CS60050
Machine Learning

Decision Trees

Somak Aditya
Assistant Professor
Department of CSE
August 16, 2023

Sudeshna Sarkar
Professor
CoE AI, Department of CSE

Recap

- Learning problem (classification)

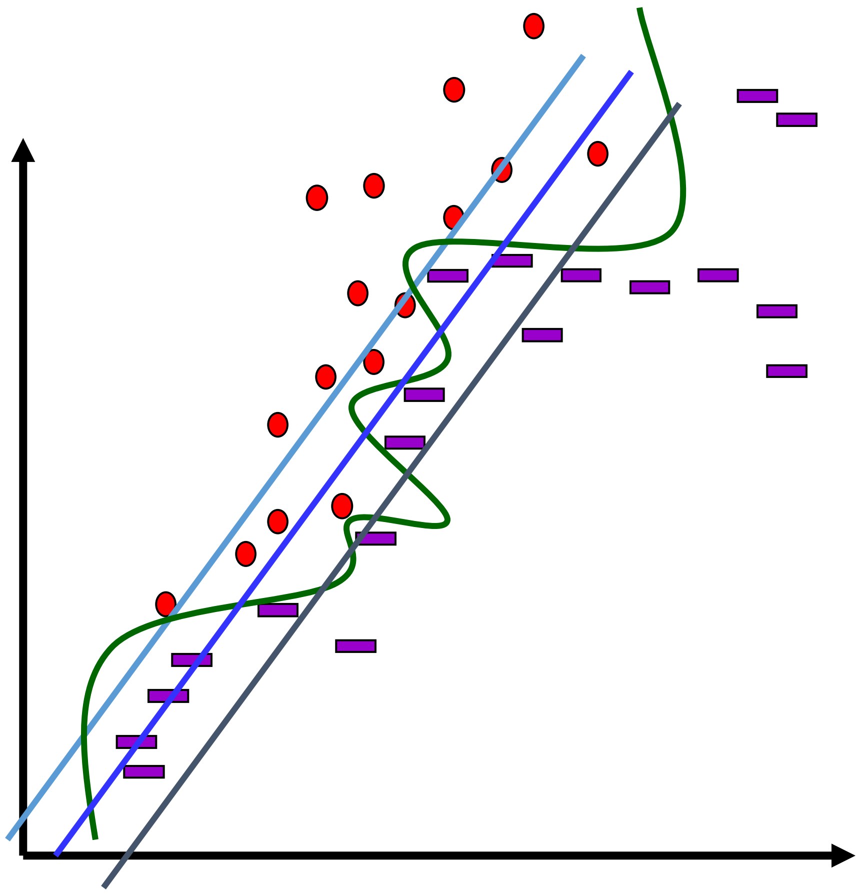
  Find a function that

  best separates the data

- What function?

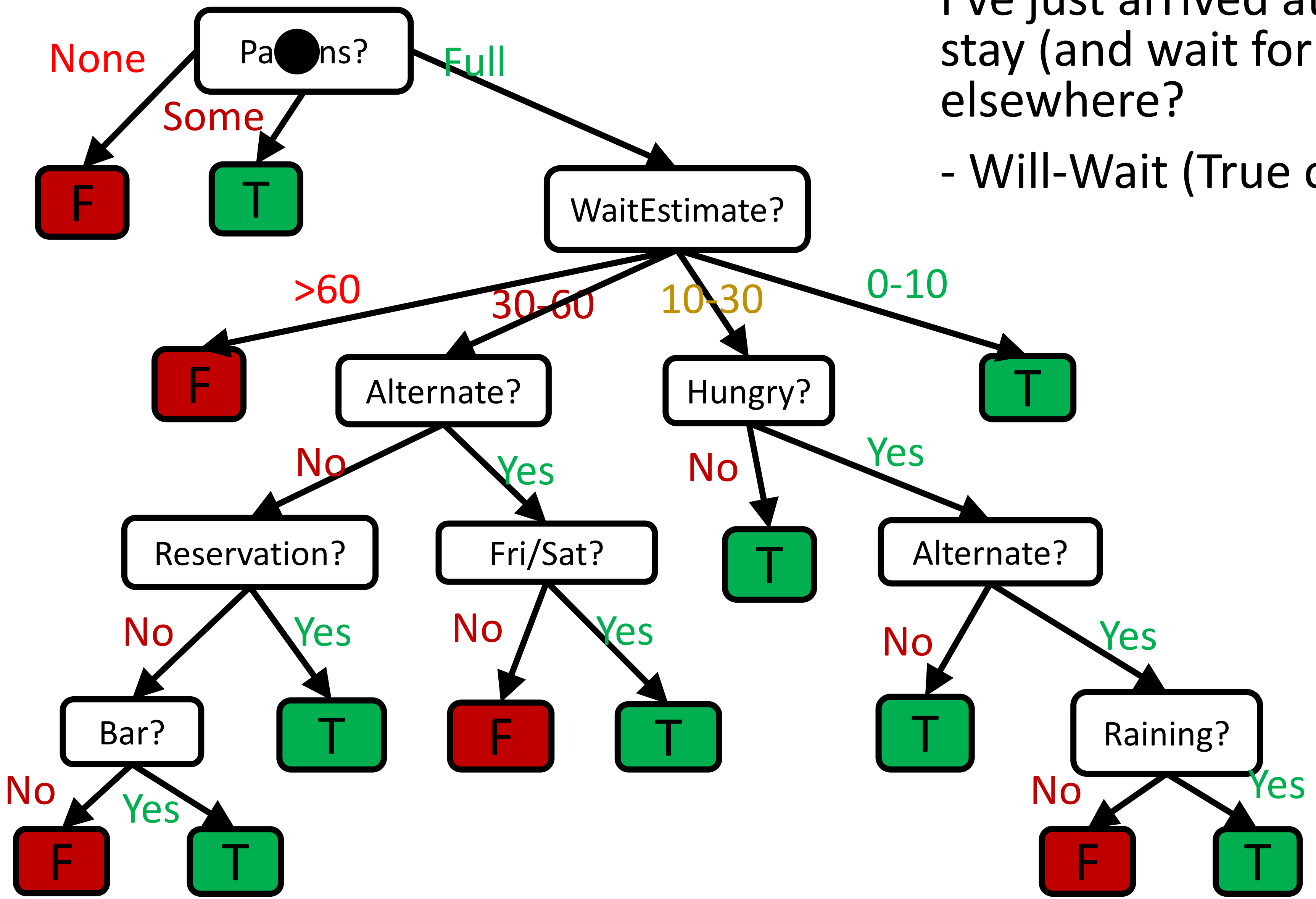
Linear:

$$Y = \mathbf{sign}\left(\boldsymbol{\theta}^{T}\boldsymbol{X}\right)$$



- **Limitations of Linear Functions**

Decision Trees



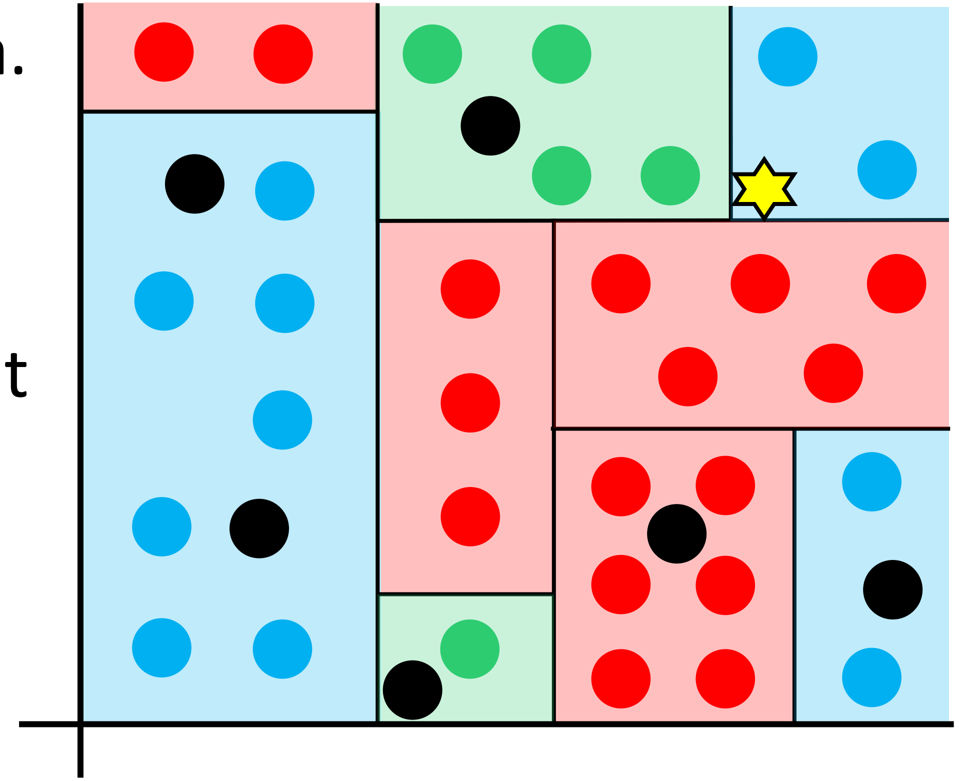
I've just arrived at a restaurant: should I stay (and wait for a table) or go elsewhere?

- Will-Wait (True or False?)

Slide credit: ai.berkeley.edu

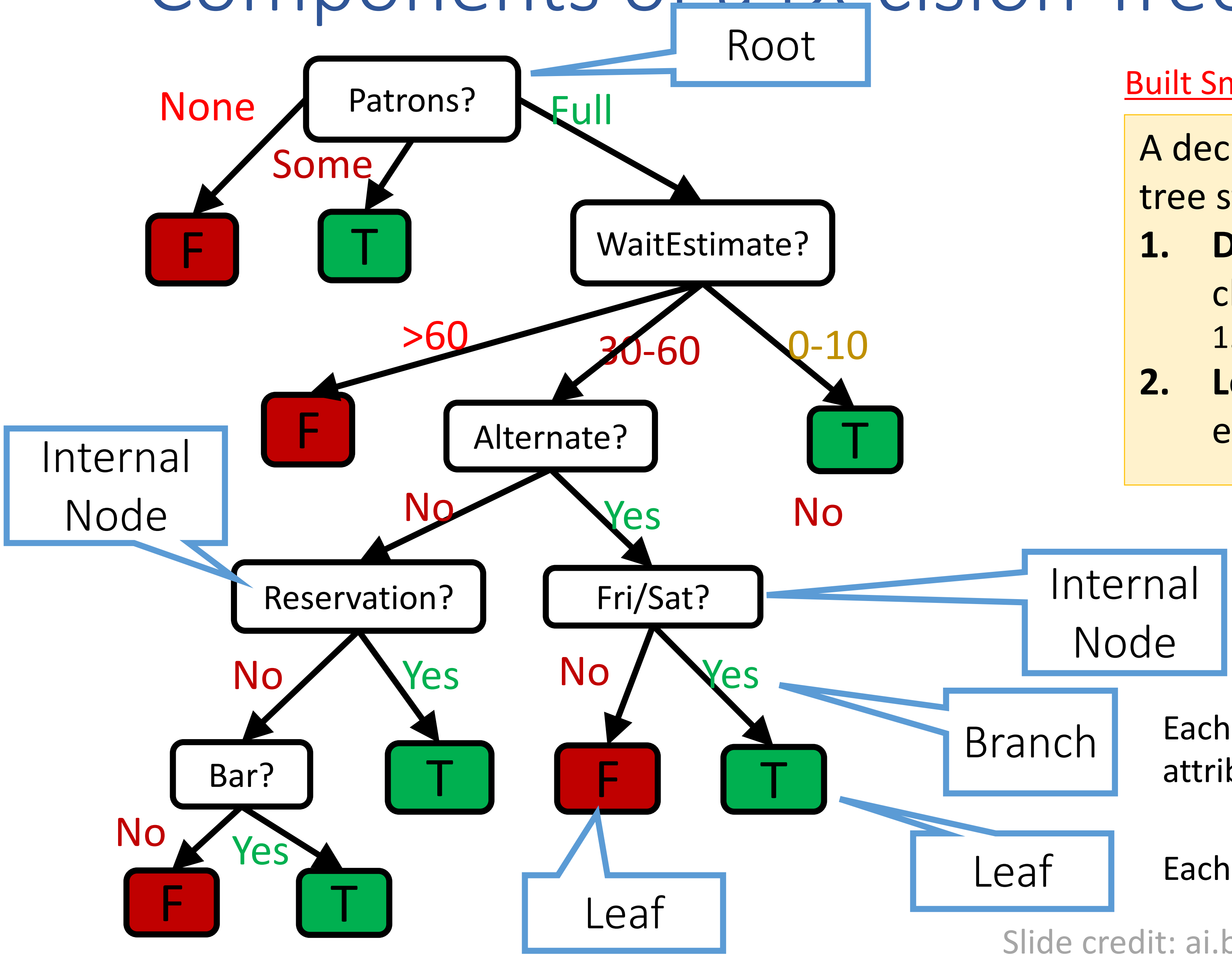
Decision Trees for Classification

- Find ”many” lines that best “separates” the data.
- Repeatedly partition feature space $\mathbb{R}^d$
- Assign a label to each partition.
- For test data point, easy to find which partition it lies



This illustration’s credit: Purushottam Kar

Components of a Decision Tree



Built Smaller for Illustration

A decision tree is a classifier in the form of a tree structure with two types of nodes:

1. **Decision node (Internal)**: Specifies a choice or test of some attribute
   1. An outcome ➔ A branch
2. **Leaf node**: Indicates classification of an example

Each internal node tests an attribute

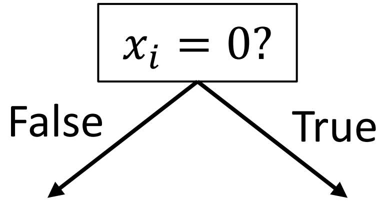
Each branch corresponds to an attribute value node

Each leaf node assigns a classification

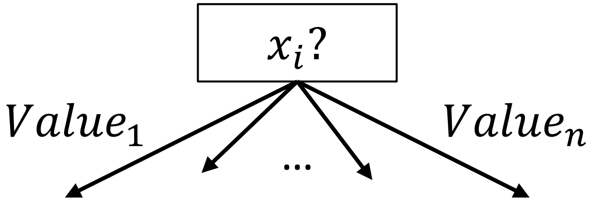
Slide credit: ai.berkeley.edu, Illustration: Purushottam Kar, IITK

Type of Internal Tests

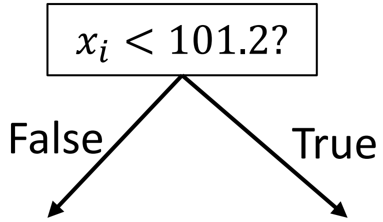
Binary Feature



Categorical Feature



Numeric Feature



Types of Leaves

Classification

$\boxed{y = POS}$

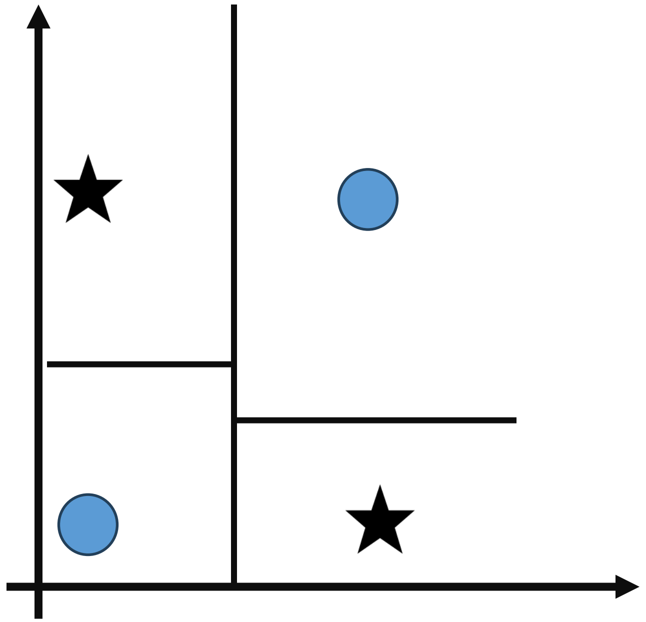
Regression

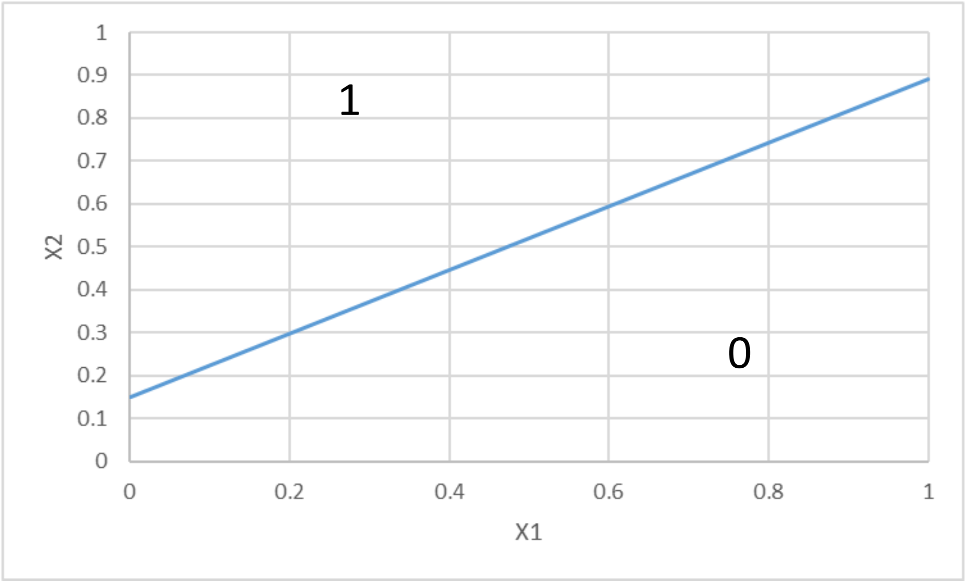
$\boxed{y = 5.2}$

Probability Estimate

$$\boxed{\begin{array}{l} \mathrm{p}(y = 0) = \ .3 \\ p(y = 1) = \ .3 \\ p(y = 2) = \ .4 \end{array}}$$

Decision Trees vs Linear Models



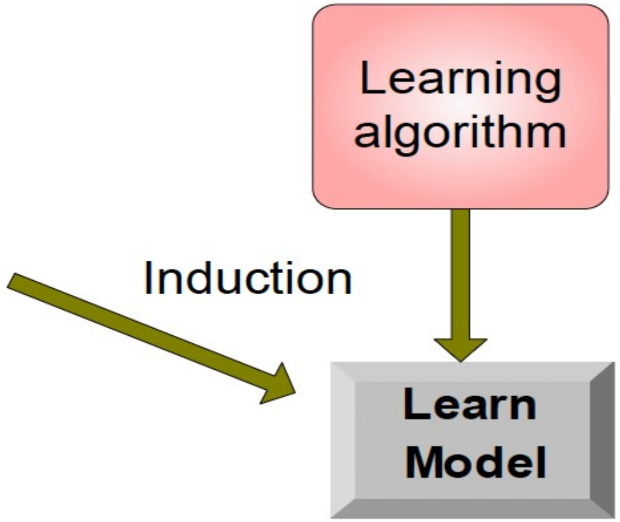


Adding nodes (structure) allows more powerful representation

Classification in a Nutshell

Tid	Attrib1	Attrib2	Attrib3	Class
1	Yes	Large	125K	No
2	No	Medium	100K	No
3	No	Small	70K	No
4	Yes	Medium	120K	No
5	No	Large	95K	Yes
6	No	Medium	60K	No
7	Yes	Large	220K	No
8	No	Small	85K	Yes
9	No	Medium	75K	No
10	No	Small	90K	Yes

Training Set



Tid	Attrib1	Attrib2	Attrib3	Class
11	No	Small	55K	?
12	Yes	Medium	80K	?
13	Yes	Large	110K	?
14	No	Small	95K	?
15	No	Large	67K	?

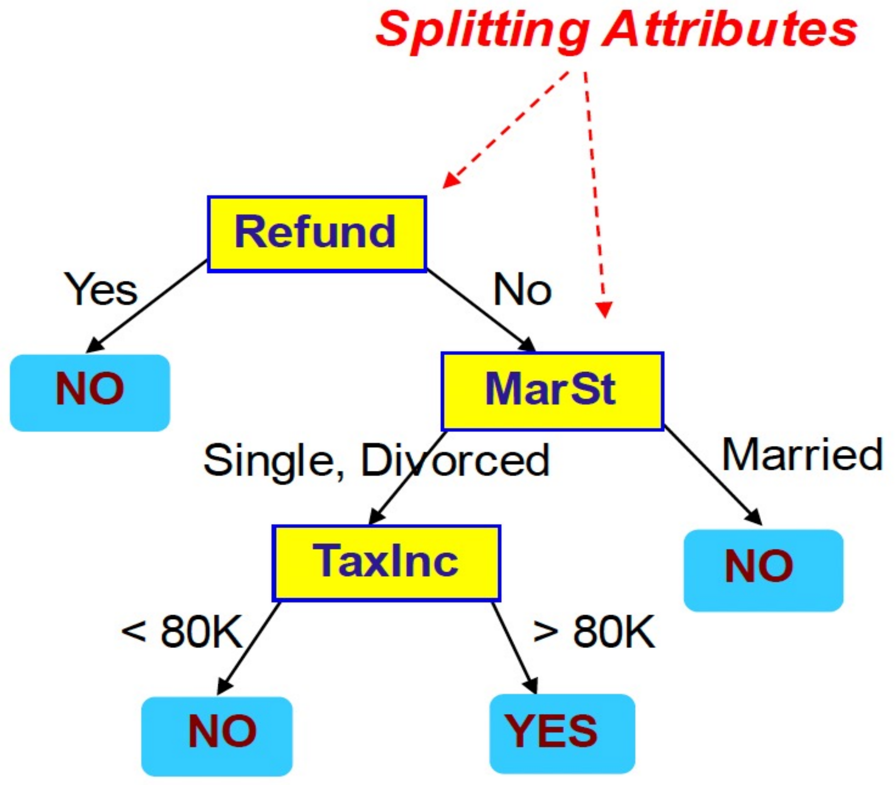
Test Set

Learning Decision Tree from Data

categorical categorical continuous class

Tid	Refund	Marital Status	Taxable Income	Cheat
1	Yes	Single	125K	No
2	No	Married	100K	No
3	No	Single	70K	No
4	Yes	Married	120K	No
5	No	Divorced	95K	Yes
6	No	Married	60K	No
7	Yes	Divorced	220K	No
8	No	Single	85K	Yes
9	No	Married	75K	No
10	No	Single	90K	Yes

Training Data



Model: Decision Tree

Issues

- Given some training examples, what decision tree should be generated?
- One proposal: learn the smallest tree that is fits the data
- Possible method:
  - Exhaustive search over the space of decision trees
  - This is NP-hard.

- *Efficient algorithms available to learn a reasonably accurate (potentially suboptimal) decision tree in reasonable time*
  - *Employs greedy strategy*
  - *Locally optimal choices about which attribute to use next to partition the data*

Building a Decision Tree (GREEDY)

Function BuildTree(dataset,attributes) returns a DT

dataset : dataset at current node, *attributes*: current set of attributes

If *attributes* is empty OR

all labels in *dataset* are the same:

Leaf node

class = most common class in *dataset*

else

Internal node

att ⇐ CHOOSE-BEST-ATTRIBUTE(*dataset*, *attributes*)

Binary Test

tree ← A new DT with root test *att*

LeftNode = BuildTree(*dataset*(*att* =1), *attributes* −{*att*})

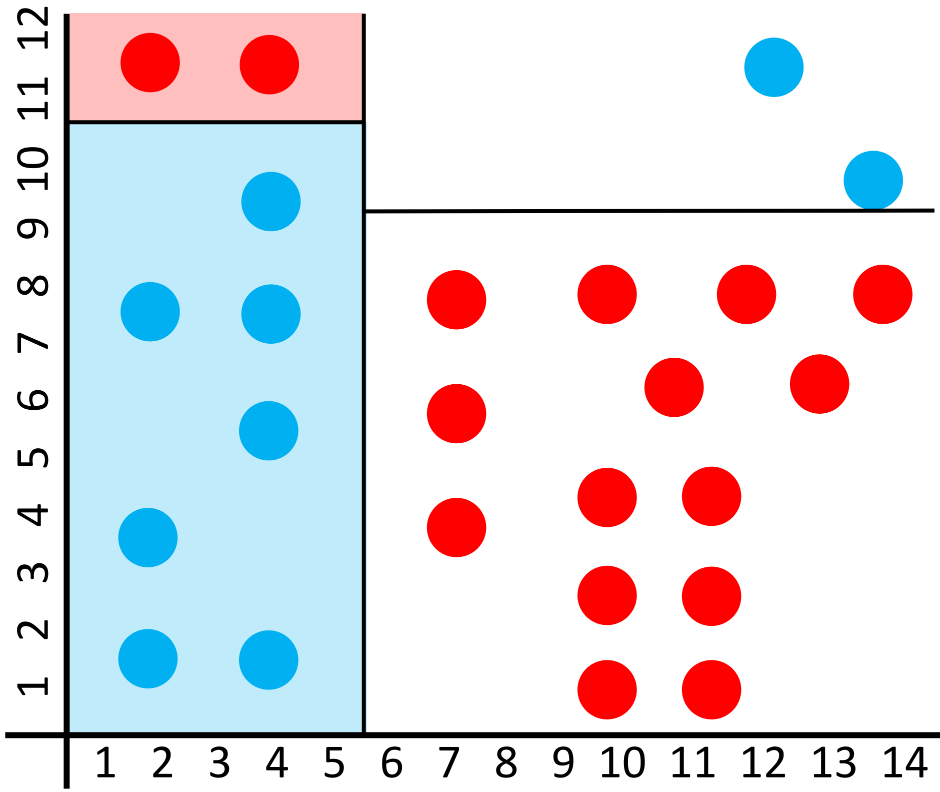
RightNode = BuildTree(*dataset*(*att* =0), *attributes* −{*att*})

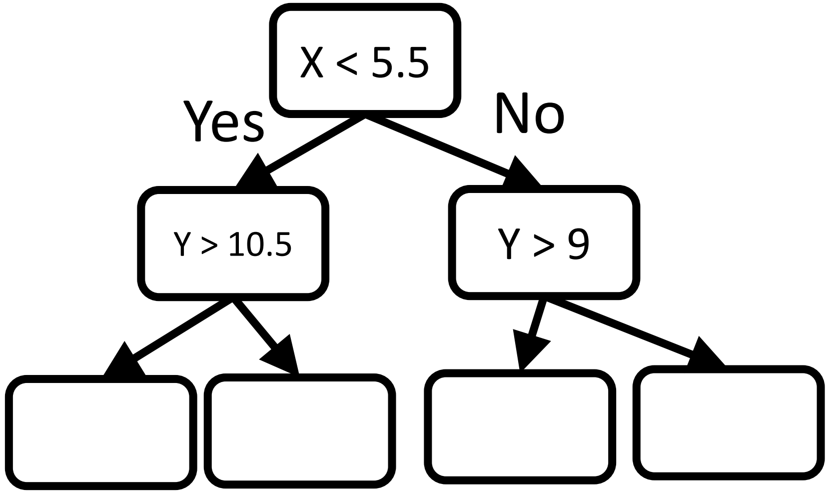
add branch to tree with value 1, subtree LeftNode

add branch to tree with value 0, subtree RightNode

generalize for multiple values

return tree





Decision Tree (Learn & Predict)

Function BuildTree(dataset,attributes) returns a DT

dataset : dataset at current node, *attributes*: current set of attributes

If *attributes* is empty OR

all labels in *dataset* are the same:

Leaf node

class = most common class in *dataset*

else

Internal node

att ⇐ CHOOSE-BEST-ATTRIBUTE(*dataset*, *attributes*)

tree ← A new DT with root test *att*

For each value v_j of attribute *att*:

ChildNode$_j$ = BuildTree(D(*att*= v_j), attributes−{att})

add branch to tree with value v_j, subtree ChildNode$_j$

return tree

Prediction

def f(x'):

Let *current node* = root

while(true):

- if *current node* is internal (non-leaf):
  - Let a = attribute associated with current node
  - Go down branch labeled with value x'_a
- if *current node* is a leaf:
  - return label y stored at that leaf

Decision Tree (Choices)

Function BuildTree(dataset,attributes) returns a DT

dataset : dataset at current node, *attributes*: current set of attributes

If *attributes* is empty OR

all labels in *dataset* are the same:

\# Leaf node

class = most common class in *dataset*

else

\# Internal node

att ⇐ CHOOSE-BEST-ATTRIBUTE(*dataset*, *attributes*)

tree ← A new DT with root test *att*

For each value v_j of attribute *att*:

ChildNode$_j$ = BuildTree(D(*att*= v_j), attributes−{att})

add branch to tree with value v_j, subtree ChildNode$_j$

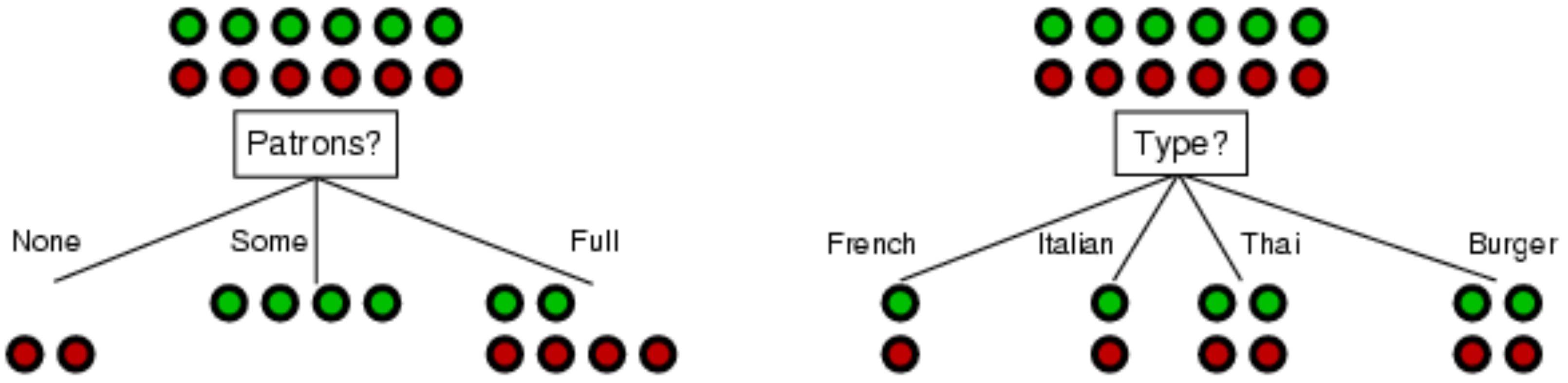
return tree

Choices

1. When to stop
   - no more input features
   - all examples are classified the same
   - too few examples to make an informative split
2. Which test to split on
   - split gives smallest error.

Choosing an attribute

Idea: good attribute splits examples into subsets that are (ideally) *all positive* or *all negative*

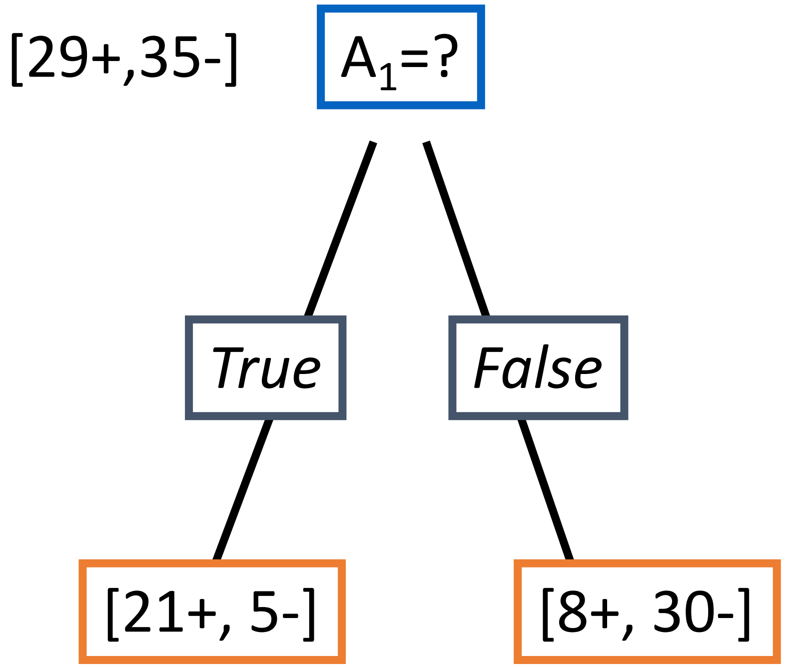


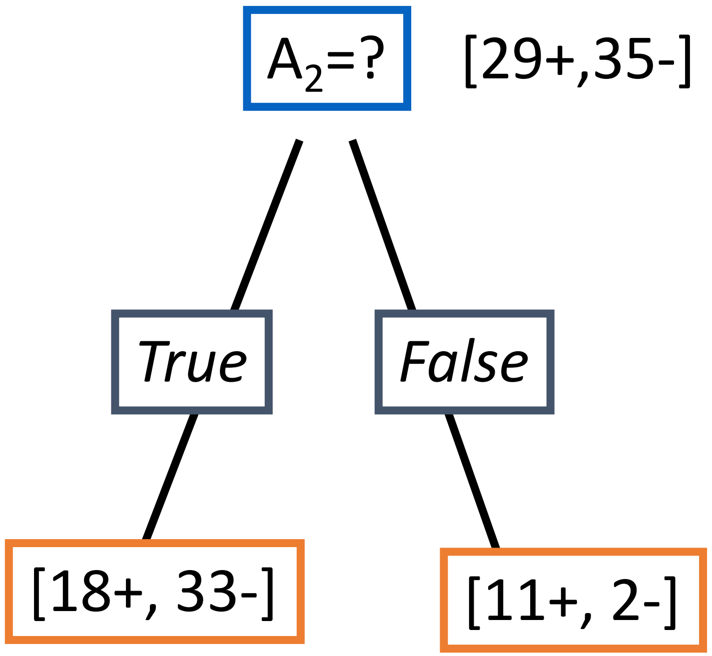
Which is better: *Patrons?* or *Type?*

Heuristic based on "information gain".

- We want attributes that split the examples to sets that are relatively pure in one label; this way we are closer to a leaf node.

Which Attribute is "best"?





How to determine the Best Split?

- *Greedy approach:*
  - *Nodes with homogeneous class distribution are preferred*

- *Need a measure of node impurity:*

C0: 5	C0: 9
C1: 5	C1: 1
Non-homogeneous,	**Homogeneous,**
High degree of impurity	**Low degree of impurity**

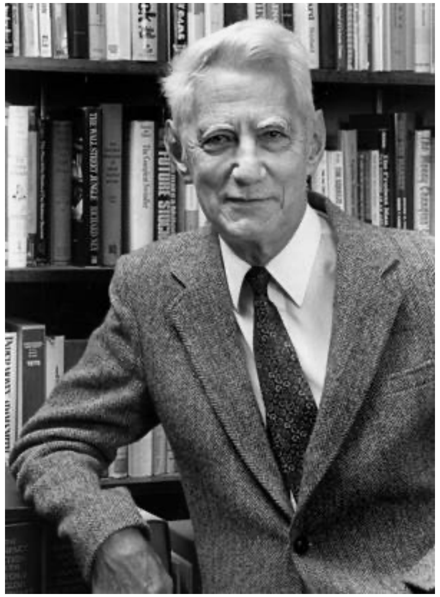
Information gain: measures how well a given attribute separates the training examples according to their target classification

Gini Index: At each node measures, what is the error if you use the most prevalent label

Background: Information theory

- Claude Shannon's seminal work: Mathematical Theory of Communication in 1948
- Information in a message (information entropy)
  - ➔ minimum #bits needed to store/send using a good encoding
- If probability distribution $P(p_1, p_2, \ldots, p_n)$ for n messages, its information (or *entropy*) is:

$$H(P) = -(p_1 \log p_1 + p_2 \log p_2 + \cdots + p_n \log p_n)$$



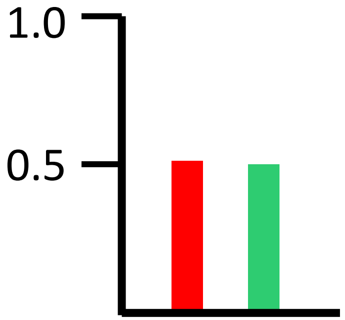
Claude Shannon

Entropy of a Distribution

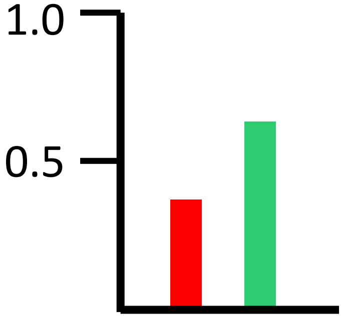
- Quantifies the amount of uncertainty associated with a specific probability distribution

$$H(X) = \sum_x p(X=x)\log_2 \frac{1}{p(X=x)}$$

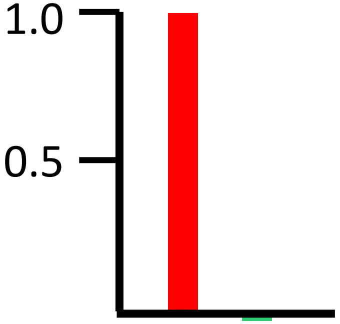
$$H(X) = -\sum_x p(X=x)\log_2 p(X=x)$$



$H(P)$
$= -.5 * (-1) + 0.5$
$* (-1)$
$= 1$



$H(P)$
$= -\left(\frac{2}{3} * \log\left(\frac{2}{3}\right) + \frac{1}{3} * \log\left(\frac{1}{3}\right)\right)$
= 0.92



$H(P)$
$= -(1 * 1 + 0 * \log(0))$
$= 0$

Entropy (Measure I)

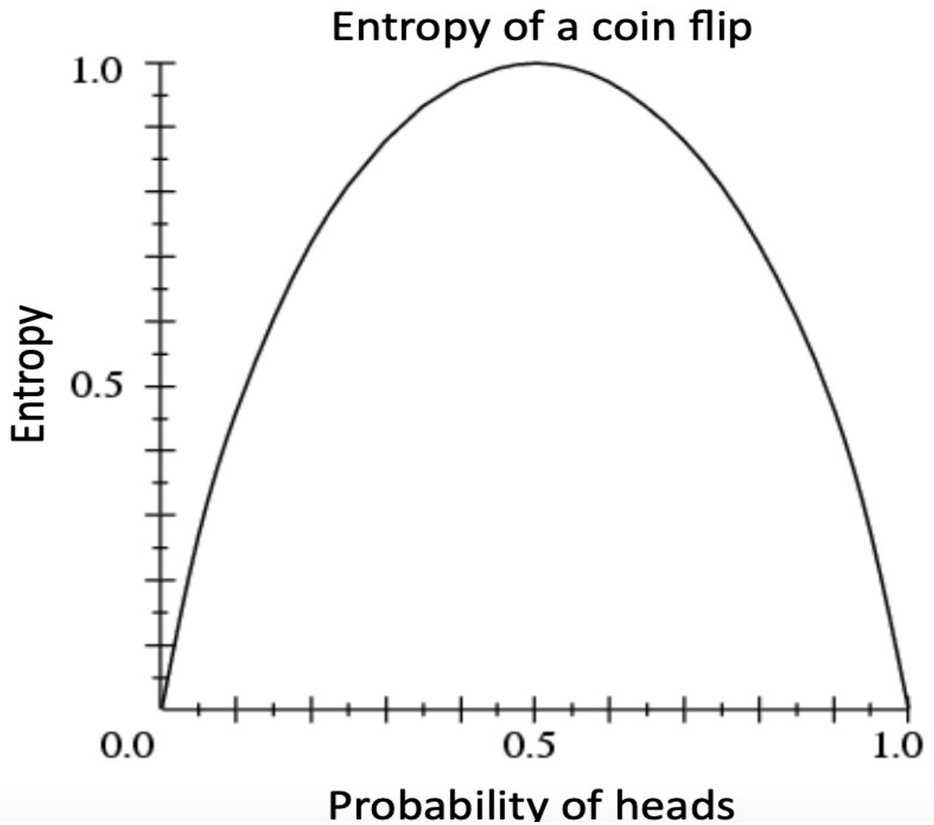
A measure for
- uncertainty
- purity
- information content

Entropy $H(Y)$ of a random variable Y

$$H(Y) = -\sum_{i=1}^{k} p(Y = y_i) \log_2 p(Y = y_i)$$

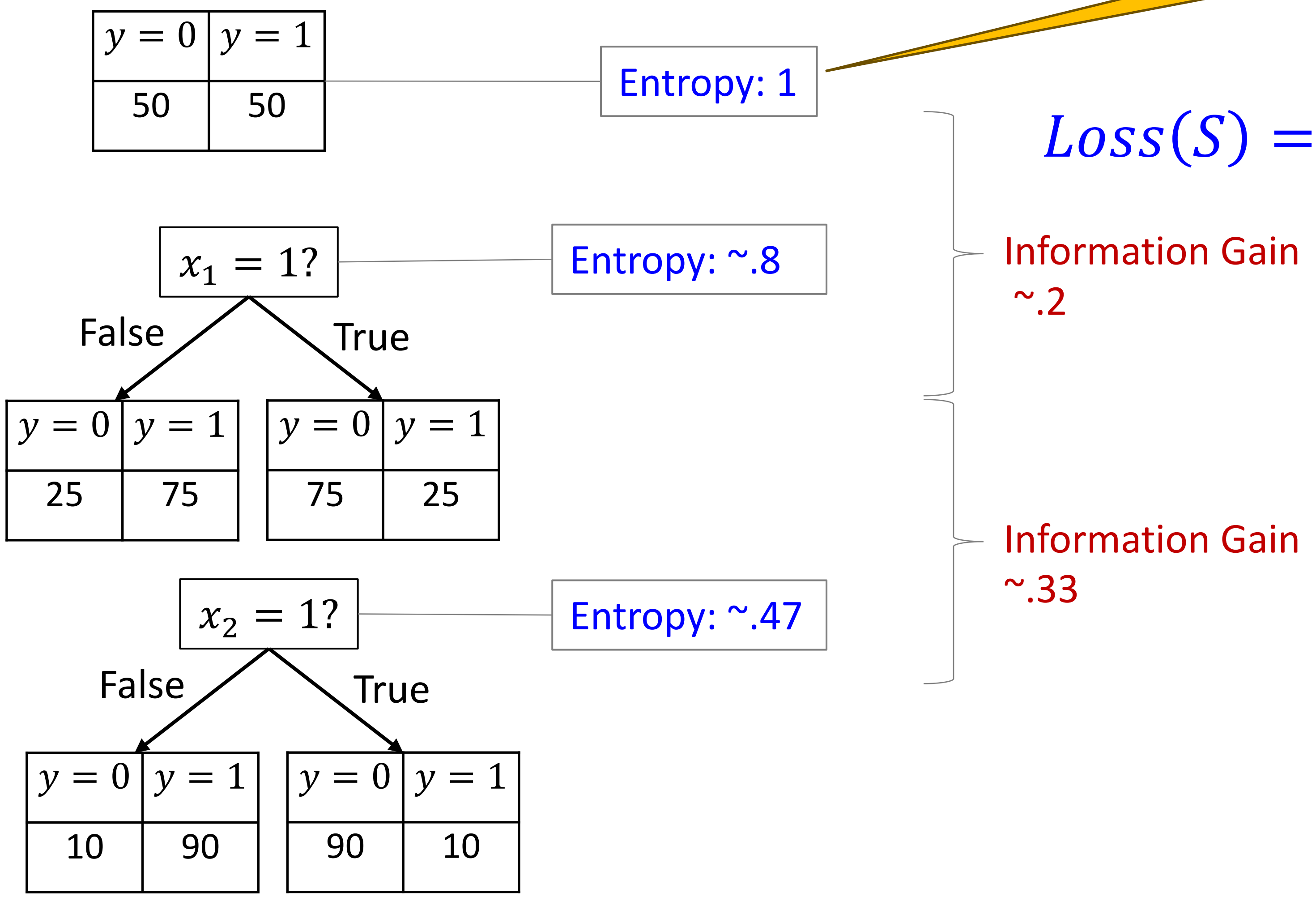
More uncertainty, more entropy!

Information Theory interpretation:
H(Y) is the expected number of bits needed to encode a randomly drawn value of Y (under most efficient code)



Loss for Decision Trees

Should we stop splitting (in the first place)? Or continue?



$$Loss(S) = \frac{1}{n}\sum_{i=1}^{n} Entropy(Leaf(S_i))$$

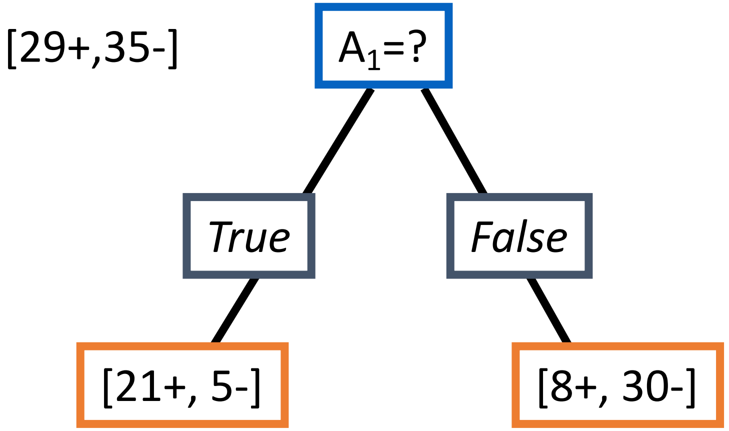
Information Gain – reduction in Entropy (loss) from a change to the model

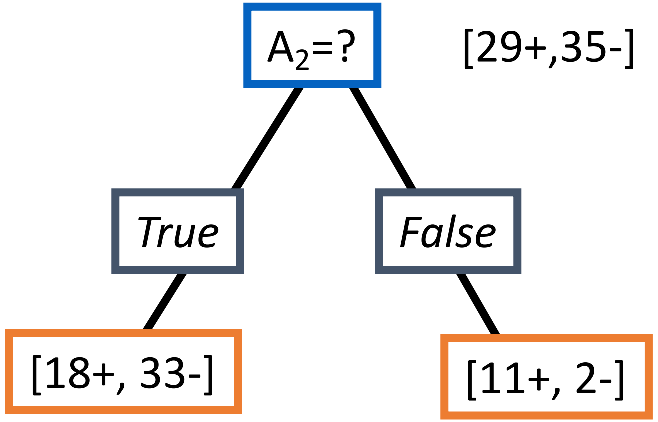
Information Gain

Gain(S,A): expected reduction in entropy due to splitting S on attribute A

$$Gain(S,A) = Entropy(S) - \sum_{v \in values(A)} \frac{|S_v|}{|S|} \times Entropy(Sv)$$

S_v is the subset of S for which attribute A has value v, and

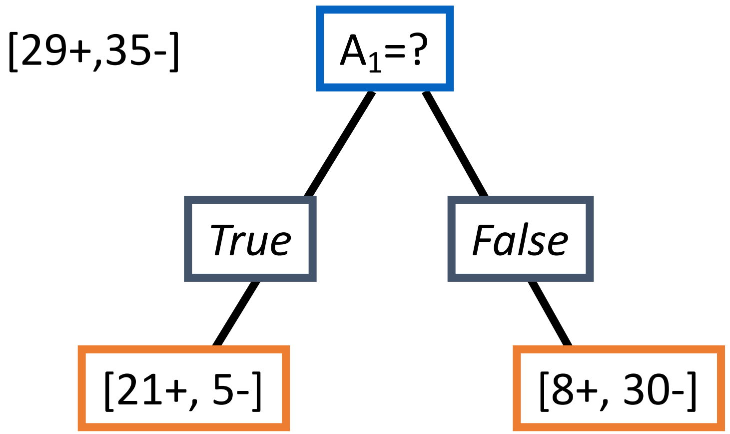


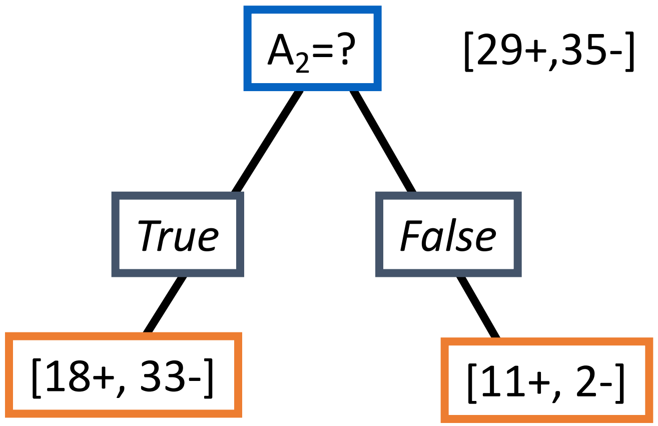


$$Entropy([29+, 35-])$$
$$= -\frac{29}{64}\log_2\frac{29}{64} - \frac{35}{64}\log_2\frac{35}{64}$$
$$= 0.99$$

Information Gain Computation

$$Entropy([29+, 35-]) = -\frac{29}{64}\log_2\frac{29}{64} - \frac{35}{64}\log_2\frac{35}{64} = 0.99$$





Entropy([21+,5-]) = 0.71

Entropy([8+,30-]) = 0.74

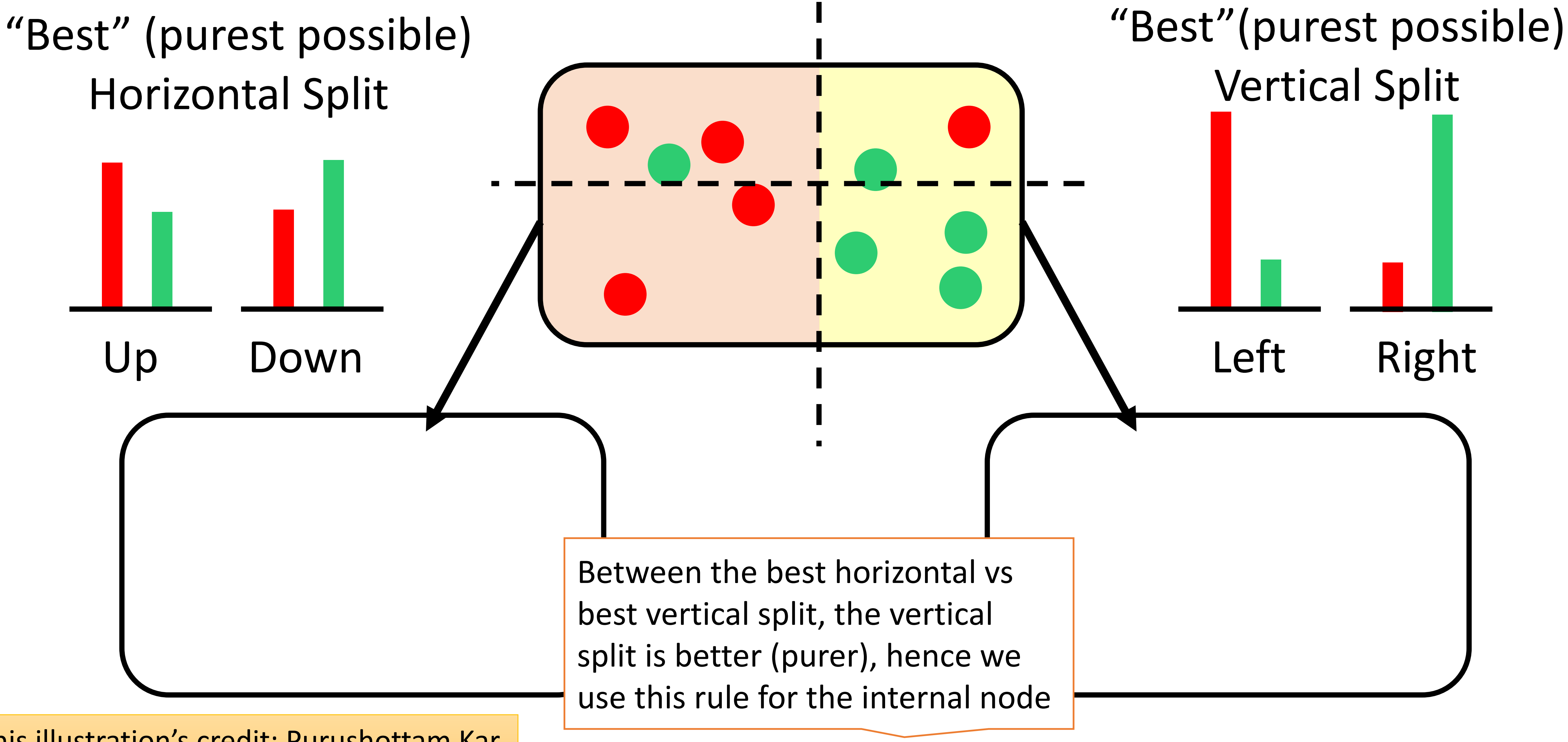
$$Gain(S, A_1) = Entropy(S) - \frac{26}{64} * Entropy([21+, 5-]) - \frac{38}{64} * Entropy([8+, 30-]) = 0.27$$

Entropy([18+,33-]) = 0.94

Entropy([8+,30-]) = 0.62

$$Gain(S, A_2) = Entropy(S) - \frac{51}{64} * Entropy([18+, 33-]) - \frac{13}{64} * Entropy([11+, 2-]) = 0.12$$

An Illustration: DT with Real-Valued Features



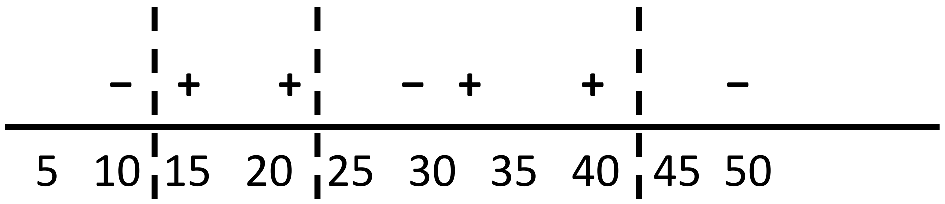
This illustration’s credit: Purushottam Kar

DT with Real-Valued Features

Example:

- Length (L): 10 15 21 28 32 40 50
- Class: − + + − + + −
- Check thresholds:

  L < 12.5; L < 24.5; L < 45



How to find the split with the highest gain ?

For each continuous feature A:

- Sort examples according to the value of A
- For each ordered pair (x,y) with different labels
- Check the mid-point as a possible threshold.

Gini Impurity: Decision Trees (Measure II)

- Gini impurity estimates the following
  - Choose an element randomly.
  - Label it using the distribution of labels on the set.
  - How often the element is incorrectly labeled?
- For a set of items with C classes, with relative frequency p_c for class c, the probability of choosing an item with label c is p_c, and the probability of misclassifying the item is

$$\sum_{k \neq c} p_k = 1 - p_c$$

- The Gini Index is computed by summing pairwise products of these probabilities for each class label:

$$GINI(p) = \sum_{c=1}^{C} p_c(1 - p_c) = 1 - \sum_{c=1}^{C} p_c^2$$

Examples of Computing GINI

$$GINI(t) = 1 - \sum_j [p(j \mid t)]^2$$

C1	0
C2	6

P(C1) = 0/6 = 0 P(C2) = 6/6 = 1

Gini = 1 – $P(C1)^2$ – $P(C2)^2$ = 1 – 0 – 1 = 0

C1	1
C2	5

P(C1) = 1/6 P(C2) = 5/6

Gini = 1 – $(1/6)^2$ – $(5/6)^2$ = 0.278

C1	2
C2	4

P(C1) = 2/6 P(C2) = 4/6

Gini = 1 – $(2/6)^2$ – $(4/6)^2$ = 0.444

Measure of Impurity: Gini Index

Gini Index for a given node t :

$$GINI(t) = 1 - \sum_j [p(j \mid t)]^2$$

$p(j \mid t)$ is the relative frequency of class j at node t

- Maximum ($1 - 1/n_c$) when records are equally distributed among all classes, implying least interesting information [n_c: number of classes]
- Minimum (0.0) when all records belong to one class, implying most interesting information

C1	0
C2	6
Gini=0.000	

C1	1
C2	5
Gini=0.278	

C1	2
C2	4
Gini=0.444	

C1	3
C2	3
Gini=0.500	

Splitting Based on GINI

Used in CART, SLIQ, SPRINT.

When a node p is split into k partitions (children), the quality of split is computed as,

$$\boxed{GINI_{split} = \sum_{i=1}^{k} \frac{n_i}{n} GINI(i)}$$

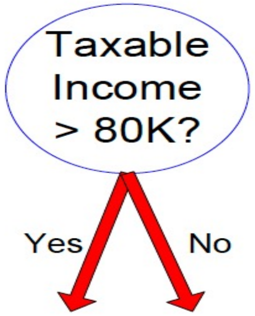
where, n_i = number of records at child i,

n = number of records at node p.

Continuous Attributes: Computing Gini Index

- Use binary decisions (A<v and A>=v)
- Many choice.
- Each value v has a count matrix associated with it
  - Class counts with A >= v
  - Class counts with A < v
- Method to choose best v
  - For each v, scan the dataset to get the count matrix. Compute Gini Index.
  - Choose the one with min. Gini Index.
  - **Inefficient. Repetition of work!**

Tid	Refund	Marital Status	Taxable Income	Cheat
1	Yes	Single	125K	No
2	No	Married	100K	No
3	No	Single	70K	No
4	Yes	Married	120K	No
5	No	Divorced	95K	Yes
6	No	Married	60K	No
7	Yes	Divorced	220K	No
8	No	Single	85K	Yes
9	No	Married	75K	No
10	No	Single	90K	Yes



Continuous Attributes: Computing Gini Index...

- For efficient computation: for each attribute,
  - Sort the attribute on values
  - Linearly scan these values, each time updating the count matrix and computing gini index
  - Choose the split position that has the least gini index

Cheat	No	No	No	Yes	Yes	Yes	No	No	No	No
	Taxable Income									
Sorted Values →	60	70	75	85	90	95	100	120	125	220

Split Positions →	55		65		72		80		87		92		97		110		122		172		230	
	<=	>	<=	>	<=	>	<=	>	<=	>	<=	>	<=	>	<=	>	<=	>	<=	>	<=	>
Yes	0	3	0	3	0	3	0	3	1	2	2	1	3	0	3	0	3	0	3	0	3	0
No	0	7	1	6	2	5	3	4	3	4	3	4	3	4	4	3	5	2	6	1	7	0
Gini	0.420		0.400		0.375		0.343		0.417		0.400		***0.300***		0.343		0.375		0.400		0.420	

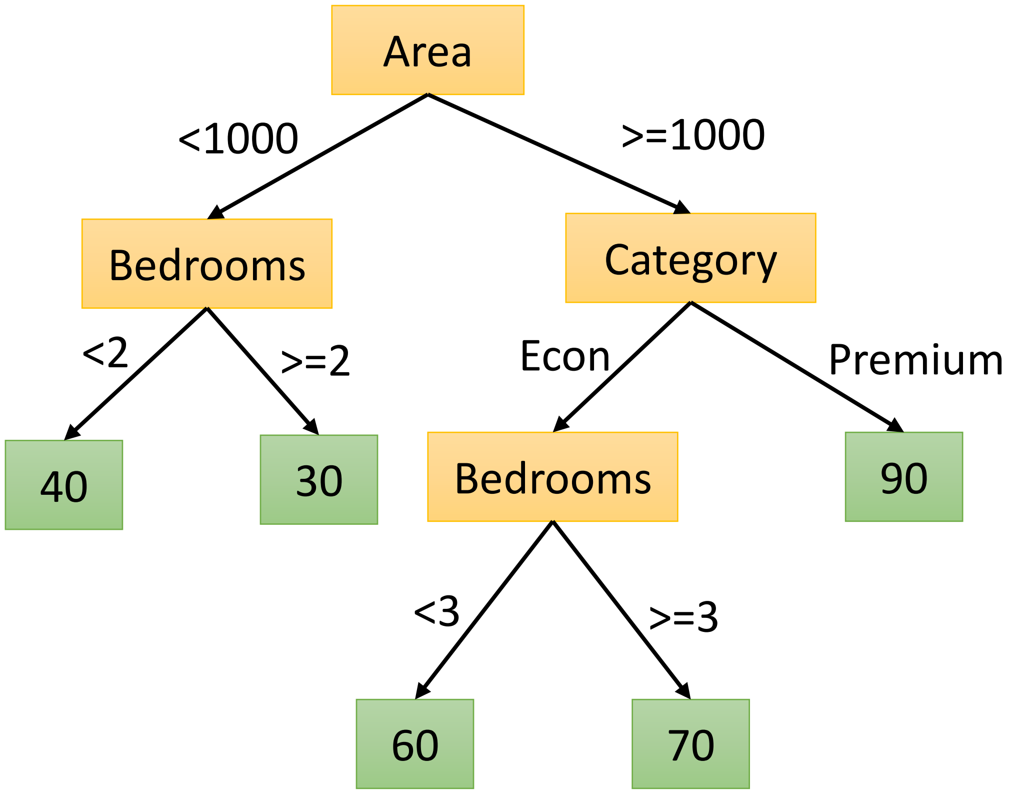
Continuous Attributes: Variance (Measure III)

Another Example of Splitting Criteria:

Variance Reduction

If a node is entirely homogeneous, then the variance is zero.

1. For each split, individually calculate the variance of each child node
2. Calculate the variance of each split as the weighted average variance of child nodes
3. Select the split with the lowest variance



Practical Issues

- Missing Values
- Attributes with different costs
  - Change information gain so that low cost attribute are preferred
- Dealing with features with different # of values

Experimental Machine Learning

- Machine Learning is an Experimental Field
- Basics:
  - Split your data into two (or three) sets:
    - Training data (often 70-90%)
    - Test data (often 10-20%)
    - Development data (10-20%)
- You need to report performance on test data, but you are not allowed to look at it.
  - You are allowed to look at the development data (and use it to tweak parameters)