THE UNIVERSITY OF CHICAGO

STAT 37710 / CMSC 35400 / CAAM 37710 Machine Learning

Decision Trees

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Outline

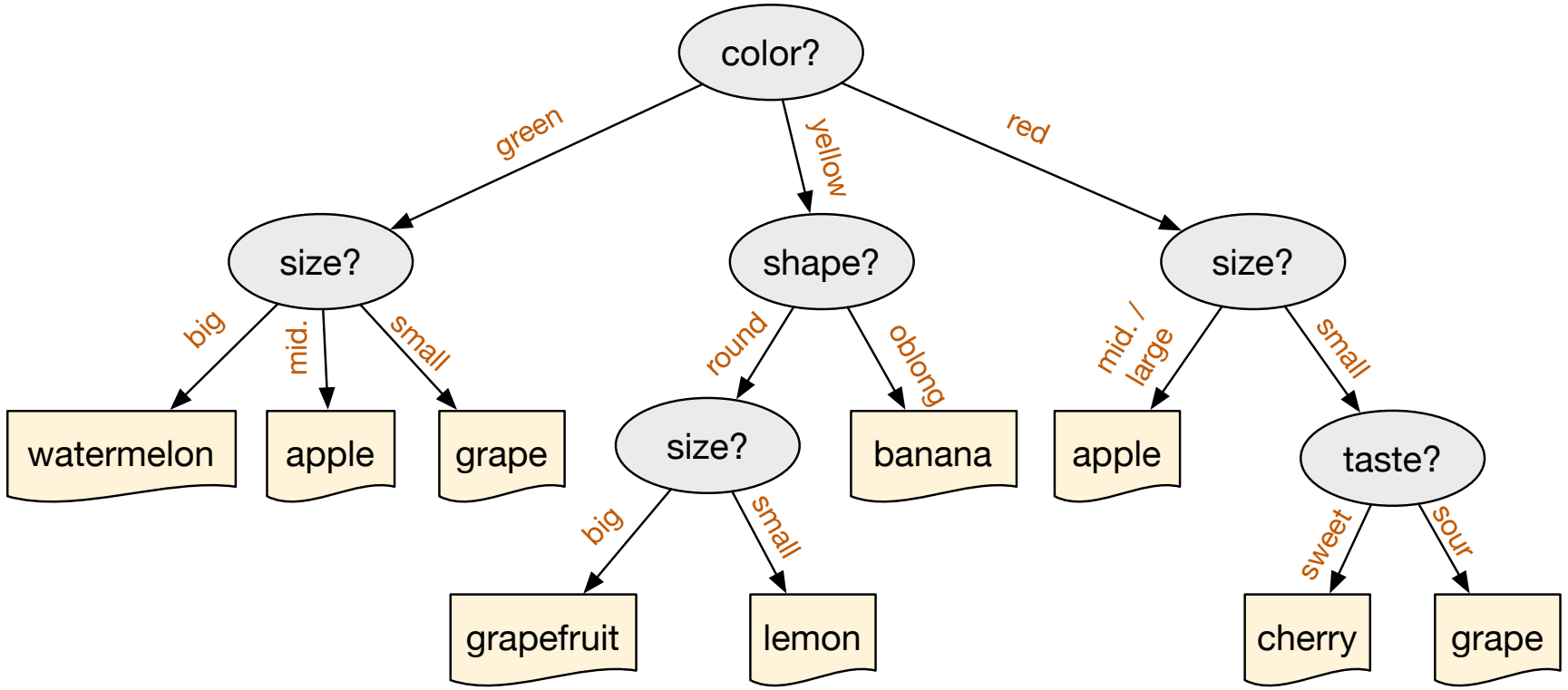
- What's a decision tree?
- Regression tree:
  - How to grow a tree: decrease in squared error
  - How to prune a tree
  - How to predict given a tree
- Classification tree
  - How to grow a tree: misclassification rate, information gain, Gini index
  - How to predict
- Summary

Tree based methods

- Divide the input space into a number of simple regions
- Use simple prediction rules in each region

Adaptive feature selection

- Prediction based on (a sequence of) decision rules

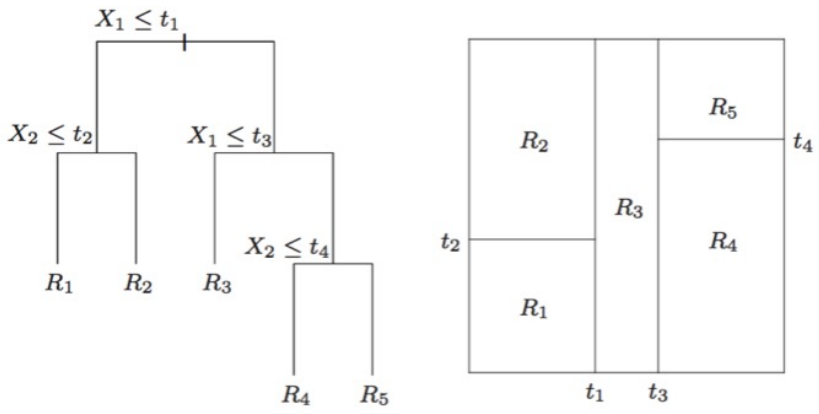


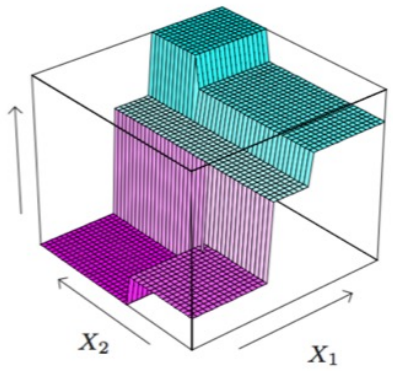
Regression trees

Trees

$$f(x) = \sum_{m=1}^{M} c_m I(x \in R_m).$$

Build a binary tree, splitting along axes





Goal

- The goal is to find boxes $R_1, \ldots, R_J$ that minimize the RSS, given by

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

where $\hat{y}_{R_j}$ is the mean response for the training observations within the jth box.

More details of the tree-building process

- Unfortunately, it is computationally infeasible to consider every possible partition of the feature space into J boxes.
- For this reason, we take a *top-down*, *greedy* approach that is known as recursive binary splitting.
- The approach is *top-down* because it begins at the top of the tree and then successively splits the predictor space; each split is indicated via two new branches further down on the tree.
- It is *greedy* because at each step of the tree-building process, the *best* split is made at that particular step, rather than looking ahead and picking a split that will lead to a better tree in some future step.

How to grow a regression tree

$$R_1(j,s) = \{X|X_j \leq s\} \text{ and } R_2(j,s) = \{X|X_j > s\}.$$

Then we seek the splitting variable j and split point s that solve

$$\min_{j,\ s}\left[\min_{c_1}\sum_{x_i\in R_1(j,s)}(y_i-c_1)^2+\min_{c_2}\sum_{x_i\in R_2(j,s)}(y_i-c_2)^2\right].$$

Pruning a tree

- The process described above may produce good predictions on the training set, but is likely to *overfit* the data, leading to poor test set performance. *Why?*
- A smaller tree with fewer splits (that is, fewer regions $R_1, \ldots, R_J$) might lead to lower variance and better interpretation at the cost of a little bias.
- One possible alternative to the process described above is to grow the tree only so long as the decrease in the RSS due to each split exceeds some (high) threshold.
- This strategy will result in smaller trees, but is too *short-sighted:* a seemingly worthless split early on in the tree might be followed by a very good split — that is, a split that leads to a large reduction in RSS later on.

Tree pruning

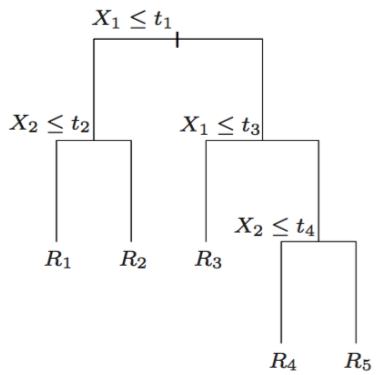
- Greedily grow the tree is prone to overfitting
- Tree pruning phase
  - Searching over all trees $\mathcal{T}$ and find the one with the best fit to data and smallest size

$$\min_{\mathcal{T}} -\sum_{v \in \mathcal{T}} L(S_v) + \lambda |\mathcal{T}|$$

- We can prune back tree branches (i.e. merge a pair of leaf nodes) recursively to choose the tree that minimizes the above objective
  - Due to the greedy nature for the growth phase, the combined growth + pruning process is not guaranteed to find the optimal tree

Learning decision trees

- Start from empty decision tree
- Split on next best attribute (feature)
  - Use, for example, information gain to select attribute
  - Split on $\arg\max_i IG(X_i) = \arg\max_i H(Y) - H(Y \mid X_i)$
- Recurse
- Prune



$$f(x) = \sum_{m=1}^{M} c_m I(x \in R_m).$$

Classification tree

- How to split a node?
- How to predict in the end?

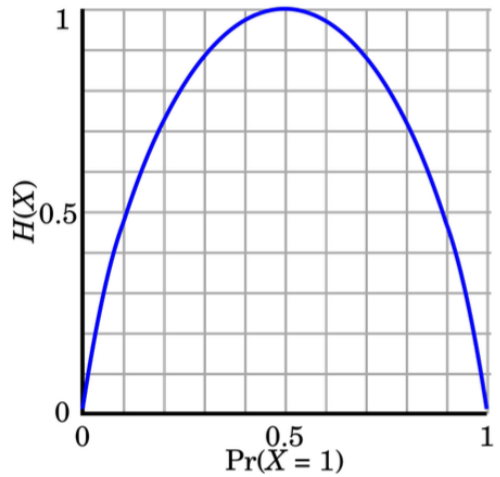
From Entropy to Info Gain: A Brief Review of Entropy

- Entropy (Information Theory)
  - A measure of uncertainty associated with a random number
  - Calculation: For a discrete random variable Y taking m distinct values $\{y_1, y_2, \ldots, y_m\}$

$$H(Y) = -\sum_{i=1}^{m} p_i \log(p_i) \quad where\ p_i = P(Y = y_i)$$

  - Interpretation
    - Higher entropy → higher uncertainty
    - Lower entropy → lower uncertainty
- Conditional entropy

$$H(Y|X) = \sum_{x} p(x) H(Y|X = x)$$



m = 2

Information Gain: An Attribute Selection Measure

- Select the attribute with the highest information gain (used in typical decision tree induction algorithm: ID3/C4.5)
- Let p_i be the probability that an arbitrary tuple in D belongs to class C_i, estimated by $|C_{i,D}|/|D|$
- Expected information (entropy) needed to classify a tuple in D:

$$Info(D) = -\sum_{i=1}^{m} p_i \log_2(p_i)$$

- Information needed (after using A to split D into v partitions) to classify D:

$$Info_A(D) = \sum_{j=1}^{v} \frac{|D_j|}{|D|} \times Info(D_j)$$

- Information gained by branching on attribute A

$$Gain(A) = Info(D) - Info_A(D)$$

Example: Attribute Selection with Information Gain

- Class P: buys_computer = "yes"
- Class N: buys_computer = "no"

$$Info(D) = I(9,5) = -\frac{9}{14}\log_2(\frac{9}{14}) - \frac{5}{14}\log_2(\frac{5}{14}) = 0.940$$

age	p_i	n_i	$I(p_i, n_i)$
<=30	2	3	0.971
31…40	4	0	0
>40	3	2	0.971

age	income	student	credit_rating	buys_computer
<=30	high	no	fair	no
<=30	high	no	excellent	no
31…40	high	no	fair	yes
>40	medium	no	fair	yes
>40	low	yes	fair	yes
>40	low	yes	excellent	no
31…40	low	yes	excellent	yes
<=30	medium	no	fair	no
<=30	low	yes	fair	yes
>40	medium	yes	fair	yes
<=30	medium	yes	excellent	yes
31…40	medium	no	excellent	yes
31…40	high	yes	fair	yes
>40	medium	no	excellent	no

12

$$Info_{age}(D) = \frac{5}{14}I(2,3) + \frac{4}{14}I(4,0) + \frac{5}{14}I(3,2) = 0.694$$

$\frac{5}{14}I(2,3)$ means "age <=30" has 5 out of 14 samples, with 2 yes'es and 3 no's.

Hence

$$Gain(age) = Info(D) - Info_{age}(D) = 0.246$$

Similarly, we can get

$$Gain(income) = 0.029$$

$$Gain(student) = 0.151$$

$$Gain(credit\_rating) = 0.048$$

Another Measure: Gini Index

- Gini index: Used in CART, and also in IBM IntelligentMiner
- If a data set D contains examples from n classes, gini index, $gini(D)$ is defined as
  - $gini(D) = 1 - \sum_{j=1}^{n} p_j^2$
    - p_j is the relative frequency of class j in D
- If a data set D is split on A into two subsets D_1 and D_2, the $gini$ index $gini(D)$ is defined as
  - $gini_A(D) = \frac{|D_1|}{|D|} gini(D_1) + \frac{|D_2|}{|D|} gini(D_2)$
- Reduction in Impurity:
  - $\Delta gini(A) = gini(D) - gini_A(D)$
- The attribute provides the smallest $gini_{split}(D)$ (or the largest reduction in impurity) is chosen to split the node (*need to enumerate all the possible splitting points for each attribute*)

16

Computation of Gini Index

- Example: D has 9 tuples in buys_computer = "yes" and 5 in "no"

$$gini(D) = 1 - \left(\frac{9}{14}\right)^2 - \left(\frac{5}{14}\right)^2 = 0.459$$

- Suppose the attribute income partitions D into 10 in D_1: {low, medium} and 4 in D_2
  - $gini_{income \in \{low,medium\}}(D) = \frac{10}{14} gini(D_1) + \frac{4}{14} gini(D_2)$

$$= \frac{10}{14}\left(1 - \left(\frac{7}{10}\right)^2 - \left(\frac{3}{10}\right)^2\right) + \frac{4}{14}\left(1 - \left(\frac{2}{4}\right)^2 - \left(\frac{2}{4}\right)^2\right) = 0.443$$

$$= Gini_{income \in \{high\}}(D)$$

  - $Gini_{\{low,high\}}$ is 0.458; $Gini_{\{medium,high\}}$ is 0.450
  - Thus, split on the {low,medium} (and {high}) since it has the lowest Gini index
- All attributes are assumed continuous-valued
- May need other tools, e.g., clustering, to get the possible split values
- Can be modified for categorical attributes

17

References & acknowledgement

- Hastie et al. (2021). “The Elements of Statistical Learning”
  - Ch 9.2 , “Tree-Based Methods”
- Willett & Chen (2020). “CMSC 35400: Machine Learning”