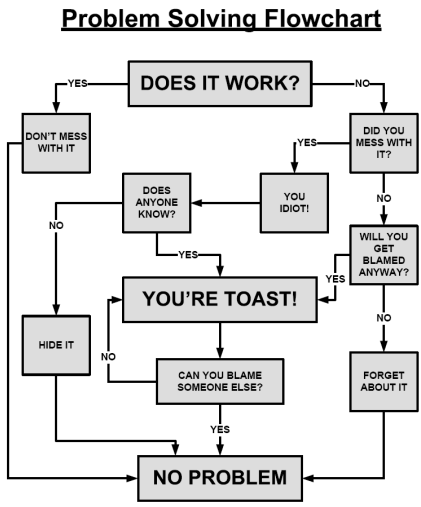
Data, Environment and Society: Lecture 16: Regression trees

Instructor: Duncan Callaway
GSI: Salma Elmallah

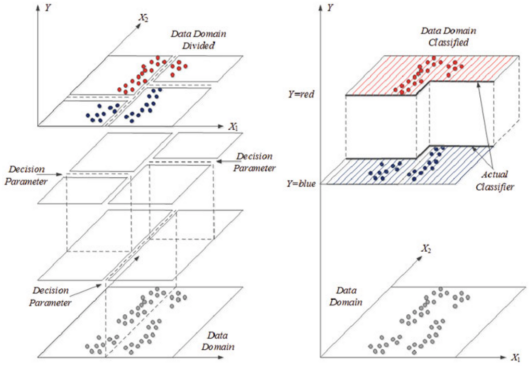
October 24, 2019



https://thenexttobestblogever.wordpress.com/2009/11/07/problem-solving-flowchart-2/

Objectives

- Introduction to regression trees
  - Terminology
  - How they are built
  - How to choose with cross validation
- Next week, we'll discuss classification trees
  - Same as regression, just different loss functions



(medium.com)

Terminology we'll cover...

- Terminal node
- Internal node
- Branches
- Leaves
- Binary splits
- Recursive binary splitting $\leftrightarrow$ Top-down greedy
- Cost complexity pruning

Basic idea for regression trees

All we are doing is "splitting" the observations into regions in the predictor space, and averaging the response variable within each region.

Basic idea for regression trees

All we are doing is "splitting" the observations into regions in the predictor space, and averaging the response variable within each region.

Doing predictions with the model just involves

- locating a set of **predictors** in a region,
- then setting the response variable equal to the average from the training **response** variable in that region.

Basic idea for regression trees

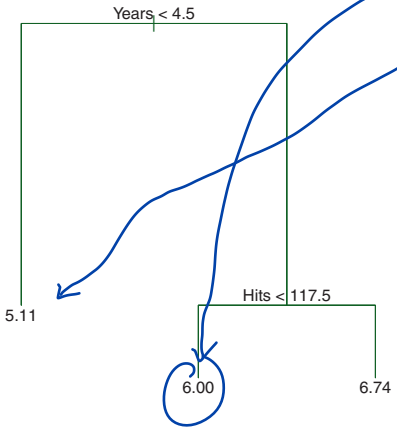
All we are doing is "splitting" the observations into regions in the predictor space, and averaging the response variable within each region.

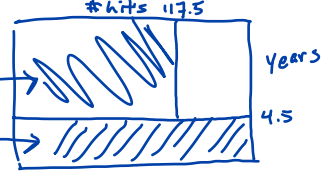
Doing predictions with the model just involves

- locating a set of **predictors** in a region,
- then setting the response variable equal to the average from the training **response** variable in that region.

Big decision in regression trees: *What are the regions we should use?*

Example, from the textbook





"Hitters" data from ISLR.

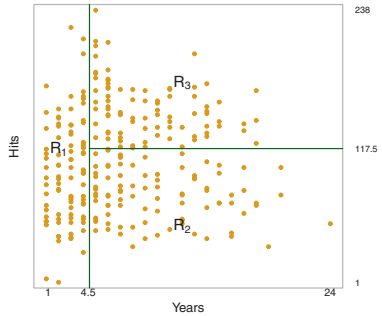
263 major league players stats.

Here, this tree is "spliting" on two variables – years in league and number of hits

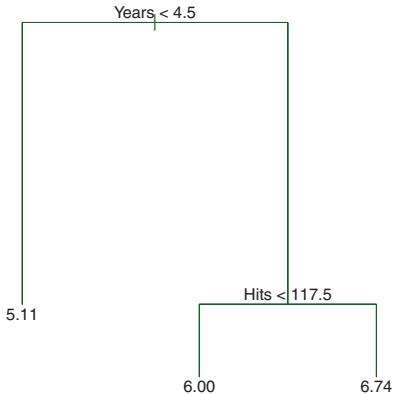
The numbers at the ends are the average (log-transformed) average salaries for players

Example, from the textbook, ctd

$$R_1 = \{X | \text{years} < 4.5\}$$
$$R_2 = \{X | \text{years} \geq 4.5, \text{hits} < 117.5\}$$
$$R_3 = \{X | \text{years} \geq 4.5, \text{hits} \geq 117.5\}$$



Terminology

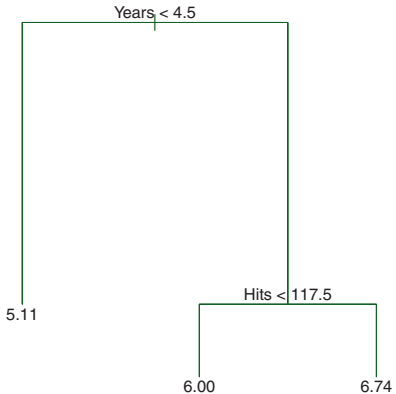


Each region R_i is a *terminal node*

Each numeric value at which a split happens is an *internal node*

Segments connecting nodes (terminal or internal) are...

Terminology

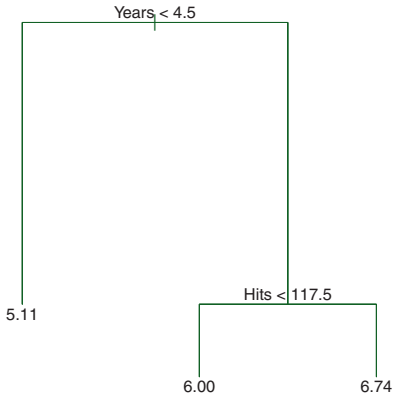


Each region R_i is a *terminal node*

Each numeric value at which a split happens is an *internal node*

Segments connecting nodes (terminal or internal) are...*branches*

Terminology



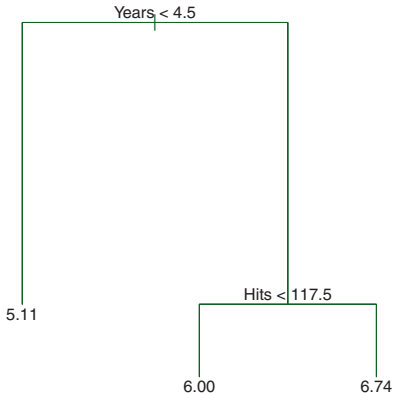
Each region R_i is a *terminal node*

Each numeric value at which a split happens is an *internal node*

Segments connecting nodes (terminal or internal) are...*branches*

The numbers at the end of the branches are also sometimes called...

Terminology



Each region R_i is a *terminal node*

Each numeric value at which a split happens is an *internal node*

Segments connecting nodes (terminal or internal) are...*branches*

The numbers at the end of the branches are also sometimes called...*leaves*

Terminology so far...

- Terminal node
- Internal node
- Branches
- Leaves

Regression trees – basic approach

1. Divide the **predictor** space into non-overlapping regions
   - This distinguishes the method from KNN regression
2. Within each region, the prediction is just the average of the **response variable** from training data.
   - This is similar to KNN regression

Regression trees – basic approach

1. Divide the **predictor** space into non-overlapping regions
   - This distinguishes the method from KNN regression
2. Within each region, the prediction is just the average of the **response variable** from training data.
   - This is similar to KNN regression

Two Basic Questions:

1. Where should I put the internal nodes?
2. How many regions should there be?

The answers are, as it turns out, really simple.

Where to put the internal nodes?

First, for simplicity, the nodes are structured to make rectangles in the a 2-D predictor space (or hyper-rectangles in higher dimensions).

How do I split regions?

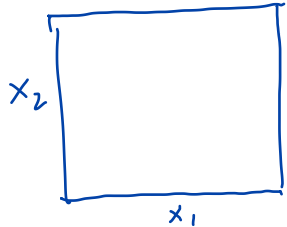
Let

- j index predictor variables
- s denote the location of the split within the region
  - (With n observations we have to consider at most $n-1$ split points; the numeric value of the split is the mid-way point between to adjacent observations.)

Then all splits can be described as:

$$R_1(j,s) = \{X|X_j < s\} \text{ and } R_2(j,s) = \{X|X_j \geq s\}$$

But where should the splits be?



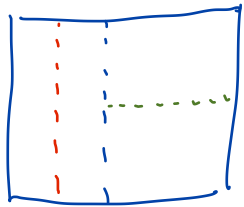
Then we partition any region by choosing j and s as follows:

$$\{j, s\} = \arg \min_{j \in J, s \in X_j} \sum_{i: x_i \in R_1(j,s)} (y_i - \hat{y}_{R_1})^2 + \sum_{i: x_i \in R_2(j,s)} (y_i - \hat{y}_{R_2})^2$$

where $\hat{y}_{R_k}$ is the mean of all response variables in region k.

It would be tedious to identify j and s by hand, but it's actually very quick computationally. (Remember, there are only $n - 1$ possible splits for each predictor.)

Ok, we've split one predictor in two. Now what?



Next choose the single best split from among *all* possible splits of the two new regions. **Now we'll have three regions.**

In general, on the n^{th} step, choose the single best possible split from among the n regions, resulting in $n + 1$ regions to take to the next step.

Repeating the splits

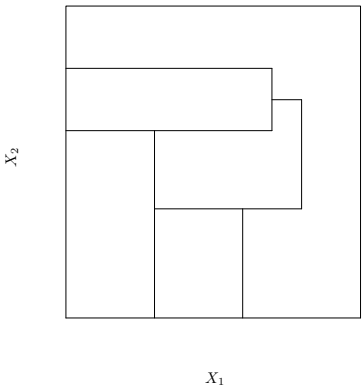
On each step, we're choosing the single best possible split from among the n regions, resulting in $n + 1$ regions to take to the next step.

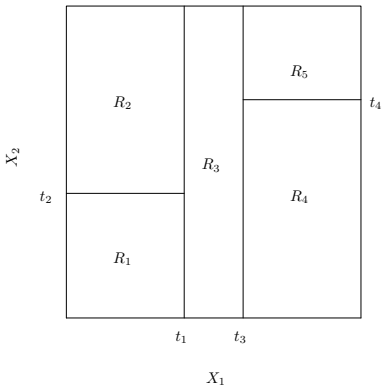
Repeat this process until you reach a stopping criterion – typically a maximum number of observations in each region. (For example all regions have no more than 5 observations.)

Call the resulting tree T_0.

We call this approach "greedy" because when we do the first partition we're not thinking ahead to future partitions to evaluate it.

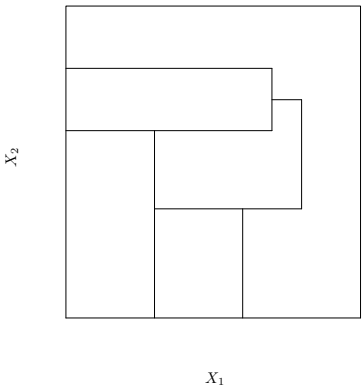
One of these doesn't belong...

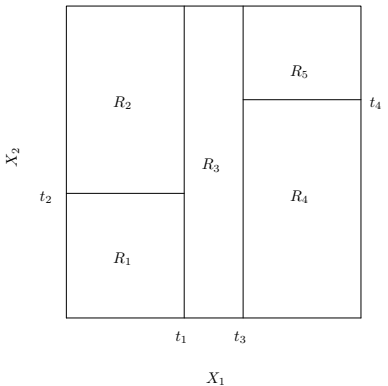




Q: Which picture results from successively splitting the regions into values greater or less than predictor values?

One of these doesn't belong...

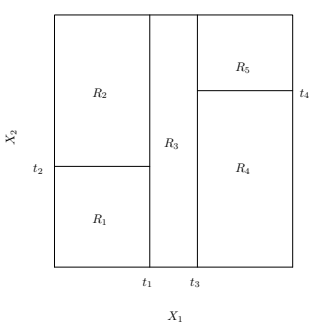


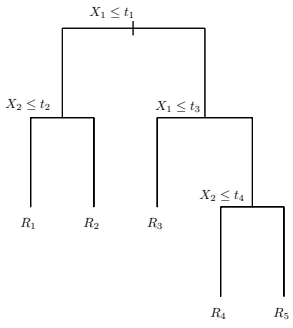


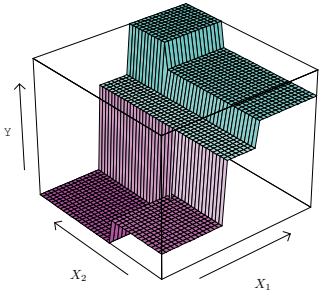
Q: Which picture results from successively splitting the regions into values greater or less than predictor values?

A: The right one. The left one is not possible with simple splitting.

A five region example... with two dimensional predictor space







What do we call it?

The process of splitting regions over and over is called...

“recursive binary splitting”

You can also call it a **“top-down greedy”** approach.

Because it’s “greedy” we can’t be sure that the splits we’re getting are the best possible splits.

Why binary?

In other words, why not multiway splits?

Why binary?

In other words, why not multiway splits?

In general multiway splits fragment the data too quickly, leaving insufficient data at the next level down

Since we do the binary splitting recursively, we get the same flexibility as a multiway split, since a region can be split a second time later.

Terminology so far...

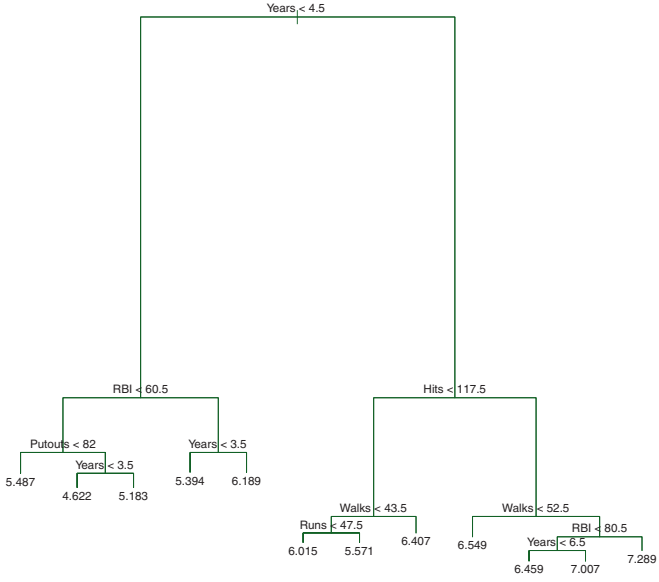
- Terminal node
- Internal node
- Branches
- Leaves

Terminology so far...

- Terminal node
- Internal node
- Branches
- Leaves
- Binary splits
- Recursive binary splitting $\leftrightarrow$ Top-down greedy

Example T_0

Remember, T_0 is the biggest tree we build. We get there by recursively splitting until we meet a threshold (often a maximum number of observations per terminal node).



When will we test?

All the steps above involve model *building*. We have yet to evaluate different models against one another. First let's build the candidate models, then we can evaluate.

Step 1: "cost complexity pruning"

We'll test models that are **subtrees** of T_0. (trees that are the same as T_0 except they are missing some internal nodes and branches).

We identify subtrees using **cost-complexity pruning** a.k.a. weakest link pruning:

- To get the first subtree, evaluate model performance for all subtrees with one leaf removed from T_0. Choose the best one, call it T_1.
  - R^2 works for measuring performance
  - ...but not for categorical variables, stay tuned!
- Then evaluate performance for all models with one leaf removed from T_1. Choose the best, call it T_2. And so on.

Step 1: "cost complexity pruning"

We'll test models that are **subtrees** of T_0. (trees that are the same as T_0 except they are missing some internal nodes and branches).

We identify subtrees using **cost-complexity pruning** a.k.a. weakest link pruning:

- To get the first subtree, evaluate model performance for all subtrees with one leaf removed from T_0. Choose the best one, call it T_1.
  - R^2 works for measuring performance
  - ...but not for categorical variables, stay tuned!
- Then evaluate performance for all models with one leaf removed from T_1. Choose the best, call it T_2. And so on.

(Smart researchers have shown that this "greedy" approach is an optimal *pruning* strategy. But recursive binary splitting is not always optimal for growth.)

Step 2: Tune up your α

Take your set of subtrees, T_0 through T_{N-2}. Call $|T|$ the number of terminal nodes in the tree.

For a given α, *one* of the T_i will minimize :

$$\sum_{m=1}^{|T|} \sum_{x_i \in R_m} (y_i - \hat{y}_{R_m})^2 + \alpha |T|$$

- $\alpha = 0$ will choose T_0, the biggest tree.
- As α grows you'll choose successively smaller trees.

Quick quiz

For a given α, *one* of the T_i will minimize :

$$\sum_{m=1}^{|T|} \sum_{x_i \in R_m} (y_i - \hat{y}_{R_m})^2 + \alpha |T|$$

Fill in the blank: As α increases, bias goes __ and variance goes _____.

Quick quiz

For a given α, *one* of the T_i will minimize :

$$\sum_{m=1}^{|T|} \sum_{x_i \in R_m} (y_i - \hat{y}_{R_m})^2 + \alpha |T|$$

Fill in the blank: As α increases, bias goes **up** and variance goes **down**. Bigger α means fewer leaves, which means more bias but less variance.

Though it seems unnecessary to define α (why not just evaluate all subtrees?), we'll see it's useful for cross validation.

The (cross validation) process

1. Split your data into K folds.
2. Repeat this process for each fold: Withhold the fold and for remaining training data:
   a. Grow a large tree via recursive binary splitting. "Large" means each leaf has some pre-specified maximum number of observations (e.g. 5)
   b. Then "prune" the tree via cost complexity pruning to get a sequence of subtrees.
   c. Choose the tree in the sequence that minimizes $\sum_{m=1}^{|T|} \sum_{x_i \in R_m} (y_i - \hat{y}_{R_m})^2 + \alpha |T|$ for each of a range of values of α.
   d. Record the test MSE for each value of α.
3. Average the test MSE across all folds *for each value of* α,
4. Choose the α that gives the lowest cross validated error,
5. Build your final model with the chosen α with *all the data.*

Why use α?

Why didn't we just evaluate cross validated error for each tree size?

That is, is α just overly complicating things?

Why use α?

Why didn't we just evaluate cross validated error for each tree size?

That is, is α just overly complicating things?

Ans: Sometimes it might. But it may be that across different folds we'd choose different subtrees. α provides a better representation of the bias-variance tradeoff across folds.

But: out of convenience the book *displays* results in terms of tree size rather than α. Argh!

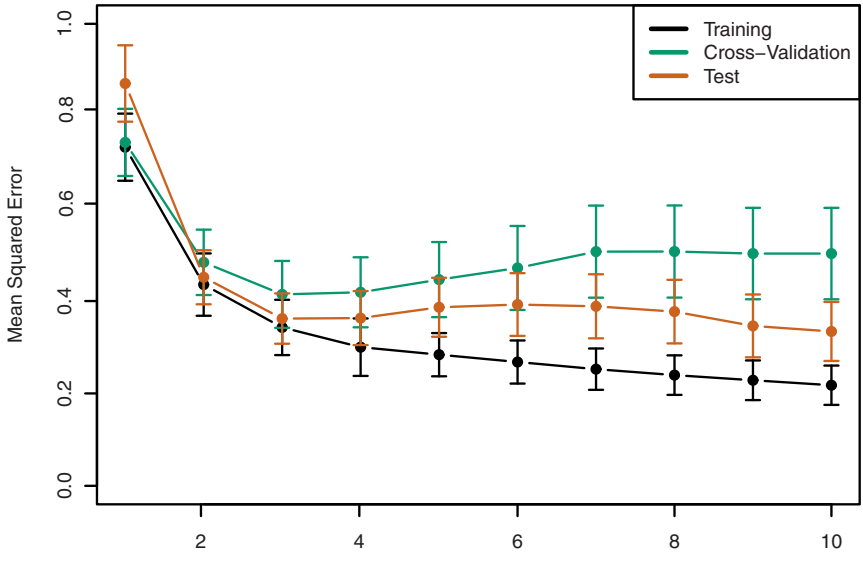
Terminology so far...

- Terminal node
- Internal node
- Branches
- Leaves
- Binary splits
- Recursive binary splitting $\leftrightarrow$ Top-down greedy

Terminology so far...

- Terminal node
- Internal node
- Branches
- Leaves
- Binary splits
- Recursive binary splitting $\leftrightarrow$ Top-down greedy
- Cost complexity pruning
- Cross validation to choose best α

Results on Hitters data



Questions

Do regression trees utilize linear regression?

Questions

Do regression trees utilize linear regression? Nope.

What do you think their advantages are (vs LASSO or nonlinear models...)?

Questions

Do regression trees utilize linear regression? Nope.

What do you think their advantages are (vs LASSO or nonlinear models...)?

- Easy to explain and non-experts can understand the results.
- They're more like human decision-making. Doctors like them.
- They easily handle qualitative predictors – no need for dummies.

Questions

Do regression trees utilize linear regression? Nope.

What do you think their advantages are (vs LASSO or nonlinear models...)?

- Easy to explain and non-experts can understand the results.
- They're more like human decision-making. Doctors like them.
- They easily handle qualitative predictors – no need for dummies.

How about some disadvantages?

Questions

Do regression trees utilize linear regression? Nope.

What do you think their advantages are (vs LASSO or nonlinear models...)?

- Easy to explain and non-experts can understand the results.
- They're more like human decision-making. Doctors like them.
- They easily handle qualitative predictors – no need for dummies.

How about some disadvantages?

- As described, they don't usually provide the same predictive power that the other tools we've studied can.
- They can be pretty sensitive to small changes in the data.
- Recursive binary splitting may generate a suboptimal tree (like forward / backward model selection). Things later in the chapter address this.