Ch 8.1: Decision Trees

Lecture 24 - CMSE 381

Prof. Elizabeth Munch

Michigan State University
::
Dept of Computational Mathematics, Science & Engineering

Mon, Nov 4, 2024

Announcements

Last time:

- Cubic Splines

This lecture:

- 8.1 Decision Trees

Announcements:

- HW #7 Sun, 11/10
- Projects

Lec #	Date			Reading	HW
21	Mon	10/28	Polynomial & Step Functions	7.1,7.2	
22	Wed	10/30	Step Functions; Basis functions; Start Splines	7.2 - 7.4	
23	Fri	11/1	Regression Splines	7.4	HW #6 Due Sun 11/3
24	Mon	11/4	Decision Trees	8.1	
25	Wed	11/6	Class Cancelled (Dr Munch out of town)		
26	Fri	11/8	Random Forests	8.2.1, 8.2.2	HW #7 Due Sun 11/10
27	Mon	11/11	Maximal Margin Classifier	9.1	
28	Wed	11/13	SVC	9.2	
29	Fri	11/15	SVM	9.3, 9.4	HW #8 Due Sun 11/17
30	Mon	11/18	Single layer NN	10.1	
31	Wed	11/20	Multi Layer NN	10.2	
32	Fri	11/22	CNN	10.3	HW #11 Due Sun 11/24
33	Mon	11/25	TBD: Unsupervised learning/clustering	12.1, 12.4?	
	Wed	11/27	Virtual: Project office hours		
	Fri	11/29	No class - Thanksgiving		
	Mon	12/2	Review		
	Wed	12/4	**Midterm #3**		
	Fri	12/6	No class - EGR Design Day		Project due

Section 1

Decision Trees

Big idea

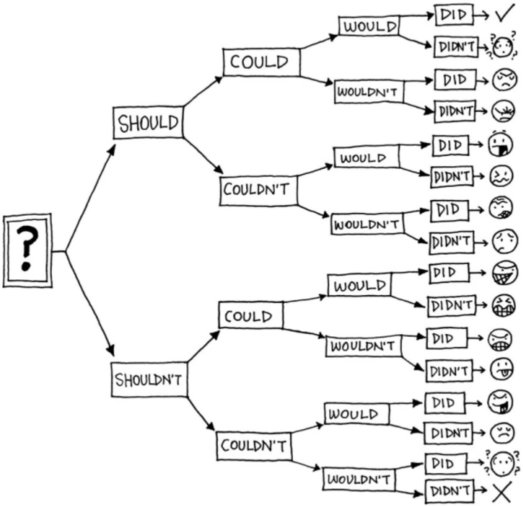


Image: https://marekbennett.com/2014/02/14/decision-tree/

Subset of Hitters data

	Hits	Years	Salary	LogSalary
1	81	14	475.0	6.163315
2	130	3	480.0	6.173786
3	141	11	500.0	6.214608
4	87	2	91.5	4.516339
5	169	11	750.0	6.620073
...	...	...	...	...
317	127	5	700.0	6.551080
318	136	12	875.0	6.774224
319	126	6	385.0	5.953243
320	144	8	960.0	6.866933
321	170	11	1000.0	6.907755

First decision tree example

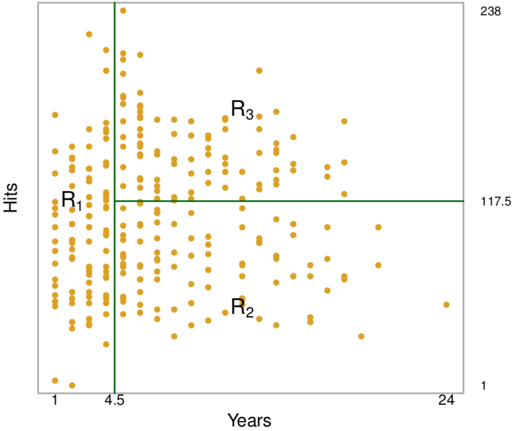
	Hits	Years	LogSalary
1	81	14	6.163315
2	130	3	6.173786
3	141	11	6.214608
4	87	2	4.516339
5	169	11	6.620073
...	...	...	...
317	127	5	6.551080
318	136	12	6.774224
319	126	6	5.953243
320	144	8	6.866933
321	170	11	6.907755

Interpretation of example

Coding a regression decision tree

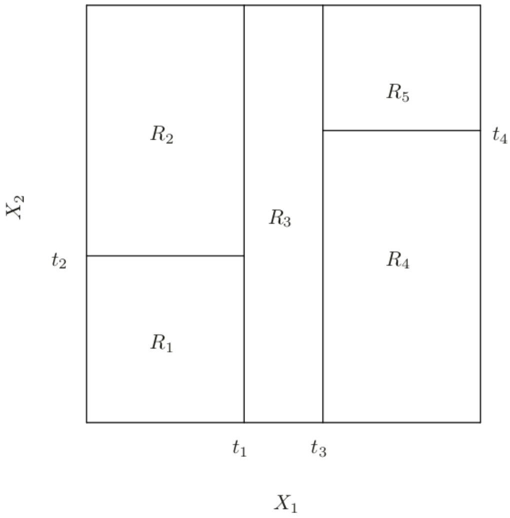
Regions defined by the tree

Viewing Regions Defined by Tree



How do we actually get the tree? Two steps

1. We divide the predictor space – that is, the set of possible values for $X_1, X_2, \cdots, X_p$ — into J distinct and non-overlapping regions, $R_1, R_2, \cdots, R_J$.
2. For every observation that falls into the region R_j, we make the same prediction = the mean of the training response values for the training observations in R_j.



Step 1: How do we decide on R_js?

Goal:

Find boxes $R_1, \cdots, R_J$ that minimize

$$\sum_{j=1}^{J} \sum_{i \in R_j} (y_i - \hat{y}_{R_j})^2$$

$\hat{y}_{R_j}$ = mean response for training observations in jth box

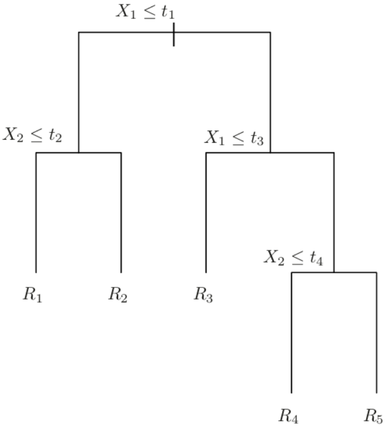
Recursive Binary Splitting

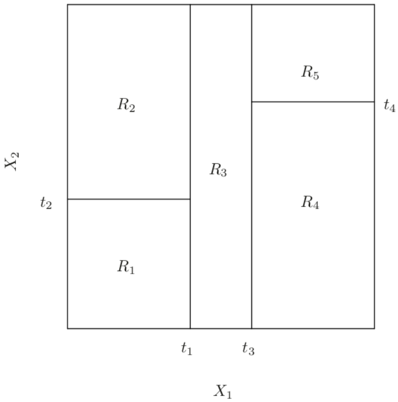
- Pick X_j
- Pick s so that splitting into $\{X \mid X_j < s\}$ and $\{X \mid X_j \geq s\}$ results in largest possible reduction in RSS

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

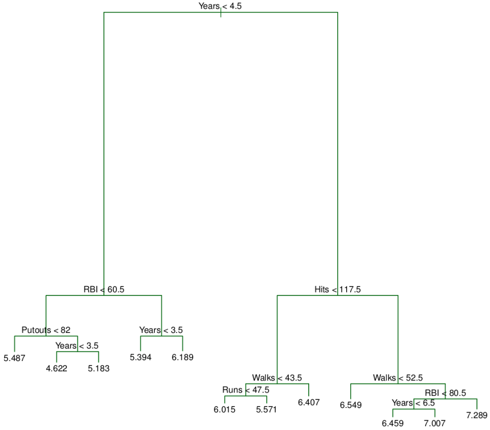
$$\sum_{i \mid x_i \in R_1(j,s)} (y_i - \hat{y}_{R_1})^2 + \sum_{i \mid x_i \in R_2(j,s)} (y_i - \hat{y}_{R_2})^2$$

Rinse and repeat





Pruning



Years < 4.5
RBI < 60.5
Hits < 117.5
Putouts < 82
Years < 3.5
Years < 3.5
5.487
4.622
5.183
5.394
6.189
Walks < 43.5
Walks < 52.5
Runs < 47.5
RBI < 80.5
Years < 6.5
6.015
5.571
6.407
6.549
6.459
7.007
7.289

Weakest Link Pruning

Also called Cost complexity pruning

For every α, there is a subtree T that minimizes:

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

- $|T|$ = number of terminal nodes of T
- R_m is rectangle for mth terminal node
- $\hat{y}_{R_m}$ is mean of training observations in R_m

Algorithm version

Algorithm 8.1 *Building a Regression Tree*

1. Use recursive binary splitting to grow a large tree on the training data, stopping only when each terminal node has fewer than some minimum number of observations.

2. Apply cost complexity pruning to the large tree in order to obtain a sequence of best subtrees, as a function of α.

3. Use K-fold cross-validation to choose α. That is, divide the training observations into K folds. For each $k = 1, \ldots, K$:

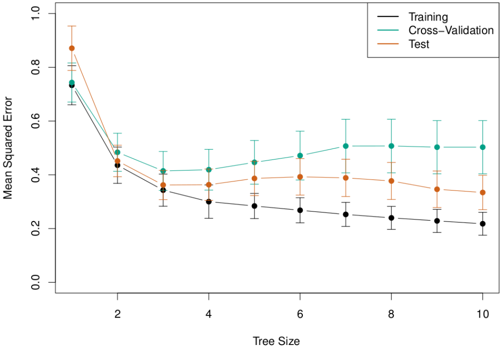
   (a) Repeat Steps 1 and 2 on all but the kth fold of the training data.

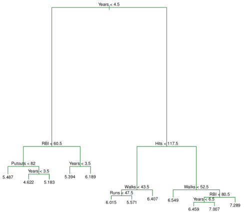
   (b) Evaluate the mean squared prediction error on the data in the left-out kth fold, as a function of α.

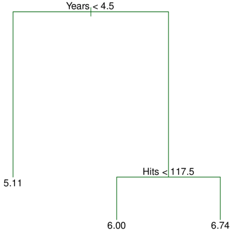
   Average the results for each value of α, and pick α to minimize the average error.

4. Return the subtree from Step 2 that corresponds to the chosen value of α.

Messing with α



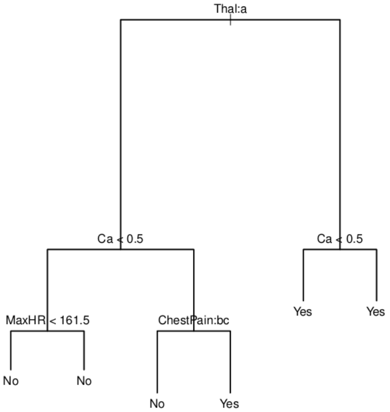




Section 2

Classification Decision Tree

Basic idea



- $\hat{p}_{mk}$ = proportion of training observations in R_m from the kth class
- $E = 1 - \max_k(\hat{p}_{mk})$

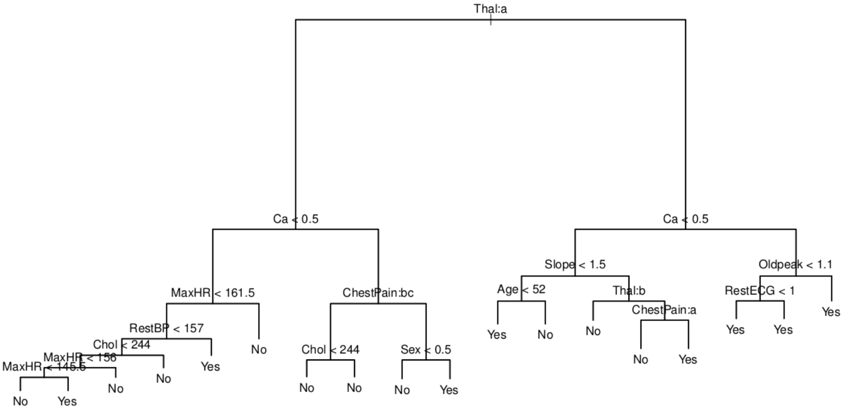
Gini index

$$G = \sum_{k=1}^{K} \hat{p}_{mk}(1 - \hat{p}_{mk})$$

Entropy

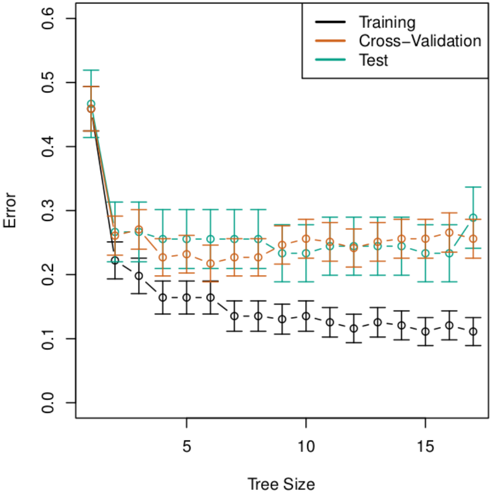
$$D = -\sum_{k=1}^{K} \hat{p}_{mk} \log \hat{p}_{mk}$$

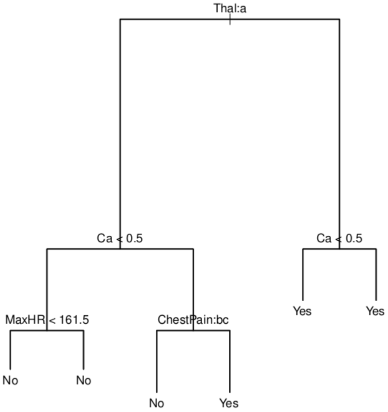
Example



Thal:a
Ca < 0.5
Ca < 0.5
MaxHR < 161.5
ChestPain:bc
Slope < 1.5
Oldpeak < 1.1
RestBP < 157
Chol < 244
MaxHR < 156
MaxHR < 145.5
No
Yes
No
No
Yes
No
Chol < 244
Sex < 0.5
No
No
No
Yes
Age < 52
Thal:b
ChestPain:a
Yes
No
No
No
Yes
RestECG < 1
Yes
Yes
Yes

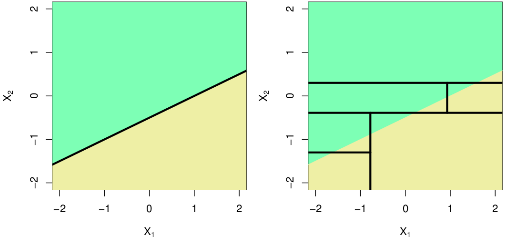
Pruning the example

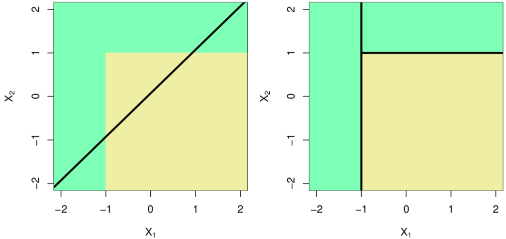




More coding!

Linear models vs trees





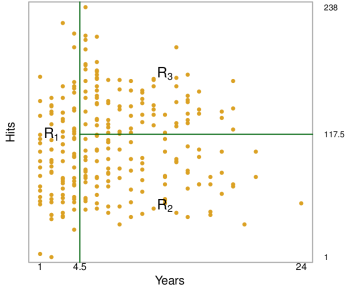
Pros/Cons

Pros:

Cons:

TL:DR

- Split into regions by greedily decreasing RSS
- Prune tree by using cost complexity
- Not robust - Next time, figure out how to aggregate trees



Next time

Lec #	Date			Reading	HW
21	Mon	10/28	Polynomial & Step Functions	7.1,7.2	
22	Wed	10/30	Step Functions; Basis functions; Start Splines	7.2 - 7.4	
23	Fri	11/1	Regression Splines	7.4	HW #6 Due Sun 11/3
24	Mon	11/4	Decision Trees	8.1	
25	Wed	11/6	Class Cancelled (Dr Munch out of town)		
26	Fri	11/8	Random Forests	8.2.1, 8.2.2	HW #7 Due Sun 11/10
27	Mon	11/11	Maximal Margin Classifier	9.1	
28	Wed	11/13	SVC	9.2	
29	Fri	11/15	SVM	9.3, 9.4	HW #8 Due Sun 11/17
30	Mon	11/18	Single layer NN	10.1	
31	Wed	11/20	Multi Layer NN	10.2	
32	Fri	11/22	CNN	10.3	HW #11 Due Sun 11/24
33	Mon	11/25	TBD: Unsupervised learning/clustering	12.1, 12.4?	
	Wed	11/27	Virtual: Project office hours		
	Fri	11/29	No class - Thanksgiving		