CSCE 421: Machine Learning

Lecture 9: Tree-Based Methods

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Goals

- Review of methods, so far!
- Feature-based challenges of linear methods
- Understand the need for non-linear methods
- Introduction to Decision Trees and models built with decision trees

- Suggested Reading: The additional, optional book "The Elements of Statistical Learning" discusses Decision Trees in great detail.

What kind of Features can Data have? A Review

Challenges of Providing Features to LR

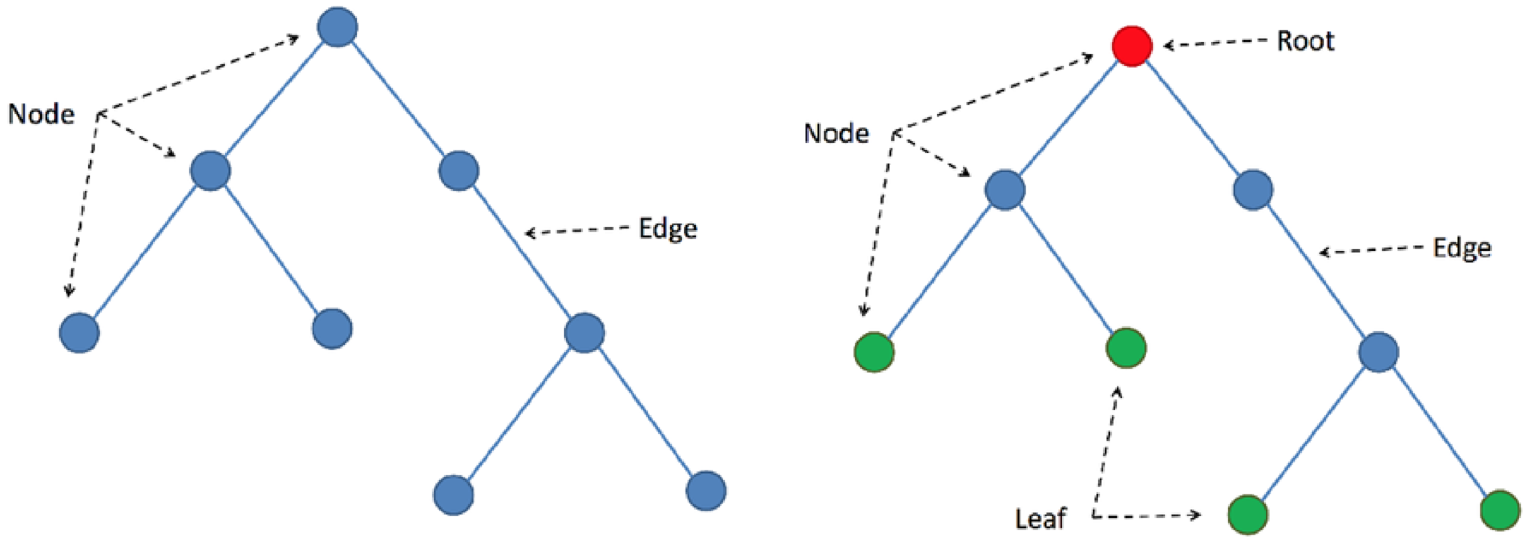
Human Decision Making: Umbrellas!

Human Decision Making: College Football

Decision Tree Data Structure

What is a decision tree

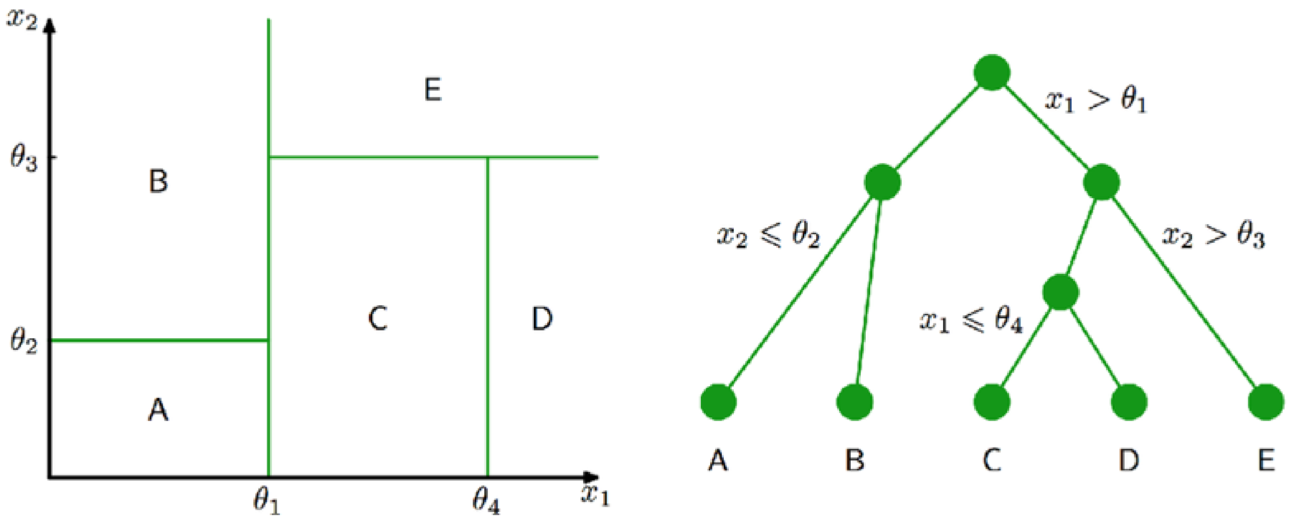
A hierarchical data structure implementing the divide-and-conquer strategy for decision making



Can be used for both classification & regression

Data Partitioning

A decision tree partitions the feature space



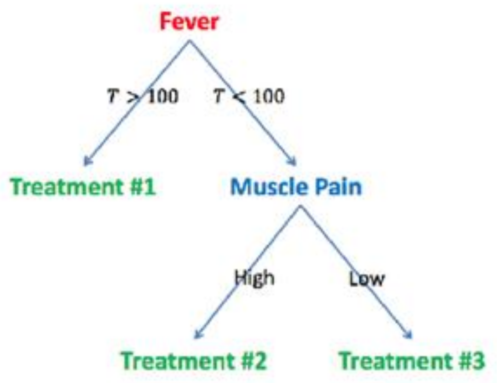
Three things to learn

- The tree structure (i.e. attributes and #branches for splitting)
- The threshold values (i.e. θ_i)
- The values of the leaves (i.e. $A, B, \ldots$)

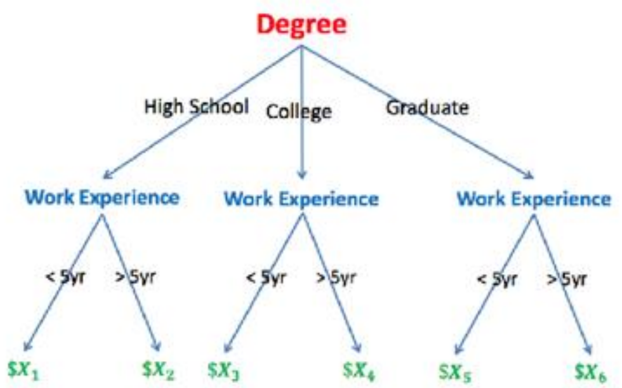
Models with Trees

Many decisions are tree-like structures

Medical treatment



Salary in a company

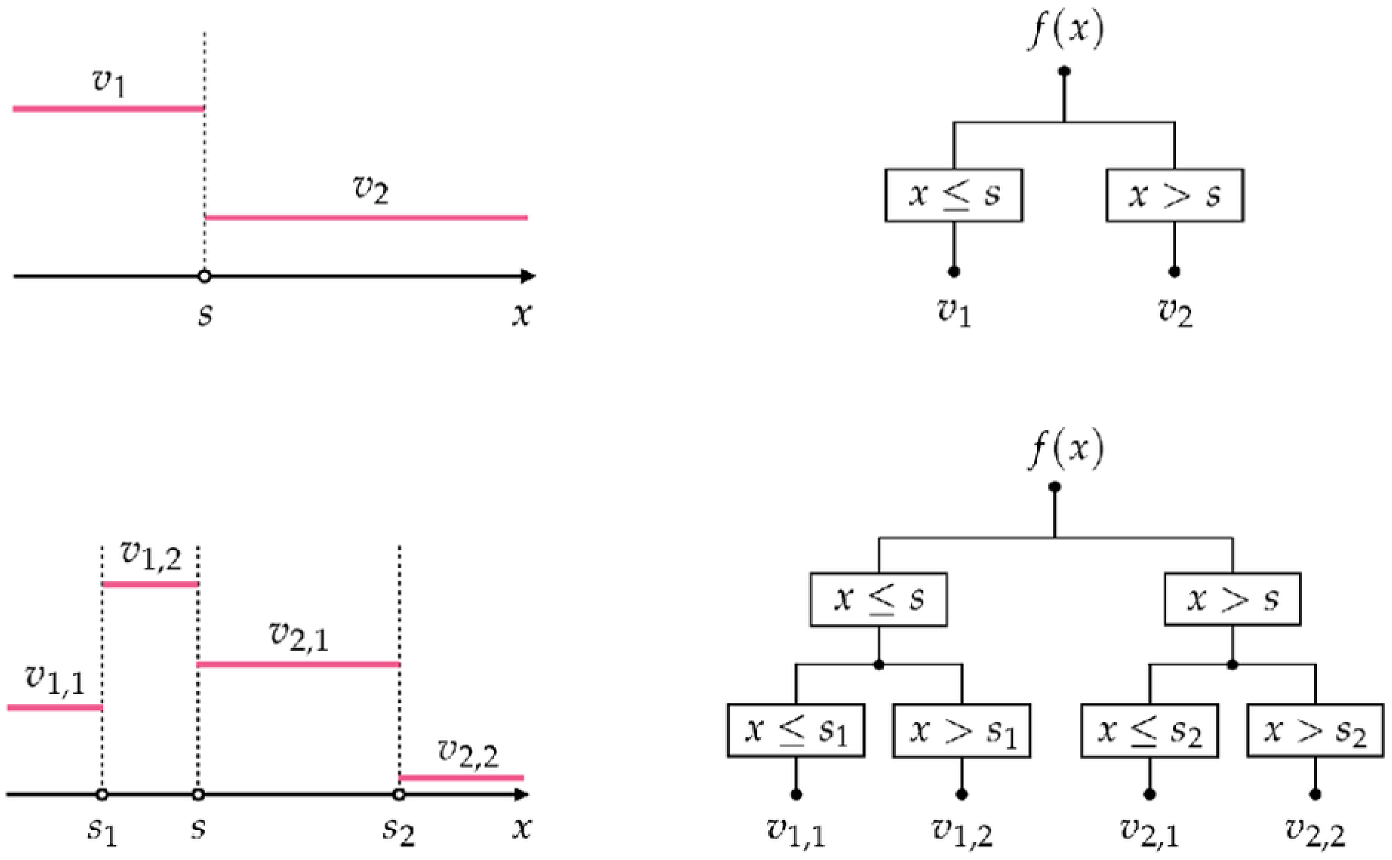


How to build trees: Decision Stumps

$$f(x) = v_1 \; if \; x \; \leq s$$
$$f(x) = \; v_2 \; if \; x > s$$

- Stump formula – this is a simple threshold for decision making
- It is easy to interpret!
- It is not very complex
- On its own, is it likely to be accurate?

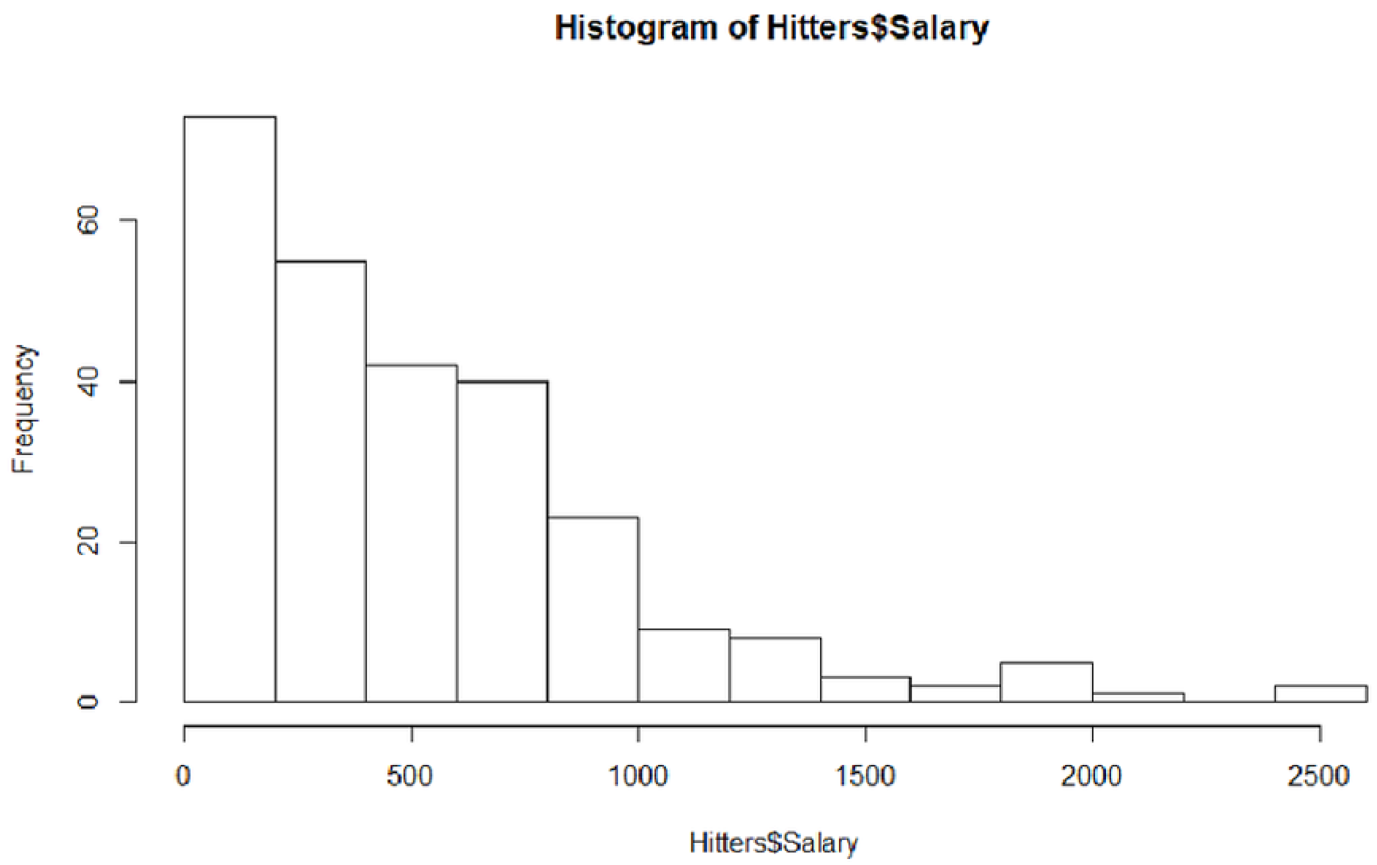
Adding Depth to Stumps



Regression for player salaries: Hitters Data

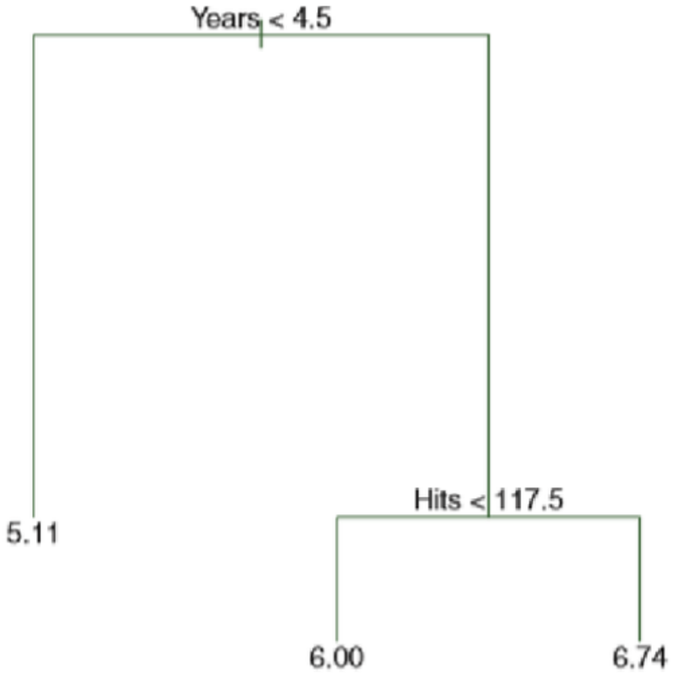
```
     AtBat            Hits          HmRun            Runs             RBI              Walks            Years       
 Min.   : 16.0   Min.   :  1   Min.   : 0.00   Min.   :  0.00   Min.   :  0.00   Min.   :  0.00   Min.   : 1.000  
 1st Qu.:255.2   1st Qu.: 64   1st Qu.: 4.00   1st Qu.: 30.25   1st Qu.: 28.00   1st Qu.: 22.00   1st Qu.: 4.000  
 Median :379.5   Median : 96   Median : 8.00   Median : 48.00   Median : 44.00   Median : 35.00   Median : 6.000  
 Mean   :380.9   Mean   :101   Mean   :10.77   Mean   : 50.91   Mean   : 48.03   Mean   : 38.74   Mean   : 7.444  
 3rd Qu.:512.0   3rd Qu.:137   3rd Qu.:16.00   3rd Qu.: 69.00   3rd Qu.: 64.75   3rd Qu.: 53.00   3rd Qu.:11.000  
 Max.   :687.0   Max.   :238   Max.   :40.00   Max.   :130.00   Max.   :121.00   Max.   :105.00   Max.   :24.000  
     CAtBat            CHits            CHmRun           CRuns             CRBI              CWalks         League 
 Min.   :   19.0   Min.   :   4.0   Min.   :  0.00   Min.   :   1.0   Min.   :   0.00   Min.   :   0.00   A:175  
 1st Qu.:  816.8   1st Qu.: 209.0   1st Qu.: 14.00   1st Qu.: 100.2   1st Qu.:  88.75   1st Qu.:  67.25   N:147  
 Median : 1928.0   Median : 508.0   Median : 37.50   Median : 247.0   Median : 220.50   Median : 170.50          
 Mean   : 2648.7   Mean   : 717.6   Mean   : 69.49   Mean   : 358.8   Mean   : 330.12   Mean   : 260.24          
 3rd Qu.: 3924.2   3rd Qu.:1059.2   3rd Qu.: 90.00   3rd Qu.: 526.2   3rd Qu.: 426.25   3rd Qu.: 339.25          
 Max.   :14053.0   Max.   :4256.0   Max.   :548.00   Max.   :2165.0   Max.   :1659.00   Max.   :1566.00          
 Division    PutOuts          Assists          Errors          Salary        NewLeague
 E:157    Min.   :   0.0   Min.   :  0.0   Min.   : 0.00   Min.   :  67.5   A:176    
 W:165    1st Qu.: 109.2   1st Qu.:  7.0   1st Qu.: 3.00   1st Qu.: 190.0   N:146    
          Median : 212.0   Median : 39.5   Median : 6.00   Median : 425.0            
          Mean   : 288.9   Mean   :106.9   Mean   : 8.04   Mean   : 535.9            
          3rd Qu.: 325.0   3rd Qu.:166.0   3rd Qu.:11.00   3rd Qu.: 750.0            
          Max.   :1378.0   Max.   :492.0   Max.   :32.00   Max.   :2460.0            
                                                           NA's   :59                
```

Salary distribution

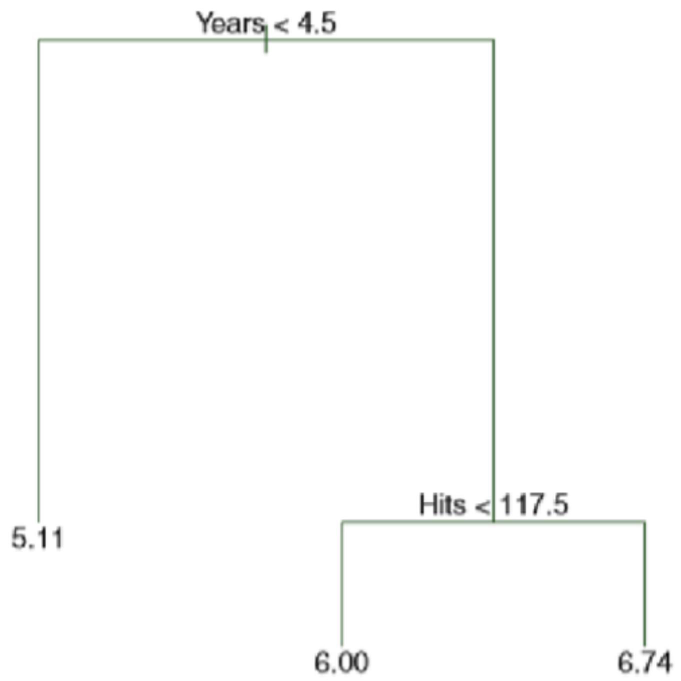


Salary distribution

Create a basic tree

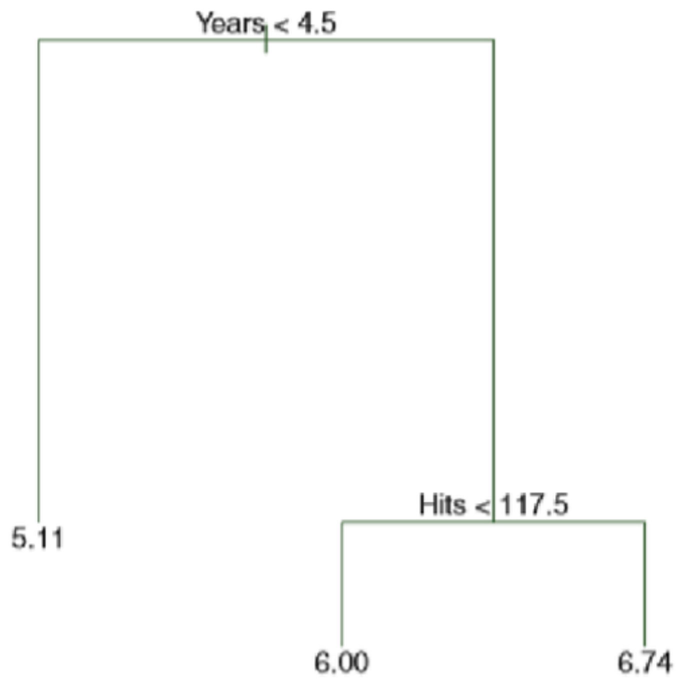


Create a basic tree



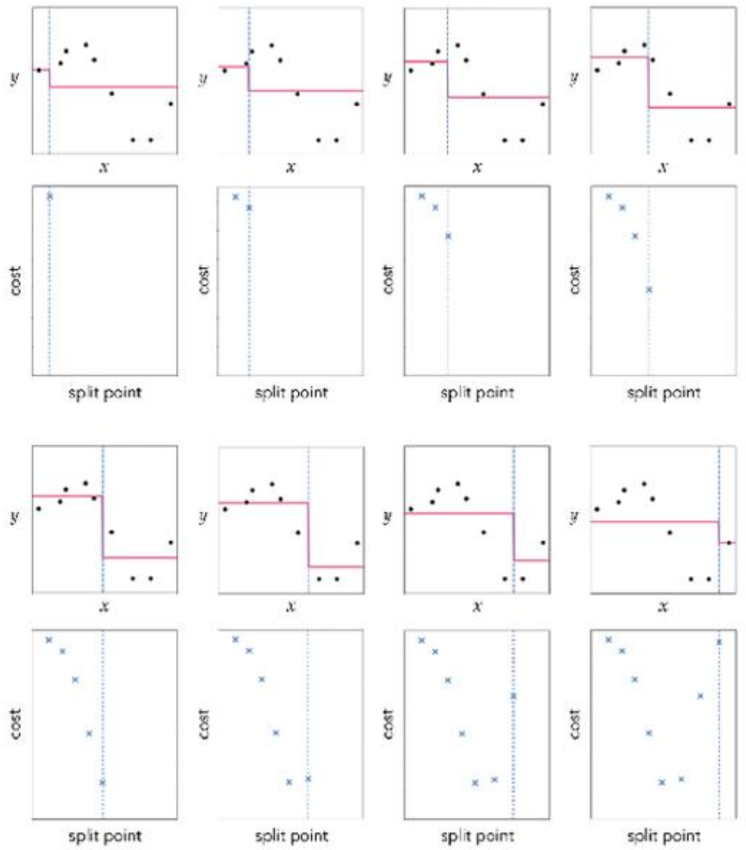
- How do we make a final prediction using this tree?

Create a basic tree

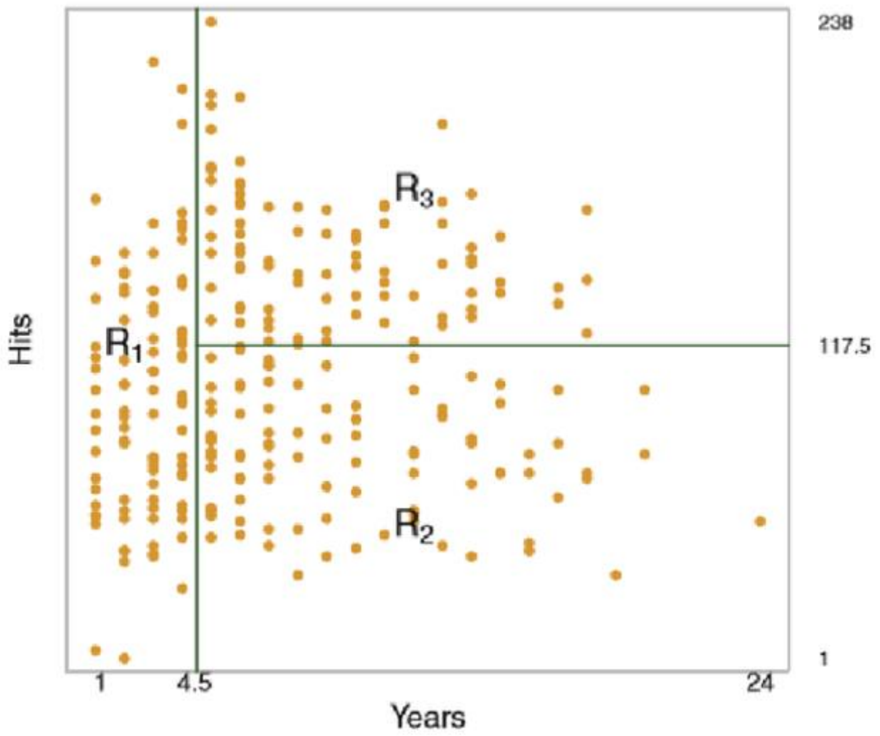


- How do we make a final prediction using this tree?
- What is the most important variable to make this prediction? Second most important variable? Third?

Partitioning the space



Partitioning hitters data



- Partition the data into regions R – again, notation check
- Each region is a leaf (or terminal) node – where decisions are made

Prediction via stratification

- Divide the predictor space $X_1, X_2,…, X_p$ into J distinct, non-overlapping regions $R_1, R_2,…, R_J$
- For every observation that falls into the region R_j we make the same prediction, which is simply the mean of the response values for the training observations partitioned into R_j
- Goal: find the partitions that minimize RSS given by:

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

Recursive Binary Splitting

- Take a top-down, greedy approach
- At each step, make the best possible split decision
- At each cut point s that splits a region into two partitions $R_1(j, s) = \{ X \mid X_j < s\}$ and $R_2(j, s) = \{ X \mid X_j \geq s\}$ that leads to the greatest minimization in RSS

Recursive Binary Splitting

- Take a top-down, greedy approach
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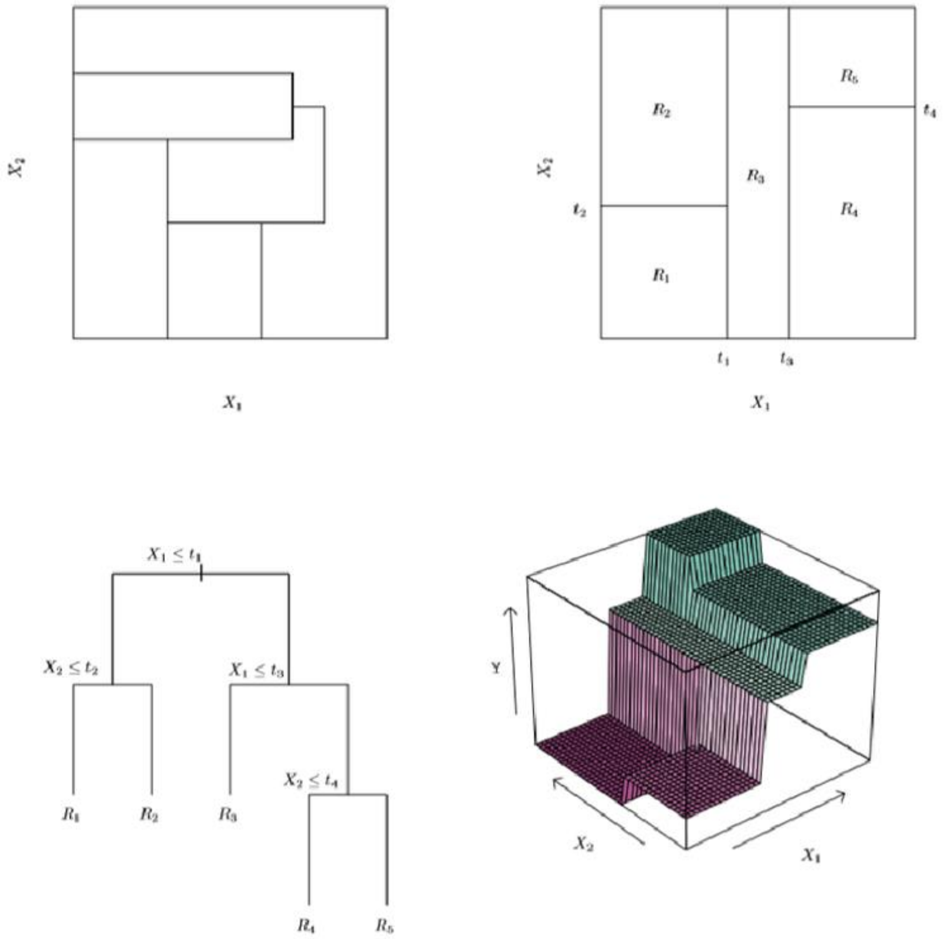
Minimize:

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

When does splitting stop?

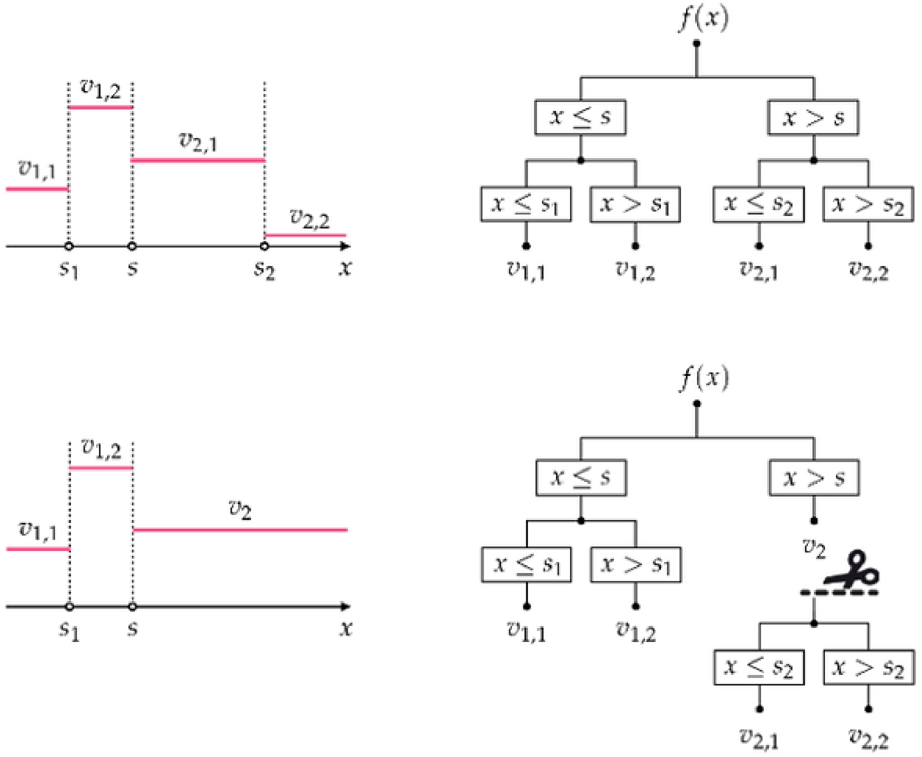


Can tree splitting lead to overfitting?

Avoiding overfitting: Pruning

- A big tree might overfit
- However, limiting the depth of a tree up front might miss key splits!
- So, best is to create the very large tree T_0 and then prune it to find the optimal subtree

Visualization: Pruning



Cost Complexity Pruning: Algorithm to build tree

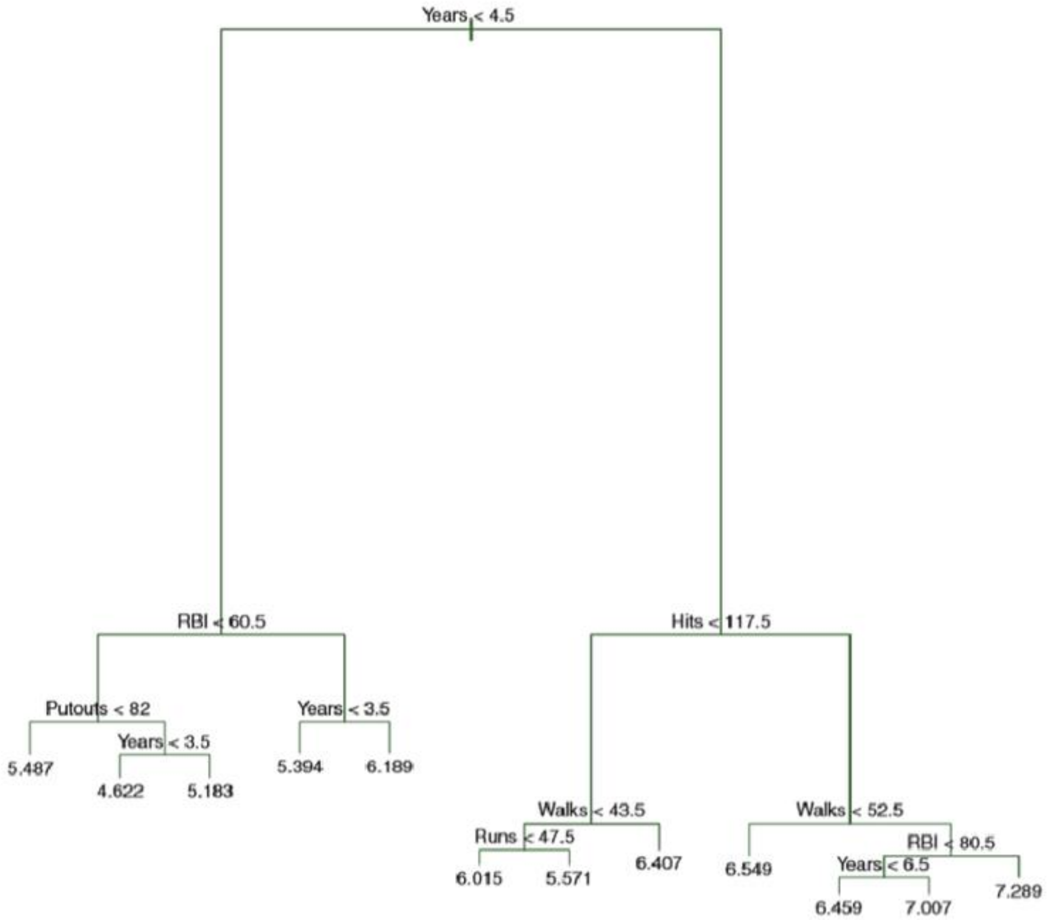
1. Use recursive binary splitting to grow a large tree on your training data
2. Stop growing tree when each terminal node has fewer than some minimum number of observations
3. Apply cost complexity pruning to the large tree in order to obtain a sequence of best subtrees, as a function of α
4. Use K-fold cross-validation to choose optimal α. That is, divide the training observations into K folds, then for each $k = 1, 2, \dots, K$:
   1. Repeat steps 1 , 2, and 3 but for the kth fold
   2. Evaluate the mean squared prediction error on the data in the left-out fold, as a function of α
   3. Average the results for each α, over all folds, and pick the α that minimizes the average error
5. Return the subtree that corresponds to the optimal α and evaluate it on your held out test set

Cost Complexity Pruning: Algorithm to build tree

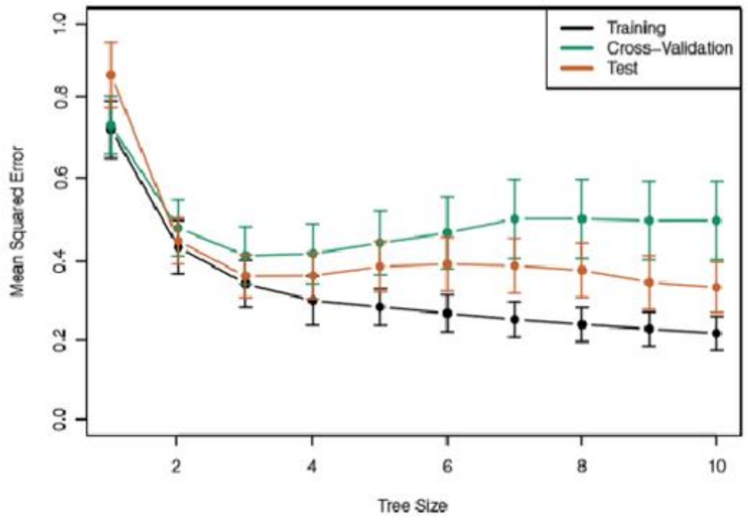
For each α, there corresponds a subtree $T \subset T_0$ with cost

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

Revisiting Baseball Salaries



Pruning hitters tree



Switching gears: Classification

- Models are the same – but rather than the mean response, we predict the most commonly-occurring class
- Much like linear regression and logistic regression, we run into trouble training with respect to the cost function:

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

Where $\hat{p}_{mk}$ is the proportion of training observations in the mth region from the kth class.
Hard to classify specific splits for each node here and grow a tree properly.

Tree-growing measures for classification

- Gini Index: measure the total variance across K classes (a measure of node purity)

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

- Entropy: takes a value near 0 if all the $\hat{p}$ are near zero or one (smaller value if the node is pure)

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

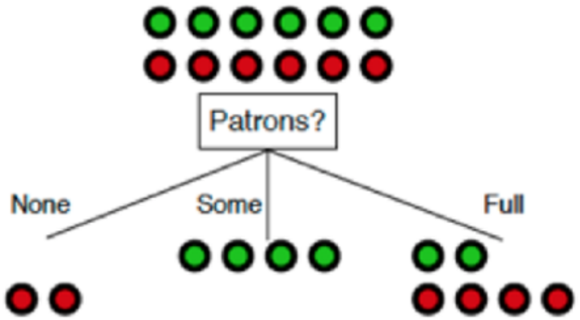
Classification: Choosing a Restaurant

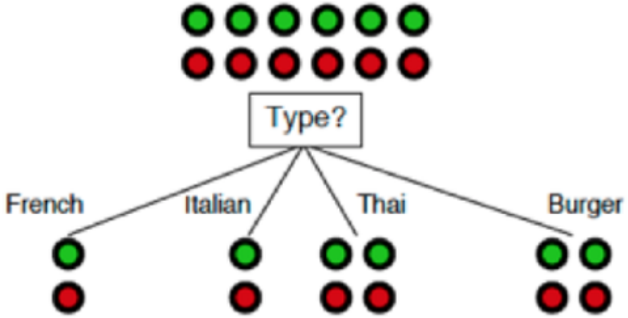
Choosing a restaurant

Example	Attributes										Target
	Alt	*Bar*	*Fri*	*Hun*	*Pat*	*Price*	*Rain*	*Res*	*Type*	*Est*	*WillWait*
X_1	*T*	*F*	*F*	*T*	*Some*	*$$$*	*F*	*T*	*French*	*0–10*	*T*
X_2	*T*	*F*	*F*	*T*	*Full*	*$*	*F*	*F*	*Thai*	*30–60*	*F*
X_3	*F*	*T*	*F*	*F*	*Some*	*$*	*F*	*F*	*Burger*	*0–10*	*T*
X_4	*T*	*F*	*T*	*T*	*Full*	*$*	*F*	*F*	*Thai*	*10–30*	*T*
X_5	*T*	*F*	*T*	*F*	*Full*	*$$$*	*F*	*T*	*French*	*>60*	*F*
X_6	*F*	*T*	*F*	*T*	*Some*	*$$*	*T*	*T*	*Italian*	*0–10*	*T*
X_7	*F*	*T*	*F*	*F*	*None*	*$*	*T*	*F*	*Burger*	*0–10*	*F*
X_8	*F*	*F*	*F*	*T*	*Some*	*$$*	*T*	*T*	*Thai*	*0–10*	*T*
X_9	*F*	*T*	*T*	*F*	*Full*	*$*	*T*	*F*	*Burger*	*>60*	*F*
X_{10}	*T*	*T*	*T*	*T*	*Full*	*$$$*	*F*	*T*	*Italian*	*10–30*	*F*
X_{11}	*F*	*F*	*F*	*F*	*None*	*$*	*F*	*F*	*Thai*	*0–10*	*F*
X_{12}	*T*	*T*	*T*	*T*	*Full*	*$*	*F*	*F*	*Burger*	*30–60*	*T*

Choosing the right split

Example	Alt	Bar	Fri	Hun	Pat	Price	Rain	Res	Type	Est	WillWait
	Attributes										Target
X_1	T	F	F	T	Some	$$$	F	T	French	0–10	T
X_2	T	F	F	T	Full	$	F	F	Thai	30–60	F
X_3	F	T	F	F	Some	$	F	F	Burger	0–10	T
X_4	T	F	T	T	Full	$	F	F	Thai	10–30	T
X_5	T	F	T	F	Full	$$$	F	T	French	>60	F
X_6	F	T	F	T	Some	$$	T	T	Italian	0–10	T
X_7	F	T	F	F	None	$	T	F	Burger	0–10	F
X_8	F	F	F	T	Some	$$	T	T	Thai	0–10	T
X_9	F	T	T	F	Full	$	T	F	Burger	>60	F
X_{10}	T	T	T	T	Full	$$$	F	T	Italian	10–30	F
X_{11}	F	F	F	F	None	$	F	F	Thai	0–10	F
X_{12}	T	T	T	T	Full	$	F	F	Burger	30–60	T





If we split the train samples with respect to the attribute "Patron", we will gain more information regarding the outcome.

Information Gain

- Intuitively, information gain tells us how important a given attribute is for predicting the outcome
- We will use it to decide the ordering of attributes in the nodes of a tree
- Main Idea: Gaining information reduces uncertainty
- From Information Theory – we learn that a measure of uncertainty is entropy

Entropy

Entropy for discrete distribution

Let X be a discrete random variable with $\{x_1, \ldots, x_N\}$ outcomes, each occurring with probability $p(x_1), \ldots, p(x_N)$.

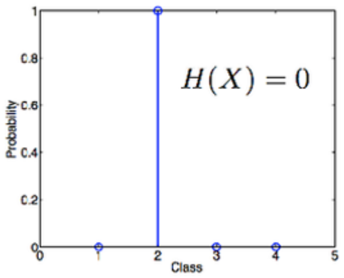
The information content of outcome x_i is inversely proportional to its probability, $h(x_i) = \log \frac{1}{p(x_i)}$

The entropy of the random variable X is the average information content of the outcomes:

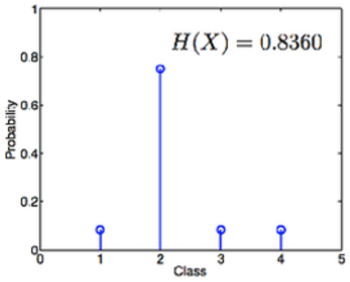
$$H(X) = \sum p(x_i) \log(\frac{1}{p(x_i)}) = -\sum p(x_i) \log(p(x_i))$$

Example

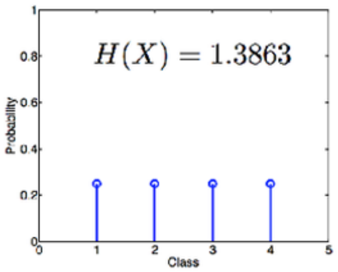
no uncertainty



some uncertainty

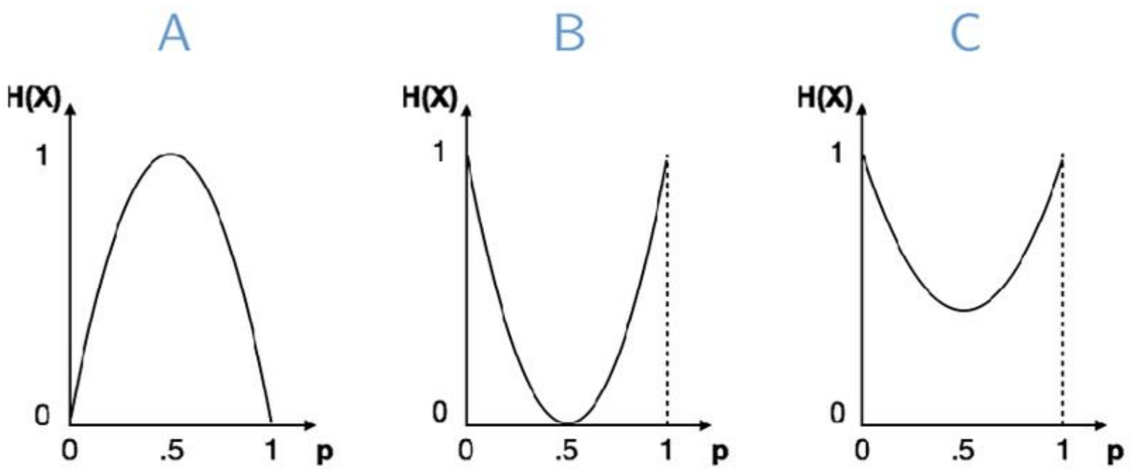


high uncertainty



Entropy: Coin Toss

Suppose $X \sim Bernoulli(p)$ with $X \in \{0, 1\}$, i.e. coin toss with probability p of getting heads and $1 - p$ of getting tails. What would be a correct plot for the entropy $H(X)$ in relation to the probability of getting heads?



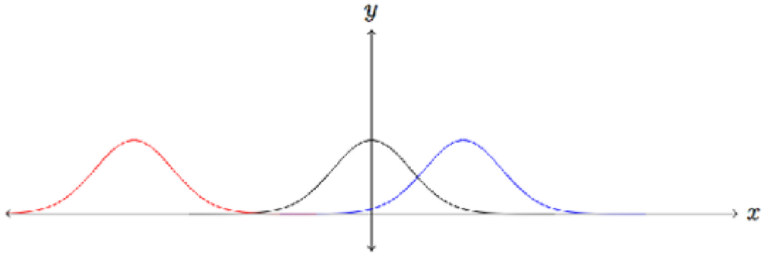
Entropy for continuous distributions

Let X be a continuous random variable with $x \in \Omega$. Its entropy is defined as follows:

$$H(X) = -\int_{x \in \Omega} p(x) \log(p(x)) dx$$

Example

If $X \sim \mathcal{N}(\mu, \sigma^2)$ its entropy is $H(X) = \frac{1}{2}(1 + \log(2\pi\sigma^2))$.
The entropy depends on the variance of the Gaussian.
i.e. higher variance $\rightarrow$ higher uncertainty, and vice-versa.



Gaussians with the same σ, therefore same entropy.

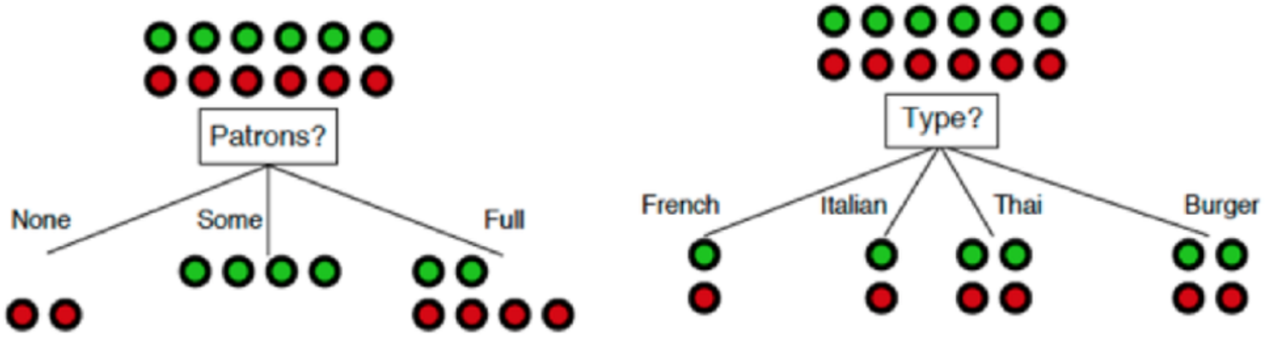
Conditional Entropy

We want to quantify how much uncertainty the realization of a random variable X has if the outcome of another random variable Y is known. The conditional entropy is defined as:

$$
\begin{aligned}
H(X|Y) &= \sum_{m=1}^{M} p_Y(y_m) H_{X|Y=y_m}(X) \\
&= \sum_{m=1}^{M} p_Y(y_m) \left(-\sum_{n=1}^{N} p_{X|Y}(x_n|y_m) \log(p_{X|Y}(x_n|y_m)) \right) \\
&= -\sum_{m=1}^{M} \sum_{n=1}^{N} p_Y(y_m) p_{X|Y}(x_n|y_m) \log(p_{X|Y}(x_n|y_m))
\end{aligned}
$$

Entropy: Choosing a restaurant

Example	Attributes										Target
	Alt	*Bar*	*Fri*	*Hun*	*Pat*	*Price*	*Rain*	*Res*	*Type*	*Est*	*WillWait*
X_1	T	F	F	T	Some	$$$	F	T	French	0–10	T
X_2	T	F	F	T	Full	$	F	F	Thai	30–60	F
X_3	F	T	F	F	Some	$	F	F	Burger	0–10	T
X_4	T	F	T	T	Full	$	F	F	Thai	10–30	T
X_5	T	F	T	F	Full	$$$	F	T	French	>60	F
X_6	F	T	F	T	Some	$$	T	T	Italian	0–10	T
X_7	F	T	F	F	None	$	T	F	Burger	0–10	F
X_8	F	F	F	T	Some	$$	T	T	Thai	0–10	T
X_9	F	T	T	F	Full	$	T	F	Burger	>60	F
X_{10}	T	T	T	T	Full	$$$	F	T	Italian	10–30	F
X_{11}	F	F	F	F	None	$	F	F	Thai	0–10	F
X_{12}	T	T	T	T	Full	$	F	F	Burger	30–60	T



If we split the train samples with respect to the attribute "Patron", we will gain more information regarding the outcome.

Entropy example: patrons

Measuring the conditional entropy on each of the "Patrons" attributes

For "None" branch

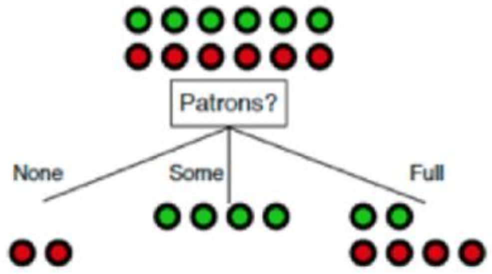
$$-\left(\frac{0}{0+2}\log\frac{0}{0+2}+\frac{2}{0+2}\log\frac{2}{0+2}\right)=0$$

For "Some" branch

$$-\left(\frac{4}{4+0}\log\frac{4}{4+0}+\frac{4}{4+0}\log\frac{4}{4+0}\right)=0$$

For "Full" branch

$$-\left(\frac{2}{2+4}\log\frac{2}{2+4}+\frac{4}{2+4}\log\frac{4}{2+4}\right)\approx 0.9$$



Measuring the conditional entropy on Patrons

$$H(Outcome|Patron)=\tfrac{2}{12}\times 0+\tfrac{4}{12}\times 0+\tfrac{6}{12}\times 0.9=0.45$$

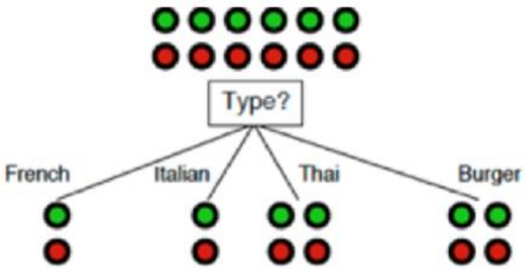
"How uncertain is the Outcome with respect to attribute Patrons"

Entropy example: type

Measuring the conditional entropy on each of the "Type" attributes

For "French" branch

$$-\left(\frac{1}{1+1}\log\frac{1}{1+1}+\frac{1}{1+1}\log\frac{1}{1+1}\right)=1$$



For "Italian" branch

$$-\left(\frac{1}{1+1}\log\frac{1}{1+1}+\frac{1}{1+1}\log\frac{1}{1+1}\right)=1$$

For "Thai" and "Burger" branches

$$-\left(\frac{2}{2+2}\log\frac{2}{2+2}+\frac{2}{2+2}\log\frac{2}{2+2}\right)=1$$

For choosing "Type"

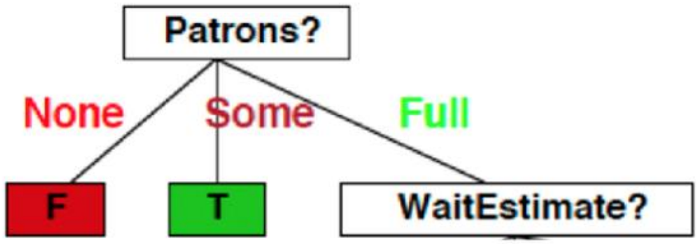
Measuring the conditional entropy on Type

$$H(Outcome|Type)=\tfrac{2}{12}\times 1+\tfrac{2}{12}\times 1+\tfrac{4}{12}\times 1+\tfrac{4}{12}\times 1=1$$

"How uncertain is the Outcome with respect to attribute Type"

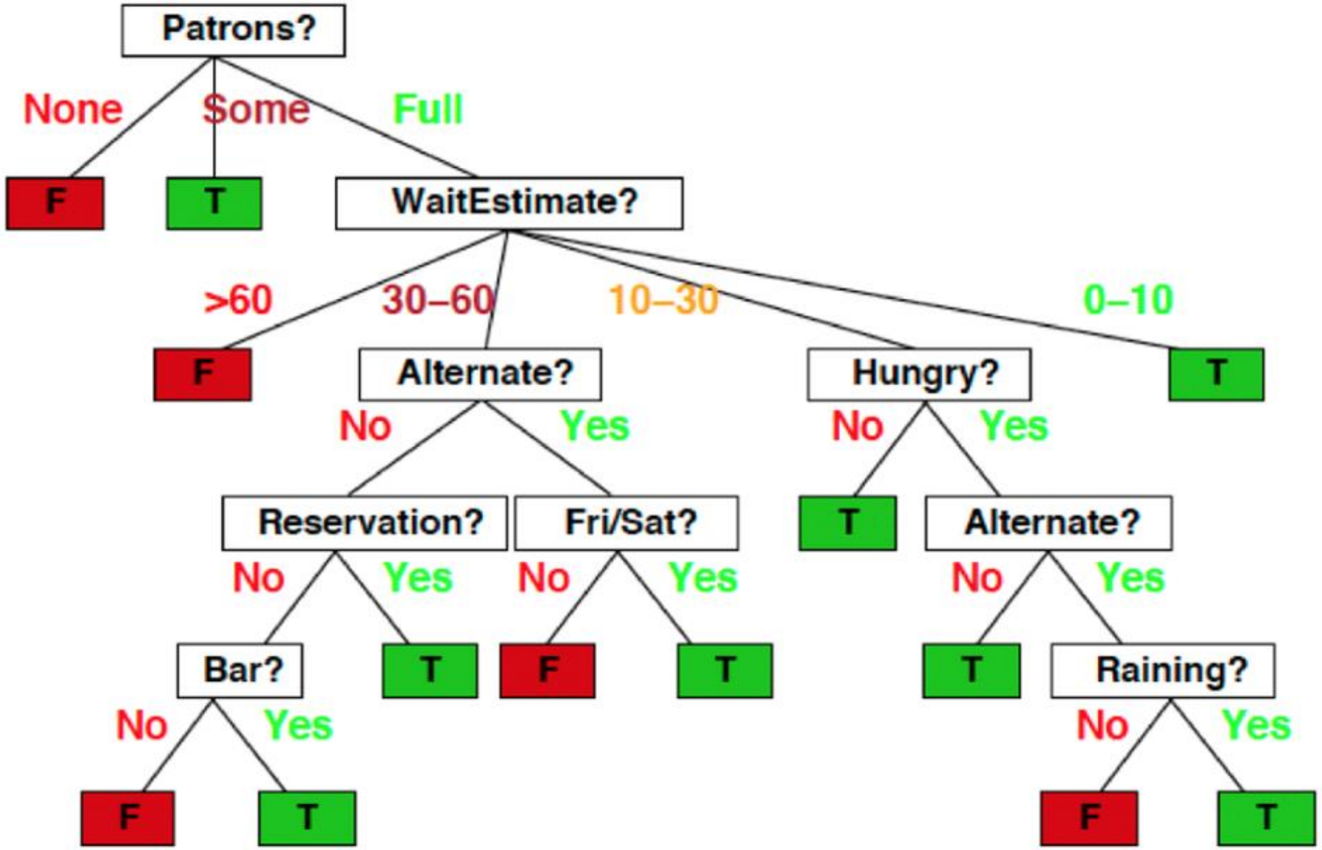
Choosing a restaurant: Building the tree

- The entropy, conditioned on outcome, for patron is the smallest
- So the first split, with respect to the tree, is performed on patrons
- We do not split the none node or some node since the decision is deterministic
- Now we need to determine the next split:



Final decision tree

Greedily we build the tree and looks like this



Classification trees

GenerateTree($\mathcal{X}$) (Input $\mathcal{X}$: training samples)

1 $i := SplitAttribute(\mathcal{X})$ (find attribute with lowest uncertainty)

2 For each branch of $\mathbf{x_i}$

  2a Find $\mathcal{X}_i$ falling in branch

  2b GenerateTree($\mathcal{X}_i$)

SplitAttribute($\mathcal{X}$) (Input $\mathcal{X}$: training samples)

1 $MinEnt := MAX$

2 For all attributes X_i, $i = 1, \ldots, D$

  2a Compute $H(Y|\mathcal{X}_i)$ (entropy of attribute X_i)

  2b If $MinEnt > H(Y|\mathcal{X}_i)$ (current attribute X_i has the lowest entropy so far)

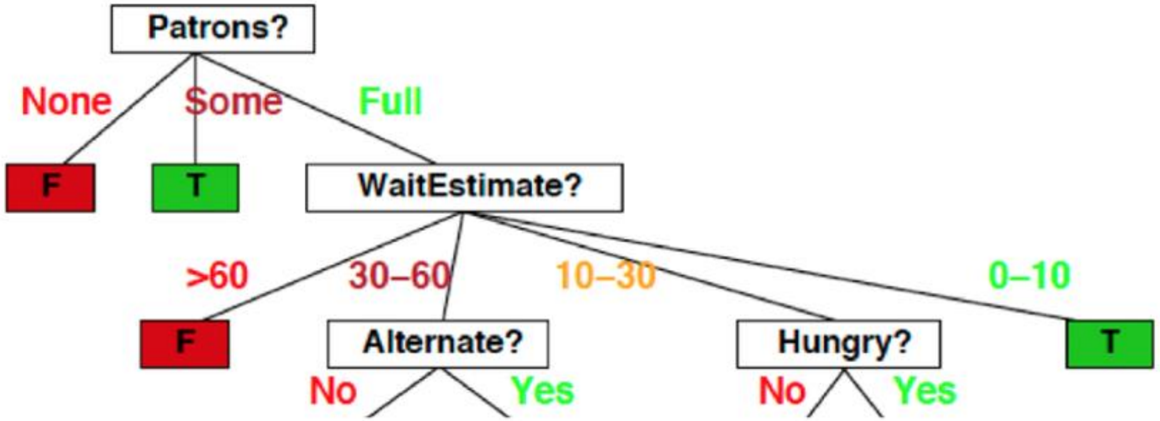
    2b.i $MinEnt := H(Y|\mathcal{X}_i)$

    2b.ii $SplitAttr := i$

3 Return $SplitAttr$

Pruning classification trees

We should prune some of the leaves of the tree to get a smaller depth



- If we stop here, not all training samples are classified correctly
- How do we classify a new instance?
  - We label the leaves of this smaller tree with the label of the majority of training samples

Two types of pruning

- Pre-Pruning
  - Stop growing the tree earlier, before it perfectly classifies the training set
  - Use a min entropy parameter θ_I
- Post-Pruning
  - Grow the tree full until no training error
  - Trim the nodes of the decision tree in a bottom-up fashion
  - If generalization error improves after trimming, replace sub-tree by a leaf node
    - Class label of leaf node is determined from majority class of instances in the sub-tree

Pre-pruning algorithm

GenerateTree($\mathcal{X}$) (Input $\mathcal{X}$: training samples)

1 If $Entropy(\mathcal{X}) < \theta_I$ (very small uncertainty)

  1a Create leaf labelled by majority class in $\mathcal{X}$

2 Else

  2a $i := SplitAttribute(\mathcal{X})$ (find attribute with lowest uncertainty)

  2b For each branch of $\mathbf{x_i}$

    2b.i Find $\mathcal{X}_i$ falling in branch

    2b.ii GenerateTree($\mathcal{X}_i$)

What if we don't use entropy?

2-class problem

$\hat{p}$, $1-\hat{p}$: frequency of class 0 and 1

- Entropy:
  $\phi(\hat{p}) =$
  $-\hat{p}\log\hat{p} - (1-\hat{p})\log(1-\hat{p})$
- Gini index:
  $\phi(\hat{p}) = 2\hat{p}(1-\hat{p})$
- Misclassification error:
  $\phi(\hat{p}) = 1 - \max(\hat{p}, 1-\hat{p})$

C-class problem

$\hat{p}_1,\ldots,\hat{p}_C$: frequency of class $1,\ldots,C$

- Entropy:
  $\phi(\hat{p}_1,\ldots,\hat{p}_C) =$
  $-\sum_c \hat{p}_c \log\hat{p}_c$
- Gini index:
  $\phi(\hat{p}_1,\ldots,\hat{p}_C) =$
  $\sum_c \hat{p}_c(1-\hat{p}_c)$
- Misclassification error:
  $\phi(\hat{p}_1,\ldots,\hat{p}_C) = 1 - \max_c(\hat{p}_c)$

Classification and Regression Trees

- Split criterion:
  - Regression tree: mean squared error between predicted and actual value of samples at that note
  - Classification tree: node purity
- Leaf node value:
  - Regression: mean of samples that have reached that node
  - Classification: majority class

Decision trees vs. other models

- Advantages:
  - Models are transparent: easily interpretable!
  - Data can contain combination of feature types: Qualitative predictors without dummy variables
  - Decision trees more closely mirror human decision making
  - Graphical representation
- Disadvantages:
  - Usually not same level of predictive accuracy
  - Not robust (small change in the data can change the tree a lot)

Building to random forests

- What if we grow a large number of trees?
- Bagging (Bootstrap Aggregating)
  - Generate independent bootstrapped datasets from the original data
  - Build decision tree on each of them
  - Predict across all the trees (majority voting)
- Randomize over the set of attributes
  - Before growing each bootstrapped decision tree, limit the features it can use
  - Don’t prune trees (keep them small)

Random Forest

- Very good performance in practice
- Runs efficiently on large data sets
- Runs efficiently on large feature sets
- Gives estimates of the most relevant variables for each problem
- NEXT TIME!

Key Takeaways

- Decision Trees
  - Hierarchical structure to perform classification and regression
  - Tree structure determined by splitting criterion
  - Pruning
    - Prevents overfitting by limiting depth of tree
    - Avoids perfect performance on the train set
  - Interpretable
- Random Forests
  - Ensemble model of lots of trees
  - Good performance in practice where individual decision trees fail