

CSC 411: Introduction to Machine Learning

Lecture 3: Decision Trees

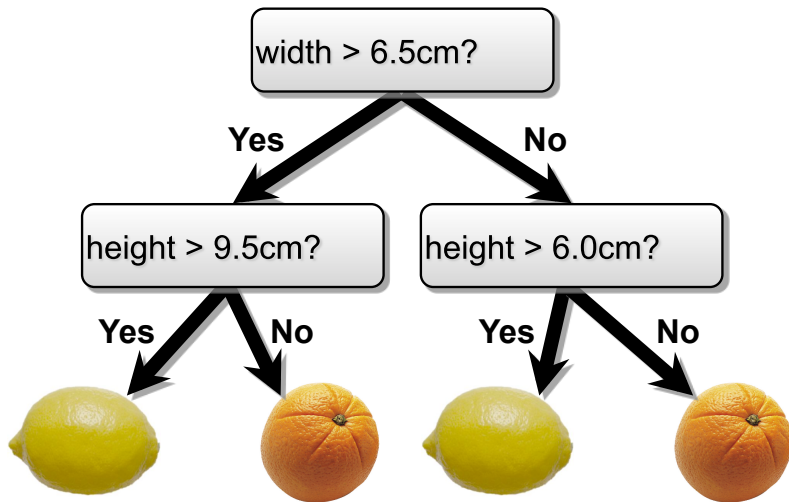
Mengye Ren and Matthew MacKay

University of Toronto

- **Decision Trees**

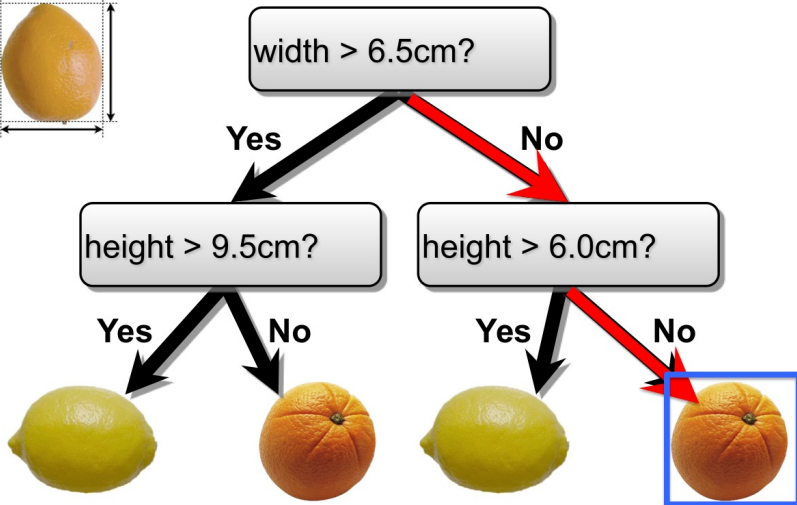
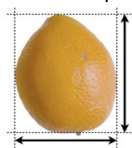
- ▶ Simple but powerful learning algorithm
- ▶ One of the most widely used learning algorithms in Kaggle competitions
- Lets us introduce ensembles (Lectures 4–5), a key idea in ML more broadly
- Useful information theoretic concepts (entropy, mutual information, etc.)

Decision Trees



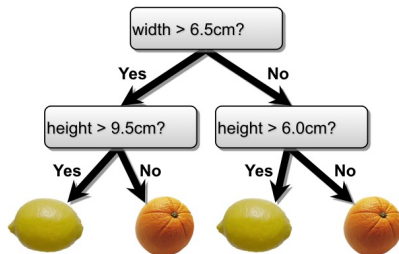
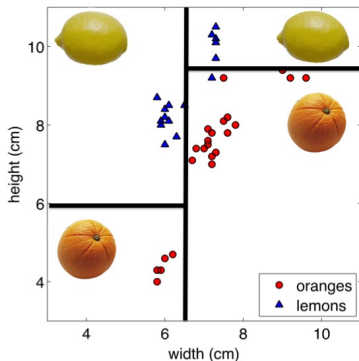
Decision Trees

Test example



Decision Trees

- **Decision trees** make predictions by recursively splitting on different attributes according to a tree structure.



Example with Discrete Inputs

- What if the attributes are discrete?

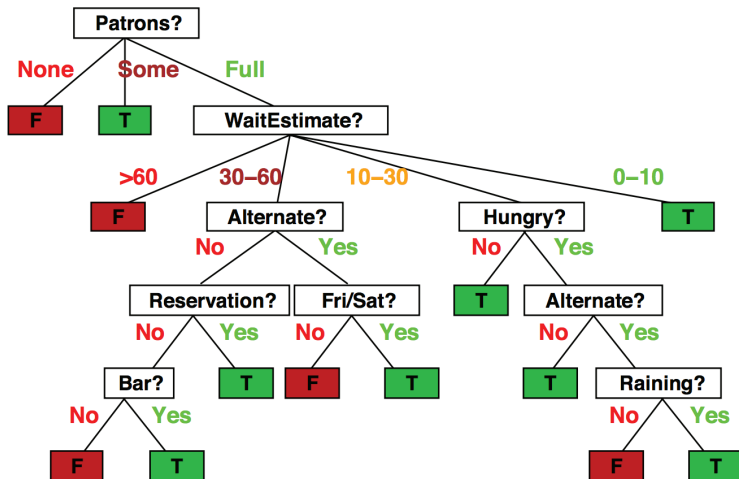
Example	Input Attributes										Goal
	<i>Alt</i>	<i>Bar</i>	<i>Fri</i>	<i>Hun</i>	<i>Pat</i>	<i>Price</i>	<i>Rain</i>	<i>Res</i>	<i>Type</i>	<i>Est</i>	<i>WillWait</i>
x_1	Yes	No	No	Yes	Some	\$\$\$	No	Yes	French	0-10	$y_1 = \text{Yes}$
x_2	Yes	No	No	Yes	Full	\$	No	No	Thai	30-60	$y_2 = \text{No}$
x_3	No	Yes	No	No	Some	\$	No	No	Burger	0-10	$y_3 = \text{Yes}$
x_4	Yes	No	Yes	Yes	Full	\$	Yes	No	Thai	10-30	$y_4 = \text{Yes}$
x_5	Yes	No	Yes	No	Full	\$\$\$	No	Yes	French	>60	$y_5 = \text{No}$
x_6	No	Yes	No	Yes	Some	\$\$	Yes	Yes	Italian	0-10	$y_6 = \text{Yes}$
x_7	No	Yes	No	No	None	\$	Yes	No	Burger	0-10	$y_7 = \text{No}$
x_8	No	No	No	Yes	Some	\$\$	Yes	Yes	Thai	0-10	$y_8 = \text{Yes}$
x_9	No	Yes	Yes	No	Full	\$	Yes	No	Burger	>60	$y_9 = \text{No}$
x_{10}	Yes	Yes	Yes	Yes	Full	\$\$\$	No	Yes	Italian	10-30	$y_{10} = \text{No}$
x_{11}	No	No	No	No	None	\$	No	No	Thai	0-10	$y_{11} = \text{No}$
x_{12}	Yes	Yes	Yes	Yes	Full	\$	No	No	Burger	30-60	$y_{12} = \text{Yes}$

1. Alternate: whether there is a suitable alternative restaurant nearby.
2. Bar: whether the restaurant has a comfortable bar area to wait in.
3. Fri/Sat: true on Fridays and Saturdays.
4. Hungry: whether we are hungry.
5. Patrons: how many people are in the restaurant (values are None, Some, and Full).
6. Price: the restaurant's price range (\$, \$\$, \$\$\$).
7. Raining: whether it is raining outside.
8. Reservation: whether we made a reservation.
9. Type: the kind of restaurant (French, Italian, Thai or Burger).
10. WaitEstimate: the wait estimated by the host (0-10 minutes, 10-30, 30-60, >60).

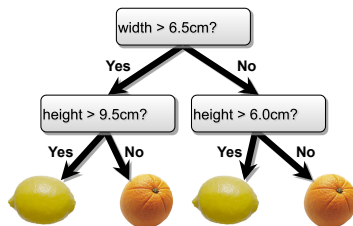
Attributes:

Decision Tree: Example with Discrete Inputs

- The tree to decide whether to wait (T) or not (F)



Decision Trees



- **Internal nodes** test **attributes**
- **Branching** is determined by **attribute value**
- **Leaf nodes** are **outputs** (predictions)

Decision Tree: Classification and Regression

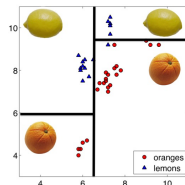
- Each path from root to a leaf defines a region R_m of input space
- Let $\{(x^{(m_1)}, t^{(m_1)}), \dots, (x^{(m_k)}, t^{(m_k)})\}$ be the training examples that fall into R_m

- **Classification tree:**

- ▶ discrete output
- ▶ leaf value y^m typically set to the most common value in $\{t^{(m_1)}, \dots, t^{(m_k)}\}$

- **Regression tree:**

- ▶ continuous output
- ▶ leaf value y^m typically set to the mean value in $\{t^{(m_1)}, \dots, t^{(m_k)}\}$

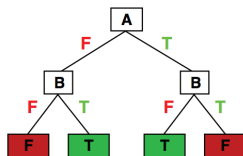


Note: We will focus on classification

- **Discrete-input, discrete-output case:**

- ▶ Decision trees can express any function of the input attributes
- ▶ E.g., for Boolean functions, truth table row \rightarrow path to leaf:

A	B	A xor B
F	F	F
F	T	T
T	F	T
T	T	F



- **Continuous-input, continuous-output case:**

- ▶ Can approximate any function arbitrarily closely
- Trivially, there is a consistent decision tree for any training set w/ one path to leaf for each example (unless f nondeterministic in x) but it probably won't generalize to new examples

[Slide credit: S. Russell]

How do we Learn a DecisionTree?

- How do we construct a useful decision tree?

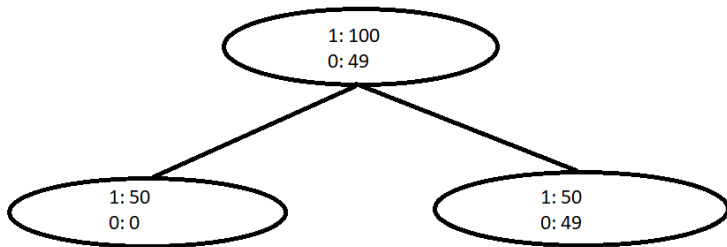
Learning Decision Trees

Learning the simplest (smallest) decision tree is an NP complete problem [if you are interested, check: Hyafil & Rivest'76]

- Resort to a **greedy heuristic**:
 - ▶ Start from an empty decision tree
 - ▶ Split on the “best” attribute
 - ▶ Recurse
- Which attribute is the “best” ?
 - ▶ Choose based on accuracy?

Choosing a Good Split

- Why isn't accuracy a good measure?



- Is this split good? Zero accuracy gain.
- Instead, we will use techniques from **information theory**

Idea: Use counts at leaves to define probability distributions, so we can measure uncertainty

Choosing a Good Split

- Which attribute is better to split on, X_1 or X_2 ?
 - ▶ Deterministic: good (all are true or false; just one class in the leaf)
 - ▶ Uniform distribution: bad (all classes in leaf equally probable)
 - ▶ What about distributions in between?

Note: Let's take a slight detour and remember concepts from information theory

[Slide credit: D. Sontag]

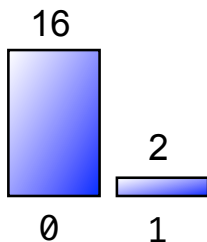
We Flip Two Different Coins

Sequence 1:

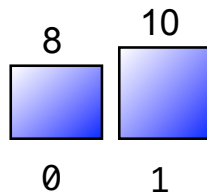
0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 1 0 0 ... ?

Sequence 2:

0 1 0 1 0 1 1 1 0 1 0 0 1 1 0 1 0 1 ... ?



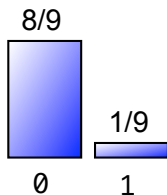
versus



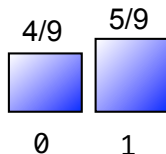
Quantifying Uncertainty

Entropy is a measure of expected “surprise”:

$$H(X) = - \sum_{x \in X} p(x) \log_2 p(x)$$



$$-\frac{8}{9} \log_2 \frac{8}{9} - \frac{1}{9} \log_2 \frac{1}{9} \approx \frac{1}{2}$$

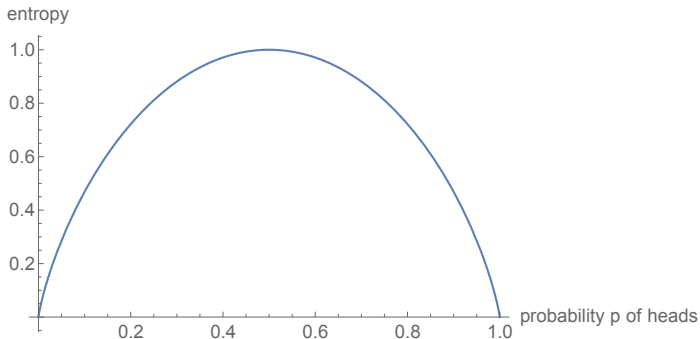


$$-\frac{4}{9} \log_2 \frac{4}{9} - \frac{5}{9} \log_2 \frac{5}{9} \approx 0.99$$

- Measures the information content of each observation
- Unit = **bits**
- A fair coin flip has 1 bit of entropy

Quantifying Uncertainty

$$H(X) = - \sum_{x \in X} p(x) \log_2 p(x)$$



- **“High Entropy”:**
 - ▶ Variable has a uniform like distribution
 - ▶ Flat histogram
 - ▶ Values sampled from it are less predictable
- **“Low Entropy”**
 - ▶ Distribution of variable has many peaks and valleys
 - ▶ Histogram has many lows and highs
 - ▶ Values sampled from it are more predictable

[Slide credit: Vibhav Gogate]

Entropy of a Joint Distribution

- Example: $X = \{\text{Raining}, \text{Not raining}\}$, $Y = \{\text{Cloudy}, \text{Not cloudy}\}$

	Cloudy	Not Cloudy
Raining	24/100	1/100
Not Raining	25/100	50/100

$$\begin{aligned} H(X, Y) &= - \sum_{x \in X} \sum_{y \in Y} p(x, y) \log_2 p(x, y) \\ &= - \frac{24}{100} \log_2 \frac{24}{100} - \frac{1}{100} \log_2 \frac{1}{100} - \frac{25}{100} \log_2 \frac{25}{100} - \frac{50}{100} \log_2 \frac{50}{100} \\ &\approx 1.56 \text{bits} \end{aligned}$$

Specific Conditional Entropy

- Example: $X = \{\text{Raining}, \text{Not raining}\}$, $Y = \{\text{Cloudy}, \text{Not cloudy}\}$

	Cloudy	Not Cloudy
Raining	24/100	1/100
Not Raining	25/100	50/100

- What is the entropy of cloudiness Y , **given that it is raining**?

$$\begin{aligned}H(Y|X = x) &= - \sum_{y \in Y} p(y|x) \log_2 p(y|x) \\&= -\frac{24}{25} \log_2 \frac{24}{25} - \frac{1}{25} \log_2 \frac{1}{25} \\&\approx 0.24\text{bits}\end{aligned}$$

- We used: $p(y|x) = \frac{p(x,y)}{p(x)}$, and $p(x) = \sum_y p(x,y)$ (sum in a row)

Conditional Entropy

	Cloudy	Not Cloudy
Raining	24/100	1/100
Not Raining	25/100	50/100

- The expected conditional entropy:

$$\begin{aligned} H(Y|X) &= \sum_{x \in X} p(x) H(Y|X = x) \\ &= - \sum_{x \in X} \sum_{y \in Y} p(x, y) \log_2 p(y|x) \end{aligned}$$

Conditional Entropy

- Example: $X = \{\text{Raining}, \text{Not raining}\}$, $Y = \{\text{Cloudy}, \text{Not cloudy}\}$

	Cloudy	Not Cloudy
Raining	24/100	1/100
Not Raining	25/100	50/100

- What is the entropy of cloudiness, given the knowledge of whether or not it is raining?

$$\begin{aligned} H(Y|X) &= \sum_{x \in X} p(x) H(Y|X=x) \\ &= \frac{1}{4} H(\text{cloudy}|\text{is raining}) + \frac{3}{4} H(\text{cloudy}|\text{not raining}) \\ &\approx 0.75 \text{ bits} \end{aligned}$$

Conditional Entropy

- Some useful properties:

- ▶ H is always non-negative
- ▶ Chain rule: $H(X, Y) = H(X|Y) + H(Y) = H(Y|X) + H(X)$
- ▶ If X and Y independent, then X doesn't tell us anything about Y :
 $H(Y|X) = H(Y)$
- ▶ But Y tells us everything about Y : $H(Y|Y) = 0$
- ▶ By knowing X , we can only decrease uncertainty about Y :
 $H(Y|X) \leq H(Y)$

Information Gain

	Cloudy	Not Cloudy
Raining	24/100	1/100
Not Raining	25/100	50/100

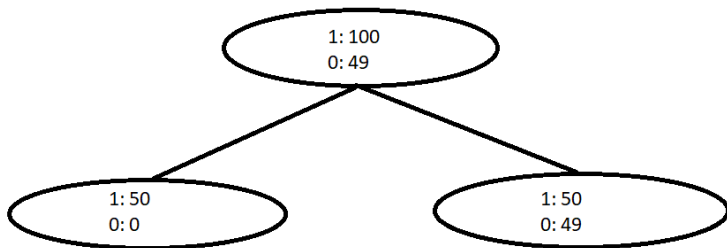
- How much information about cloudiness do we get by discovering whether it is raining?

$$\begin{aligned}IG(Y|X) &= H(Y) - H(Y|X) \\ &\approx 0.25 \text{ bits}\end{aligned}$$

- This is called the **information gain** in Y due to X , or the **mutual information** of Y and X
- If X is completely uninformative about Y : $IG(Y|X) = 0$
- If X is completely informative about Y : $IG(Y|X) = H(Y)$

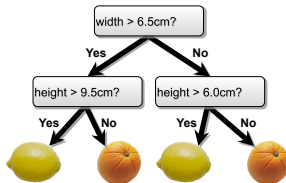
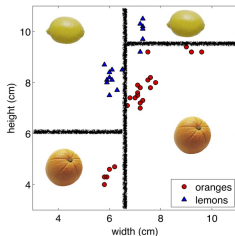
Revisiting Our Original Example

- Information gain measures the informativeness of a variable, which is exactly what we desire in a decision tree attribute!
- What is the information gain of this split?



- Root entropy: $H(Y) = -\frac{49}{149} \log_2(\frac{49}{149}) - \frac{100}{149} \log_2(\frac{100}{149}) \approx 0.91$
- Leafs entropy: $H(Y|left) = 0$, $H(Y|right) \approx 1$.
- $IG(split) \approx 0.91 - (\frac{1}{3} \cdot 0 + \frac{2}{3} \cdot 1) \approx 0.24 > 0$

Constructing Decision Trees



- At each level, one must choose:
 - Which variable to split.
 - Possibly where to split it.
- Choose them based on how much information we would gain from the decision! (choose attribute that gives the textbfest gain)

Decision Tree Construction Algorithm

- Simple, greedy, recursive approach, builds up tree node-by-node
1. pick an attribute to split at a non-terminal node
 2. split examples into groups based on attribute value
 3. for each group:
 - ▶ if no examples – return majority from parent
 - ▶ else if all examples in same class – return class
 - ▶ else loop to step 1

Back to Our Example

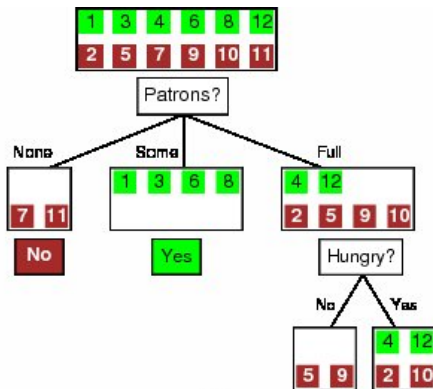
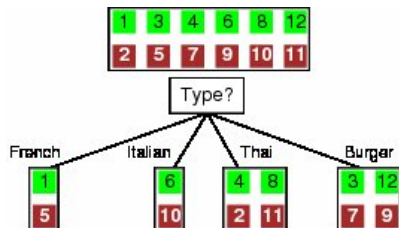
Example	Input Attributes										Goal
	<i>Alt</i>	<i>Bar</i>	<i>Fri</i>	<i>Hun</i>	<i>Pat</i>	<i>Price</i>	<i>Rain</i>	<i>Res</i>	<i>Type</i>	<i>Est</i>	<i>WillWait</i>
x_1	Yes	No	No	Yes	Some	\$\$\$	No	Yes	French	0-10	$y_1 = \text{Yes}$
x_2	Yes	No	No	Yes	Full	\$	No	No	Thai	30-60	$y_2 = \text{No}$
x_3	No	Yes	No	No	Some	\$	No	No	Burger	0-10	$y_3 = \text{Yes}$
x_4	Yes	No	Yes	Yes	Full	\$	Yes	No	Thai	10-30	$y_4 = \text{Yes}$
x_5	Yes	No	Yes	No	Full	\$\$\$	No	Yes	French	>60	$y_5 = \text{No}$
x_6	No	Yes	No	Yes	Some	\$\$	Yes	Yes	Italian	0-10	$y_6 = \text{Yes}$
x_7	No	Yes	No	No	None	\$	Yes	No	Burger	0-10	$y_7 = \text{No}$
x_8	No	No	No	Yes	Some	\$\$	Yes	Yes	Thai	0-10	$y_8 = \text{Yes}$
x_9	No	Yes	Yes	No	Full	\$	Yes	No	Burger	>60	$y_9 = \text{No}$
x_{10}	Yes	Yes	Yes	Yes	Full	\$\$\$	No	Yes	Italian	10-30	$y_{10} = \text{No}$
x_{11}	No	No	No	No	None	\$	No	No	Thai	0-10	$y_{11} = \text{No}$
x_{12}	Yes	Yes	Yes	Yes	Full	\$	No	No	Burger	30-60	$y_{12} = \text{Yes}$

1.	Alternate: whether there is a suitable alternative restaurant nearby.
2.	Bar: whether the restaurant has a comfortable bar area to wait in.
3.	Fri/Sat: true on Fridays and Saturdays.
4.	Hungry: whether we are hungry.
5.	Patrons: how many people are in the restaurant (values are None, Some, and Full).
6.	Price: the restaurant's price range (\$, \$\$, \$\$\$).
7.	Raining: whether it is raining outside.
8.	Reservation: whether we made a reservation.
9.	Type: the kind of restaurant (French, Italian, Thai or Burger).
10.	WaitEstimate: the wait estimated by the host (0-10 minutes, 10-30, 30-60, >60).

Attributes:

[from: Russell & Norvig]

Attribute Selection

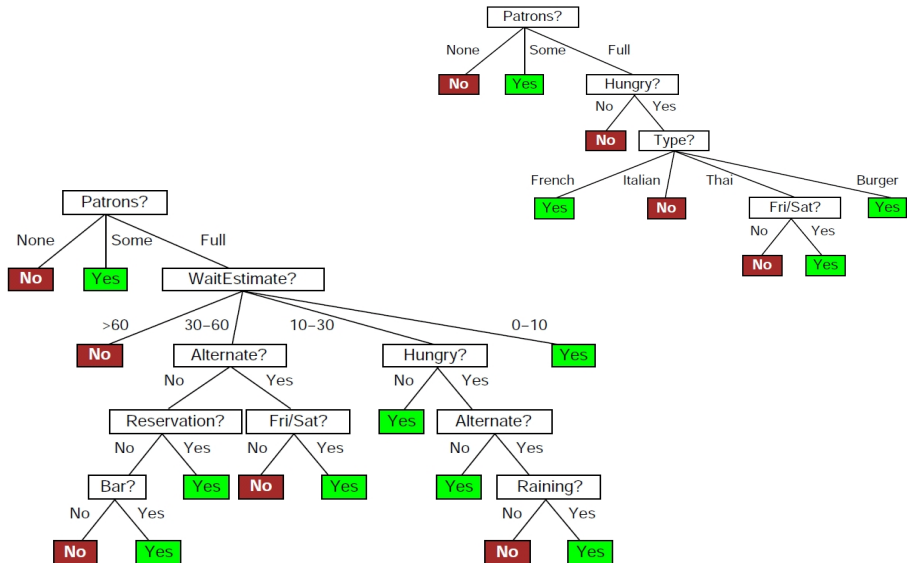


$$IG(Y) = H(Y) - H(Y|X)$$

$$IG(type) = 1 - \left[\frac{2}{12} H(Y|Fr.) + \frac{2}{12} H(Y|It.) + \frac{4}{12} H(Y|Thai) + \frac{4}{12} H(Y|Bur.) \right] = 0$$

$$IG(Patrons) = 1 - \left[\frac{2}{12} H(0, 1) + \frac{4}{12} H(1, 0) + \frac{6}{12} H\left(\frac{2}{6}, \frac{4}{6}\right) \right] \approx 0.541$$

Which Tree is Better?



What Makes a Good Tree?

- Not too small: need to handle important but possibly subtle distinctions in data
- Not too big:
 - ▶ Computational efficiency (avoid redundant, spurious attributes)
 - ▶ Avoid over-fitting training examples
 - ▶ Human interpretability
- **“Occam’s Razor”**: find the simplest hypothesis that fits the observations
 - ▶ Useful principle, but hard to formalize (how to define simplicity?)
 - ▶ See Domingos, 1999, “The role of Occam’s razor in knowledge discovery”
- We desire small trees with informative nodes near the root

- Problems:
 - ▶ You have exponentially less data at lower levels
 - ▶ Too big of a tree can overfit the data
 - ▶ Greedy algorithms don't necessarily yield the global optimum
- Handling continuous attributes
 - ▶ Split based on a threshold, chosen to maximize information gain
- Decision trees can also be used for regression on real-valued outputs. Choose splits to minimize squared error, rather than maximize information gain.

Advantages of decision trees over KNN

- Good when there are lots of attributes, but only a few are important
- Good with discrete attributes
- Easily deals with missing values (just treat as another value)
- Robust to scale of inputs
- Fast at test time
- More interpretable

Comparison to k-NN

Advantages of KNN over decision trees

- Few hyperparameters
- Able to handle attributes/features that interact in complex ways (e.g. pixels)
- Can incorporate interesting distance measures (e.g. shape contexts)
- Typically make better predictions in practice
 - ▶ As we'll see next lecture, ensembles of decision trees are much stronger. But they lose many of the advantages listed above.