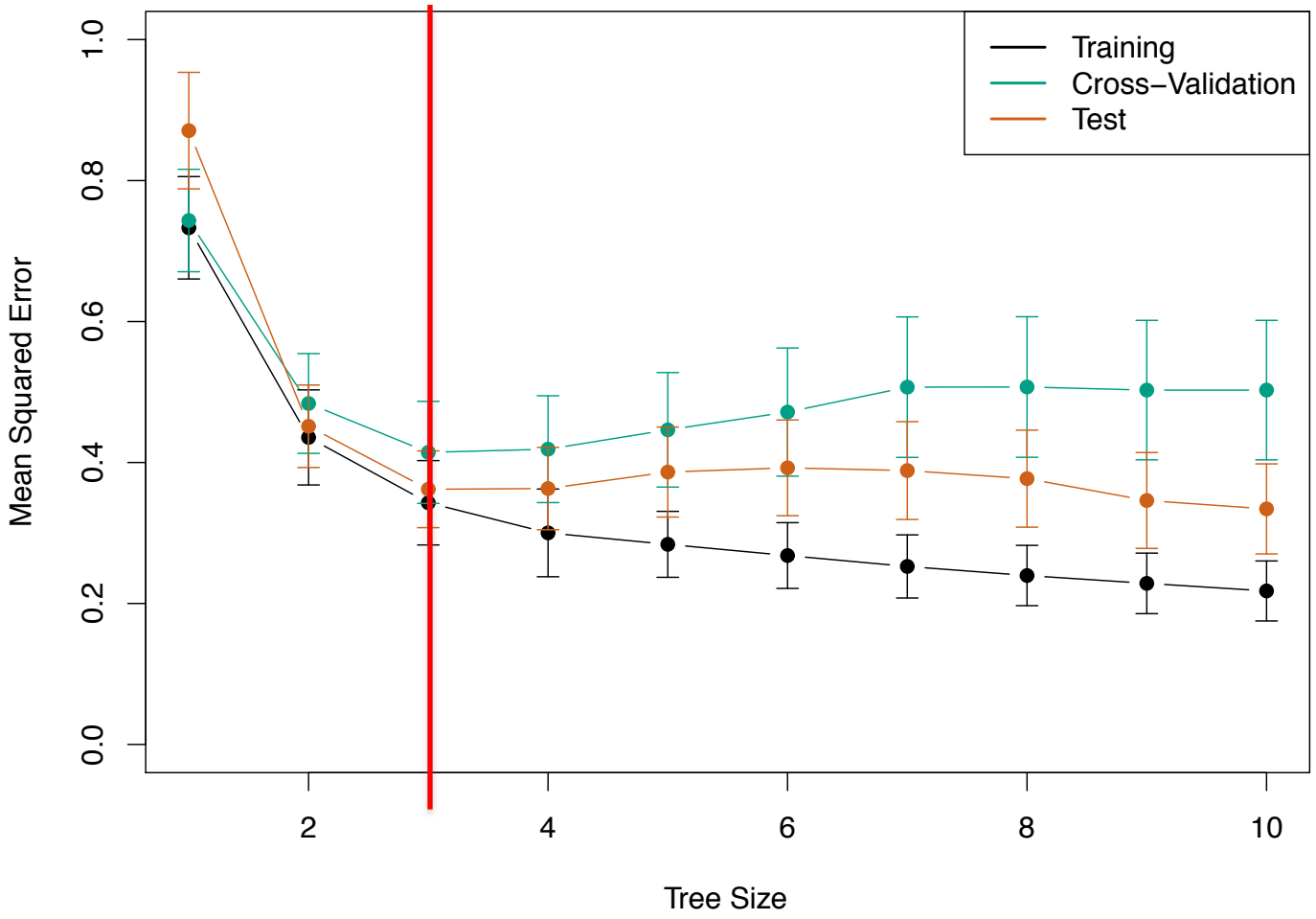
← The square root of the MSE, which means that this model leads to test predictions that are within around $\$e^{0.623}\text{K} = \$1.865\text{K} = \$1865$ of the true Salary of hitters

If using the unpruned tree to do the same, the MSE is 0.4178112.

```
yhat<-predict(tree.hitters.train, newdata=Hitters[-train,])
```

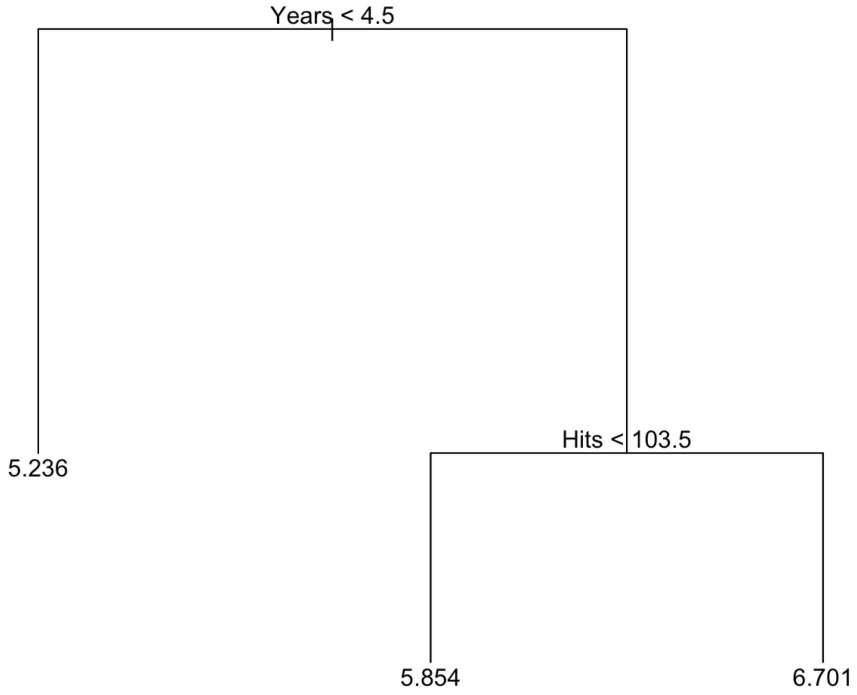
Example: Baseball Players' Salaries

- **In the book**, with an unspecified seed to random split the data set, the minimum cross validation error occurs at a tree size of 3



Example: Baseball Players' Salaries

- Cross Validation indicated that the minimum MSE is when the tree size is three (i.e. the number of leaf nodes is 3)

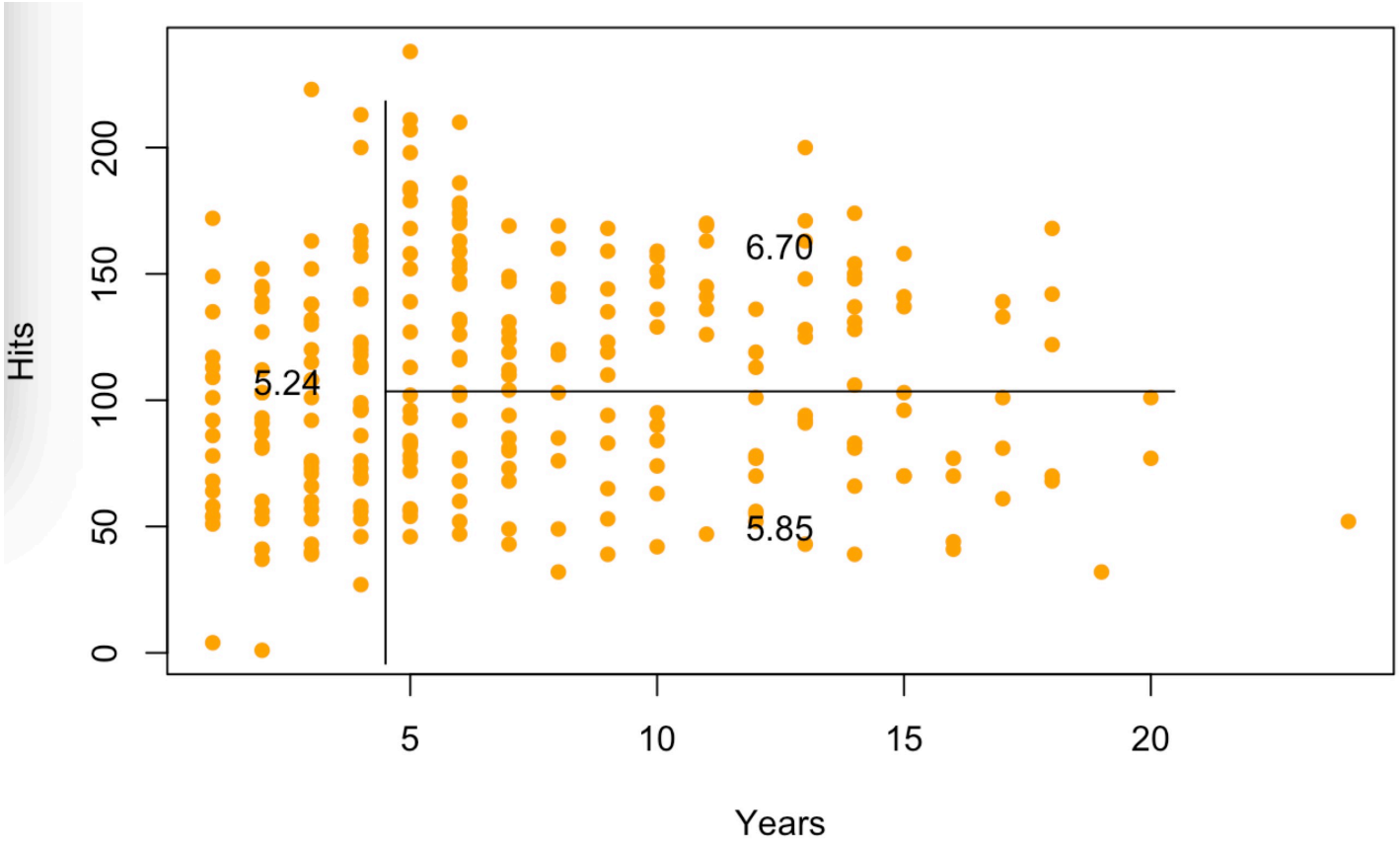


- Now, we prune the tree to be of size 3:

```
prune.hitters.3 <- prune.tree(tree.hitters.train,best=3)
plot(prune.hitters.3)
text(prune.hitters.3,pretty=0)
```

How to plot this?

```
plot(Hitters$Years,Hitters$Hits, col="orange", pch=16, xlab="Years", ylab="Hits")
partition.tree(prune.hitters, ordvars=c("Years","Hits"), add=TRUE)
```



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Classification Trees

Predicting a qualitative response

e.g., Predicting whether a customer will default,
whether an email is a spam, etc

Growing a Classification Tree

- A classification tree is very similar to a regression tree except that we try to make a prediction for a categorical rather than continuous Y.
- For each region (or node) we predict the most common category among the training data within that region.
  - What measure can it be?
- The tree is grown (i.e. the splits are chosen) in exactly the same way as with a regression tree except that minimising MSE no longer makes sense.
- There are several possible different criteria to use such as the "gini index" and "cross-entropy" but the easiest one to think about is to minimise the error rate.

Evaluation of classification models

- Recall: Counts of test records that are correctly (or incorrectly) predicted by the classification model

- **Confusion matrix**

Actual Class \ Predicted Class	Class = 1	Class = 0
Class = 1	f_{11}	f_{10}
Class = 0	f_{01}	f_{00}

$$\text{Accuracy} = \frac{\#\text{ correct predictions}}{\text{total }\#\text{ of predictions}} = \frac{f_{11} + f_{00}}{f_{11} + f_{10} + f_{01} + f_{00}}$$

$$\text{Error rate} = \frac{\#\text{ wrong predictions}}{\text{total }\#\text{ of predictions}} = \frac{f_{10} + f_{01}}{f_{11} + f_{10} + f_{01} + f_{00}}$$

Example: Carseats

- Goal: to analyse the `Carseats` data set

```
library(ISLR)
```

Sales, CompPrice, Income, Advertising, Population, Price, ShelveLoc, Age, Education, Urban, US

- `Sales` is a continuous variable, discretise it using `ifelse()`

```
High <- ifelse(Carseats$Sales<=8,"No","Yes")
```

- Merge `High` with the rest of the `Carseats` data

```
Carseats <- data.frame(Carseats,High)
```

- Fitting a classification tree

```
tree.carseats <- tree(High~.-Sales,Carseats)
summary(tree.carseats)      #How many predictors are used?
```

Example: Carseats

> summary(tree.carseats)

Classification tree:
tree(formula = High ~ . - Sales, data = Carseats)

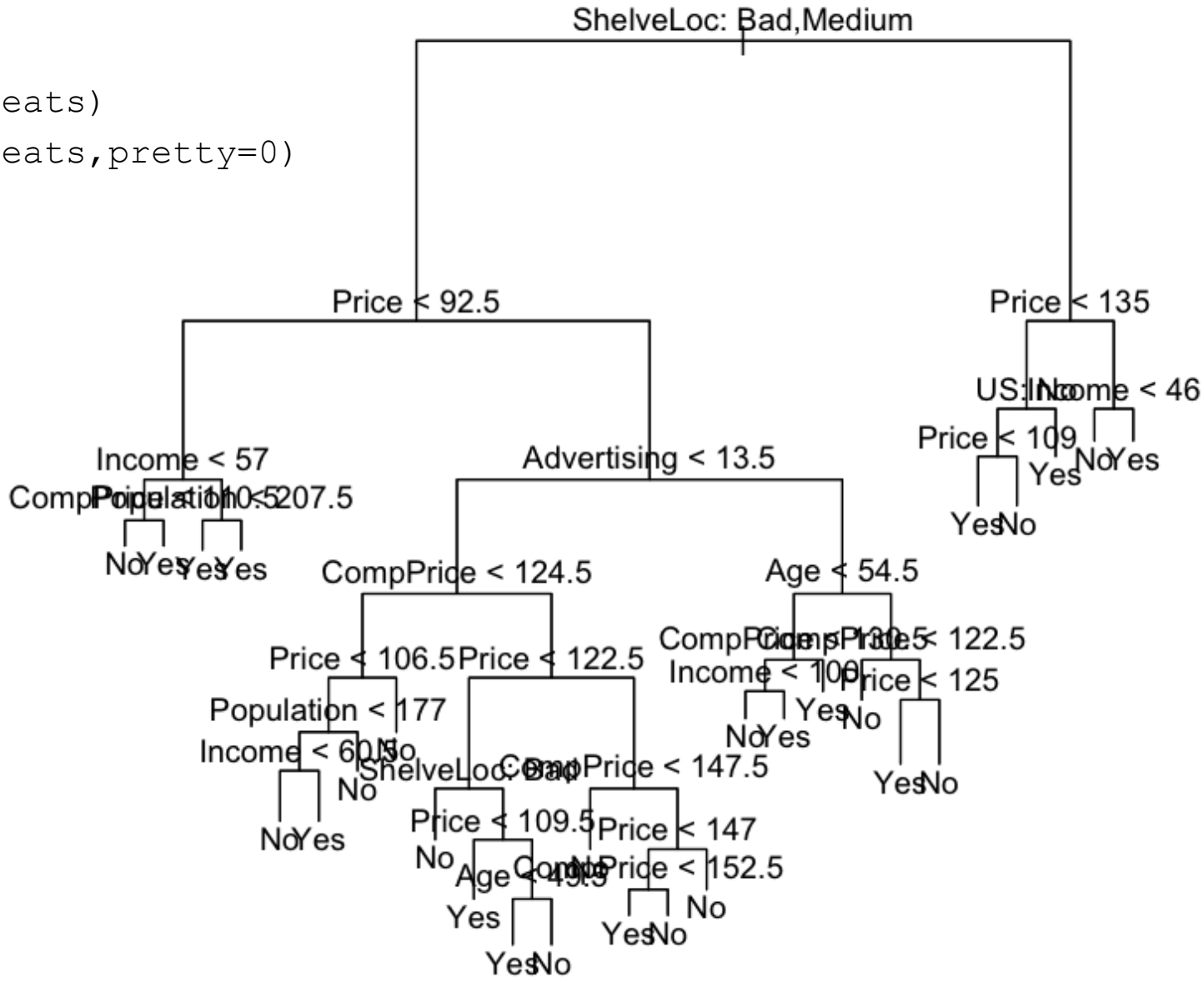
Variables actually used in tree construction:
[1] "ShelveLoc" "Price" "Income" "CompPrice" "Population"
[6] "Advertising" "Age" "US"

Number of terminal nodes: **27**

Residual mean deviance: 0.4575 = 170.7 / 373
Misclassification error rate: 0.09 = 36 / 400 ➔ training error rate is 9%

Plotting the tree

```
plot(tree.carseats)
text(tree.carseats,pretty=0)
```



Test Error Rate Estimation

- Estimate the test error rather than computing the training error
  - Split the observations into a training set and a test set
  - Build the tree using the training set
  - Evaluate its performance on the test data
    - By `predict()`, where `type="class"` returns the actual class prediction

```
set.seed(2)
train <- sample(1:nrow(Carseats),nrow(Carseats)/2)  # 1: can be omitted
Carseats.test <- Carseats[-train,]
High.test <- High[-train]
tree.carseats.train <- tree(High~.-Sales, Carseats, subset=train)
tree.pred.test <- predict(tree.carseats.train, Carseats.test, type="class")
```

```
table(tree.pred.test,High.test)
              High.test
tree.pred.test No Yes
           No  86  27
           Yes 30  57
```

Test Error Rate is 28.5%

What is training error rate? 9%

```
> (27+30)/200
[1] 0.285
```

Pruning a Tree

- Consider whether pruning the tree might lead to improved results

Step 1: Use `cv.tree()` to determine the optimal level of tree complexity

```
set.seed(3)
cv.carseats <- cv.tree(tree.carseats.train, FUN=prune.misclass)
cv.carseats
$size
 [1] 19 17 14 13  9  7  3  2  1
$dev   ← this is the cv error rate
 [1] 55 55 53 52 50 56 69 65 80
```

Step 2: Use `prune.misclass()` to prune the tree

```
prune.carseats <- prune.misclass(tree.carseats.train, best=9)
```

Step 3: Performance evaluation

```
tree.pred <- predict(prune.carseats, Carseats.test, type="class")
table(tree.pred,High.test)
         High.test
tree.pred No Yes
      No  94  24
      Yes 22  60
```

```
> (24+22)/200    test error rate
[1] 0.23   ← better than that without pruning 28.5%
```

Pruning improved interpretability and classification accuracy

Pruning a Tree

- If we increase the value of best, we obtain a larger pruned tree with lower classification accuracy

```
prune.carseats <- prune.misclass(tree.carseats, best=15)

tree.pred <- predict(prune.carseats, Carseats.test, type="class")
table(tree.pred,High.test)
         High.test
tree.pred No Yes
      No  86  22
      Yes 30  62

(30+22)/200
[1] 0.26    ➔ higher error rate than unpruned tree 0.23
```

Summary: Decision Tree Induction

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- Decision tree generation consists of two phases:
  - Tree construction
    - At start, all the training examples are at the root
    - Partition examples recursively based on selected attributes
  - Tree pruning
    - Identify and remove branches that reflect noise or outliers

- Use of decision tree:
  - Regressing or classifying an unknown sample
    - Test the attribute values of the sample against the decision tree

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Trees vs. Linear models

Trees vs. Linear Models

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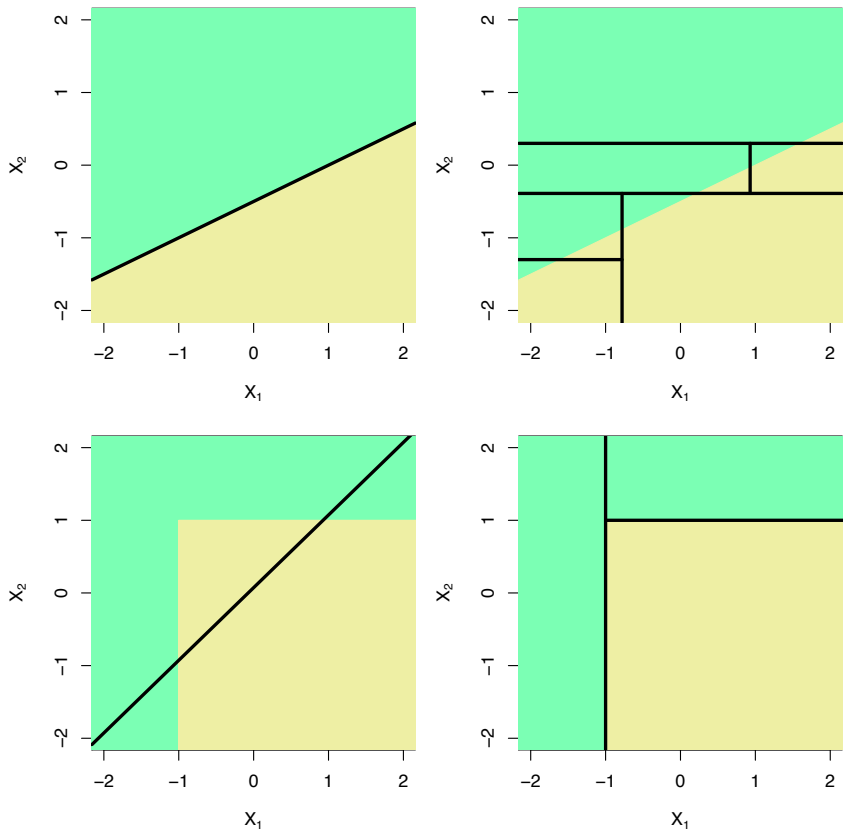
- Which model is better?
  - If the relationship between the predictors and response is linear, then classical linear models such as linear regression would outperform regression trees
  - On the other hand, if the relationship between the predictors is non-linear, then decision trees would outperform classical approaches

Trees vs. Linear Model: Classification Example

- Top row: the true decision boundary is linear
  - Left: linear model (good)
  - Right: decision tree
- Bottom row: the true decision boundary is non-linear
  - Left: linear model
  - Right: decision tree (good)



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Advantages and disadvantages of trees

Pros and Cons of Decision Trees

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- Pros:
  - Trees are very easy to explain to people (probably even easier than linear regression)
  - Trees can be plotted graphically, and are easily interpreted even by non-expert
  - They work fine on both classification and regression problems
- Cons:
  - Trees don't have the same prediction accuracy as some of the more complicated approaches that we examine in this course