Data, Environment and Society: Lecture 19: Classification and regression trees

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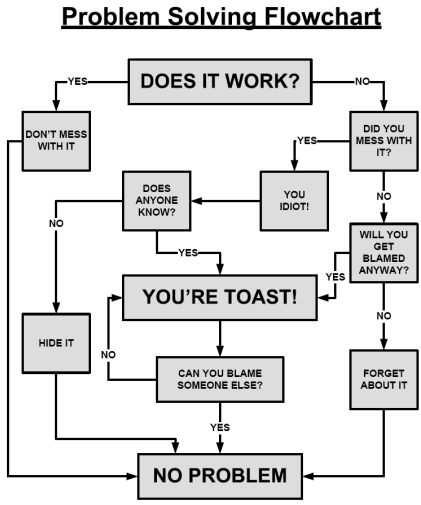
GSI: Salma Elmallah

November 5, 2019



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

Today's objectives

- Wrap up regression trees
  - How to choose with cross validation
  - Most important concept: Why we need a hyperparameter α to do cross validation
- Classification trees
  - Same as regression, just different loss functions
  - Most important concept: how the loss function affects the way you grow trees
- Boosting, bagging and random forests
  - Most important concepts: The power of crowds, and how the bias-variance tradeoff needs to be addressed.

Reading and upcoming

Reading

- Today: ISLR Ch. 8.1 - 8.2
- Next time:
  - ISLR 9.1-9.3 (Support Vector Machines)
  - Badger (NYT article on algorithm discrimination)

Upcoming

- 11/12: Guest lecture – Elinor Benami, co-author on ML for enviro monitoring paper.
- Exam review 11/14 in class, 11/18 in lab.
- Exam 11/19

Last time: where should the splits be?

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

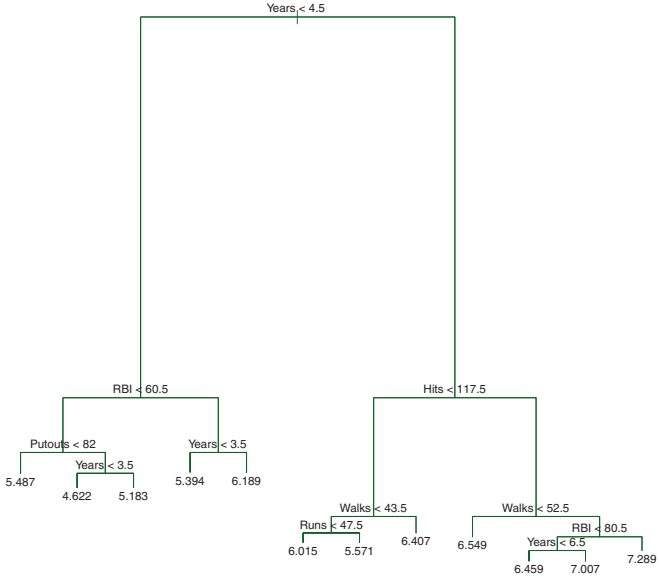
$$\{j, s\} = \arg \min_{j \in J, s \in X_j} \sum_{i: x_i \in R_1(j,s)} (y_i - \hat{y}_{R_1})^2 + \sum_{i: x_i \in R_2(j,s)} (y_i - \hat{y}_{R_2})^2$$

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.)

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).



Choosing the final tree, **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.

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- 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.)

Choosing the final tree, **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?

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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!

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Can handle nonlinear relationships better?

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.

Example: Test scores and pollution

Environmental Pollution 230 (2017) 730–740

Contents lists available at ScienceDirect

Environmental Pollution

journal homepage: www.elsevier.com/locate/envpol

Using machine learning to identify air pollution exposure profiles associated with early cognitive skills among U.S. children☆

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[b] Department of Genetics and Genomic Sciences and Icahn Institute for Genomics and Multiscale Biology, Icahn School of Medicine at Mount Sinai, New York, USA
[c] Graduate School of Biomedical Sciences, Icahn School of Medicine at Mount Sinai, New York, USA

Does pollution change cognitive ability?

Stingone et al point out that few studies have looked at the effects of multiple pollutants at once

Key data:

- Kindergarten math scores from National Center of Education Statistics Early Childhood Longitudinal Study. Randomly selected children.
- Census tract estimates of 104 toxic pollutants from U.S. Environmental Protection Agency's National Air Toxics Assessment (NATA)
- Other confounders including mother age, marital status, hhld income, etc. (Used in second stage *after* tree building.)

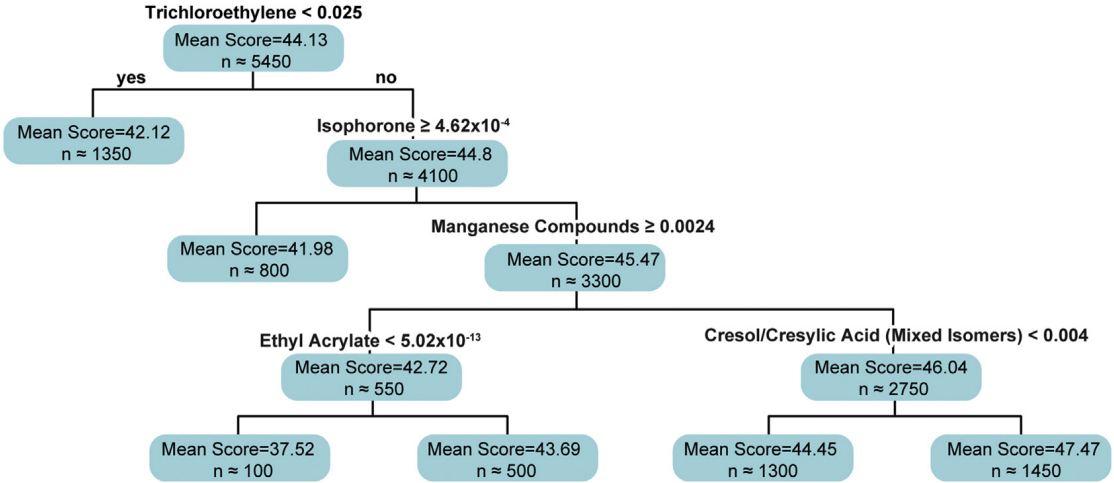
Stingone *et al* two step approach

1. Build trees for test score outcome based on pollutant exposure (what we'll focus on here)
2. Run basic multiple linear regression *within* each leaf to identify the effect of pollutants on test scores. (We won't cover this part.)

Why trees? Stingone *et al's* justification

- Easy interpretability in terms of understandable trees and/or rules,
- Ability to identify non-linear relationships between the features (exposures) and the outcome (math scores),
- Possibility of identifying interactions among the features (exposures),
- Making no/minimal assumptions about data distributions,
- Tolerance to missing values and outliers in the data,

Example result



Constructed with 10-fold cross-validation. Also used additional random partitioning – stay tuned.

A trick that Stingone *et al* used

They note that Trees are:

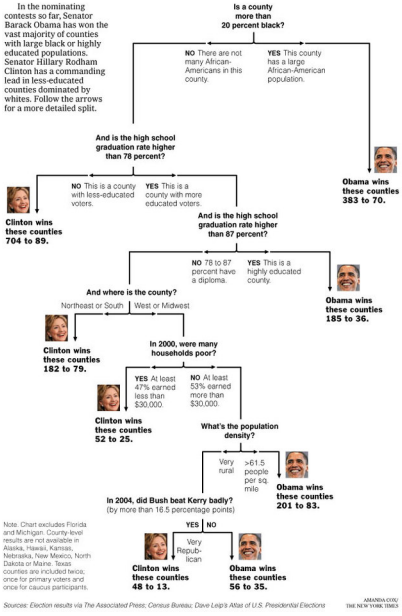
- Prone to overfitting the (training) data,
- Sensitive to small perturbations in the data and/or model/algorithm parameters

Their approach to manage this is to build a lot of different trees using random partitions of the data.

Their approach is a little unconventional (for reasons they don't provide).

Instead, we'll soon talk about formal strategies to deal with this sensitivity – boosting, bagging and random forests.

Classification trees



What's a classification tree?

As you might imagine, it's just like a regression tree, but we use it to predict a categorical or qualitative variable.

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Rather than setting the prediction equal to the mean, the prediction is:

the most commonly occurring class within the partition.

However we still use recursive binary splitting and cost-complexity pruning

Though the *criteria* for splitting and pruning will have to change

What's the error?

The typical error, RSS $= \sum_{i=1}^{N}(y_i - \hat{y}_i)^2$ won't work.

Alternatives? Let's start by defining

$$p_{mk} = \text{ fraction of observations belonging to class } k \text{ in region } m.$$

Then a simple measure is:

Classification error rate = how many training observations don't fall into the assigned class.

Within-region this is simply:

$$E_m = 1 - \max_k(\hat{p}_{mk})$$

The trouble with Classification Error

Suppose you have a two-class problem with 400 observations in each class. Consider two possible splits (S1 and S2):

S1: $R_1 : (100, 300)$, $R_2 : (300, 100) \Rightarrow$ weighted error $E_{S1} = 0.25$

S2: $R_1 : (200, 400)$, $R_2 : (200, 0) \Rightarrow$ weighted error $E_{S2} = 0.25$

$$\left[200 \times (0.33) + 200 \times (0)\right] \frac{1}{800} = 0.25$$

Can you make a case for one of these being preferable to the other?

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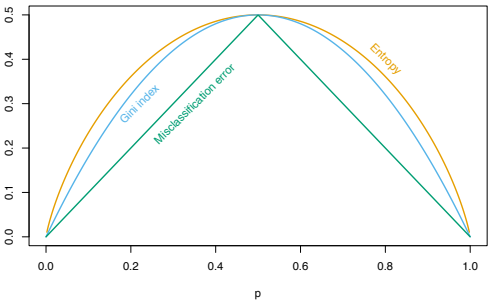
Can you make a case for one of these being preferable to the other?

S2 has a "pure" split, meaning there are *no* errors in one of the splits. You won't need to split this region any further.

Alternative errors

Remember, p_{mk} = fraction of observations in class k in region m.



(Measures for two-class classification; p is the proportion in class 2. Cross-entropy scaled to pass through (0.5, 0.5).)

$$E_m = 1 - \max_k(\hat{p}_{mk})$$

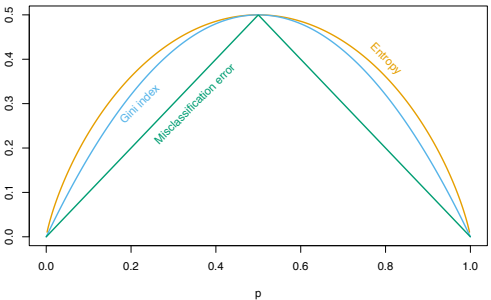
$$G_m = \sum_{k=1}^{K} \hat{p}_{mk}(1 - \hat{p}_{mk}) \quad \text{“Gini”}$$

$$D_m = -\sum_{k=1}^{K} \hat{p}_{mk} \log \hat{p}_{mk} \quad \text{“Entropy”}$$

G and D have two advantages:

1. Differentiable everywhere – good for optimization
2. Score better for “pure” splits

Why do Gini and Entropy score pure splits better?

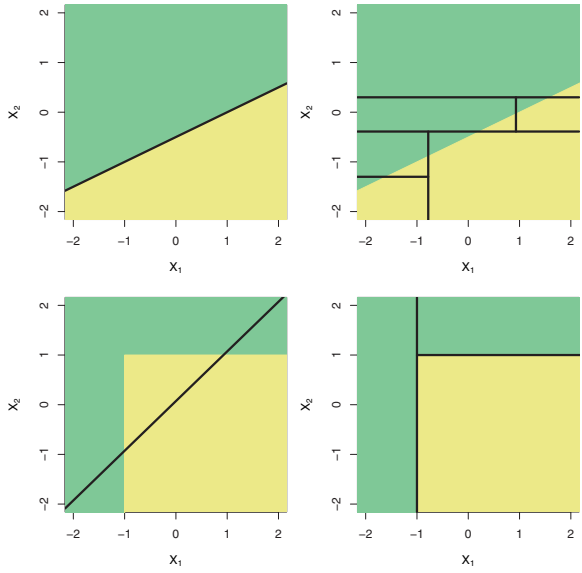


- Misclassification indifferent between
  1. two regions with $p = 0.0$ and $p = 0.4$ or
  2. two regions with $p = 0.2$ and $p = 0.2$.
- ...but Gini and cross entropy would clearly prefer the first option.

Which error rate to use?

- Since they are more "sensitive" to pure splits, it's better to use either Gini or cross-entropy when *growing* the tree.
- Any of the three measures can be used for cost-complexity pruning. Common practice is to use the misclassification rate.
  - That's because prediction is usually the final goal, and misclassification measures ability to do that.

When are trees better than linear models?



Reminder: advantages and disadvantages

Advantages

- Easy to explain and non-experts can understand the results.
- They're more like human decision-making. Doctors like them.
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Disadvantages

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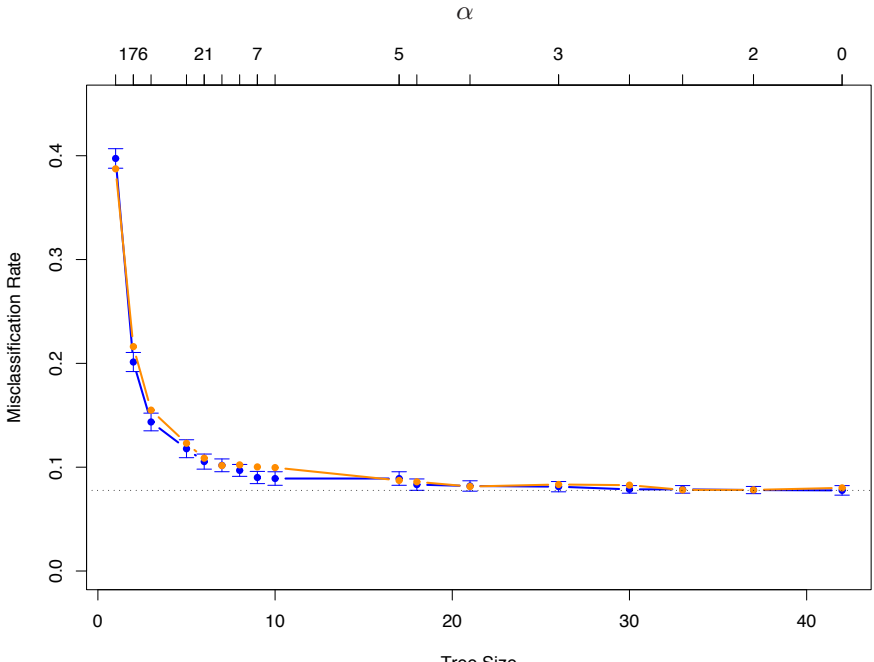
- Recursive binary splitting may generate a suboptimal tree (like forward / backward model selection). Things later in the chapter address this.

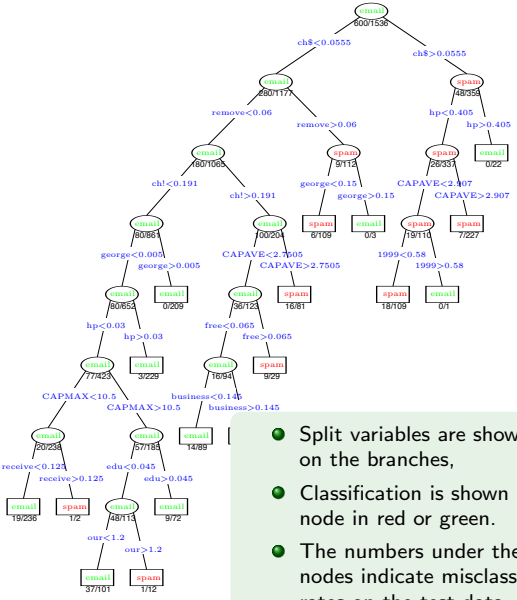
Supplemental Slides

A spam example

Email data set, donated by George Forman from HP. 4601 messages.

- 48 quantitative predictors: the percentage of words in the email that match a given word. Examples include business, address, internet, free, and george. (These could be customized for individual users.)
- 6 quantitative predictors: the percentage of characters in the email that match a given character. The characters are ch;, ch(, ch[, ch!, ch$, and ch#.
- The average length of uninterrupted sequences of capital letters: CAPAVE.
- The length of the longest uninterrupted sequence of capital letters: CAPMAX.
- The sum of the length of uninterrupted sequences of capital letters: CAPTOT.

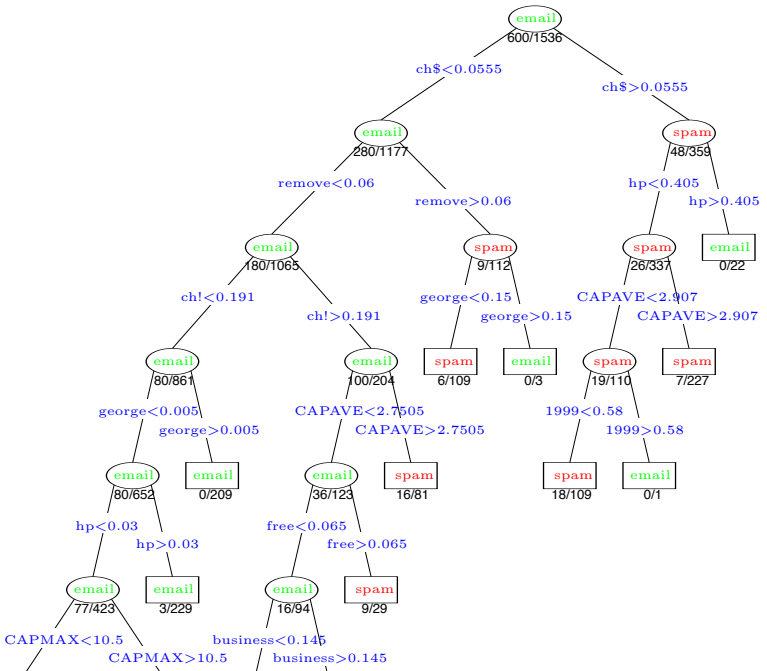

α
176
21
7
5
3
2
0
Misclassification Rate
0.0
0.1
0.2
0.3
0.4
0
10
20
30
40
Tree Size



- Split variables are shown in blue on the branches,
- Classification is shown in every node in red or green.
- The numbers under the terminal nodes indicate misclassification rates on the test data.

Figure from ESLII

A zoom in


email
600/1536
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ch$>0.0555
email
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spam
48/359
remove<0.06
remove>0.06
hp<0.405
hp>0.405
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ch!<0.191
ch!>0.191
george<0.15
george>0.15
CAPAVE<2.907
CAPAVE>2.907
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100/204
spam
6/109
email
0/3
spam
19/110
spam
7/227
george<0.005
george>0.005
CAPAVE<2.7505
CAPAVE>2.7505
1999<0.58
1999>0.58
email
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email
0/209
email
36/123
spam
16/81
spam
18/109
email
0/1
hp<0.03
hp>0.03
free<0.065
free>0.065
email
77/423
email
3/229
email
16/94
spam
9/29
CAPMAX<10.5
CAPMAX>10.5
business<0.145
business>0.145