CSC 2515: Introduction to Machine Learning

Lecture 2: Decision Trees

Amir-massoud Farahmand[1]

University of Toronto and Vector Institute

[1] Credit for slides goes to many members of the ML Group at the U of T, and beyond, including (recent past): Roger Grosse, Murat Erdogdu, Richard Zemel, Juan Felipe Carrasquilla, Emad Andrews, and myself.

Table of Contents

Today

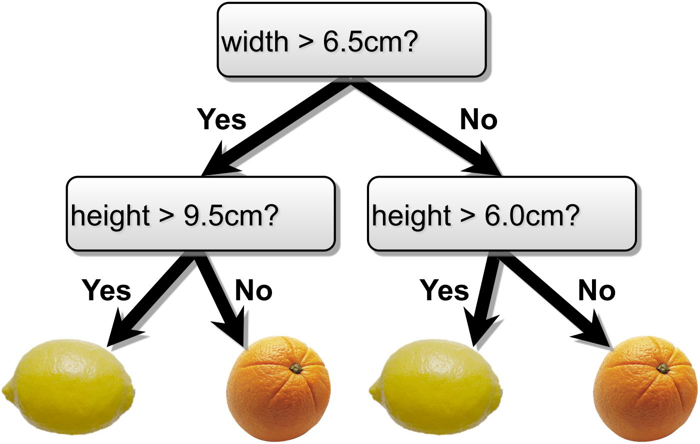
- KNN: Good method with reasonable theoretical guarantees, but not very explainable.
- **Decision Trees**
  - Simple but powerful learning algorithm
  - More explainable; somehow similar to how people make decisions
  - One of the most widely used learning algorithms in Kaggle competitions
  - Lets us introduce ensembles, a key idea in ML
- Useful Information Theoretic concepts (entropy, mutual information, etc.)

Skills to Learn:

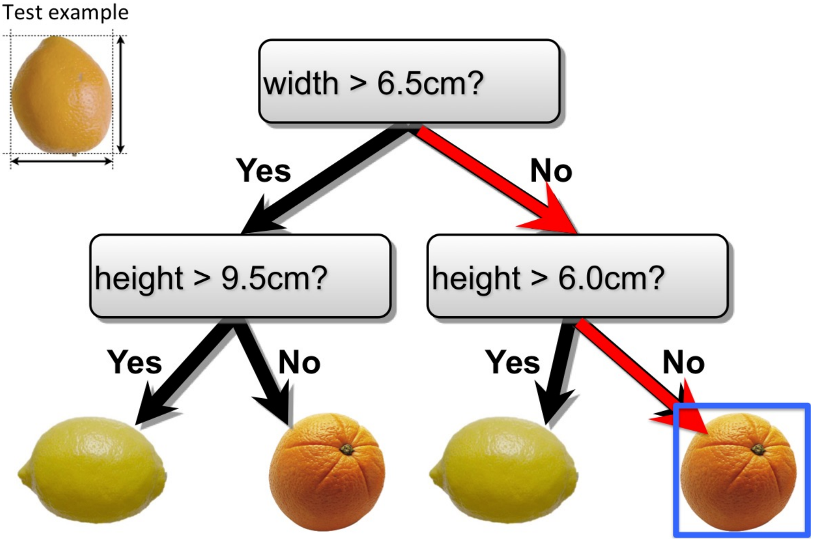
- Basic concepts of information theory
- Decision trees

Decision Trees

- Decision trees make predictions by recursively splitting on different attributes according to a tree structure.
- Example: classifying fruit as an orange or lemon based on height and width



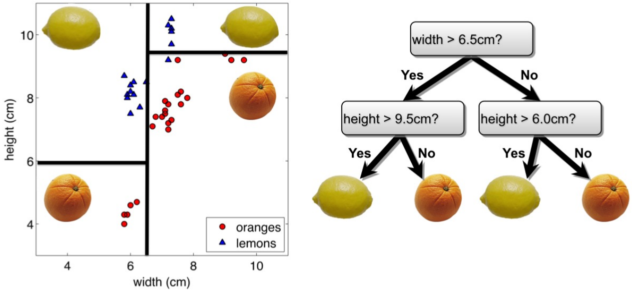
Decision Trees



Decision Trees

- For continuous attributes, split based on less than or greater than some threshold
- Thus, input space is divided into regions with boundaries parallel to axes
- The decision tree defines a function:

$$f(\mathbf{x}) = \sum_{i=1}^{r} w_i \mathbb{I}\{\mathbf{x} \in R_i\}$$



Example with Discrete Inputs

- What if the attributes are discrete?

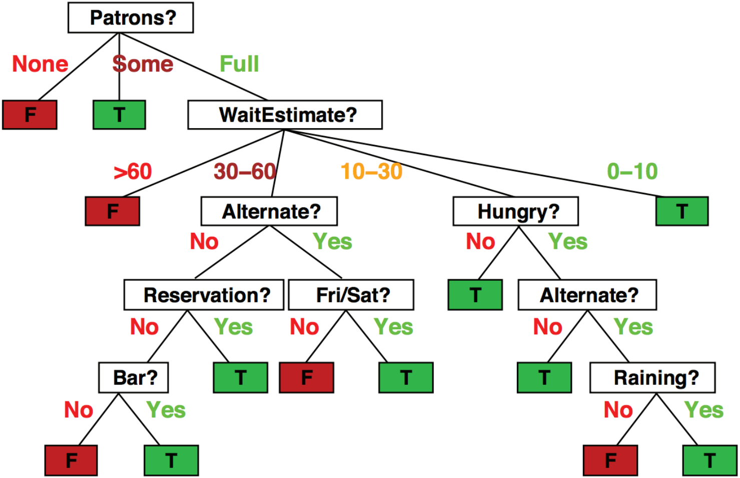
Example	Input Attributes										Goal
	Alt	*Bar*	*Fri*	*Hun*	*Pat*	*Price*	*Rain*	*Res*	*Type*	*Est*	*WillWait*
$\mathbf{x}_1$	Yes	No	No	Yes	Some	$$$	No	Yes	French	0–10	$y_1 =$ Yes
$\mathbf{x}_2$	Yes	No	No	Yes	Full	$	No	No	Thai	30–60	$y_2 =$ No
$\mathbf{x}_3$	No	Yes	No	No	Some	$	No	No	Burger	0–10	$y_3 =$ Yes
$\mathbf{x}_4$	Yes	No	Yes	Yes	Full	$	Yes	No	Thai	10–30	$y_4 =$ Yes
$\mathbf{x}_5$	Yes	No	Yes	No	Full	$$$	No	Yes	French	>60	$y_5 =$ No
$\mathbf{x}_6$	No	Yes	No	Yes	Some	$$	Yes	Yes	Italian	0–10	$y_6 =$ Yes
$\mathbf{x}_7$	No	Yes	No	No	None	$	Yes	No	Burger	0–10	$y_7 =$ No
$\mathbf{x}_8$	No	No	No	Yes	Some	$$	Yes	Yes	Thai	0–10	$y_8 =$ Yes
$\mathbf{x}_9$	No	Yes	Yes	No	Full	$	Yes	No	Burger	>60	$y_9 =$ No
$\mathbf{x}_{10}$	Yes	Yes	Yes	Yes	Full	$$$	No	Yes	Italian	10–30	$y_{10} =$ No
$\mathbf{x}_{11}$	No	No	No	No	None	$	No	No	Thai	0–10	$y_{11} =$ No
$\mathbf{x}_{12}$	Yes	Yes	Yes	Yes	Full	$	No	No	Burger	30–60	$y_{12} =$ Yes

Attributes:

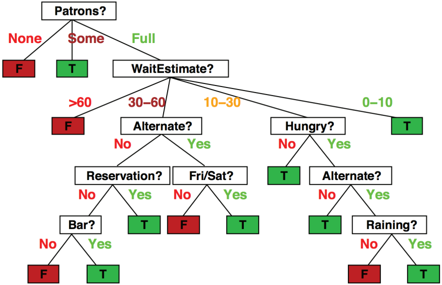
1.	Alternate: whether there is a suitable alternative restaurant nearby.
2.	Bar: whether the restaurant has a comfortable bar area to wait in.
3.	Fri/Sat: true on Fridays and Saturdays.
4.	Hungry: whether we are hungry.
5.	Patrons: how many people are in the restaurant (values are None, Some, and Full).
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).

Decision Tree: Example with Discrete Inputs

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



Decision Trees

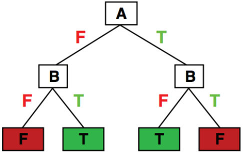


- **Internal nodes** test **attributes**
- **Branching** is determined by **attribute value**
- **Leaf nodes** are **outputs** (predictions)

Expressiveness

- **Discrete-input, discrete-output case**:
  - Decision trees can express any function of the input attributes
  - Example: For Boolean functions, the truth table row $\rightarrow$ path to leaf

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

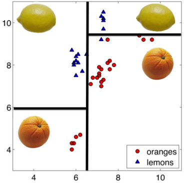


  - Q: What is the decision tree for `AND` and `OR`?

- **Continuous-input, continuous-output case**:
  - Can approximate any function arbitrarily closely

[Slide credit: S. Russell]

Decision Tree: Classification and Regression

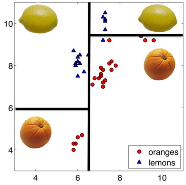


- Each path from root to a leaf defines a region R_m of input space
- Let $\{(\mathbf{x}^{(m_1)}, t^{(m_1)}), \dots, (\mathbf{x}^{(m_k)}, t^{(m_k)})\}$ be the training examples that fall into R_m
- **Classification tree**:
  - discrete output, i.e., $y \in \{1, \dots, C\}$.
  - leaf value y^m typically set to the most common value in $\{t^{(m_1)}, \dots, t^{(m_k)}\}$, i.e.,

$$y^m \leftarrow \underset{t \in \{1,\dots,C\}}{\text{argmax}} \sum_{m_i} \mathbb{I}\{t = t^{(m_i)}\}.$$

Decision Tree: Classification and Regression

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



- **Regression tree**:
  - continuous output, i.e, $y \in \mathbb{R}$.
  - leaf value y^m typically set to the mean value in $\{t^{(m_1)}, \ldots, t^{(m_k)}\}$

Note: We will focus on classification.

How do we Learn a DecisionTree?

- How do we construct a useful decision tree?
- We want to find a “simple” tree that explains data well.
  - Simple: Minimal number of nodes
  - There should be enough samples per region

Learning Decision Trees

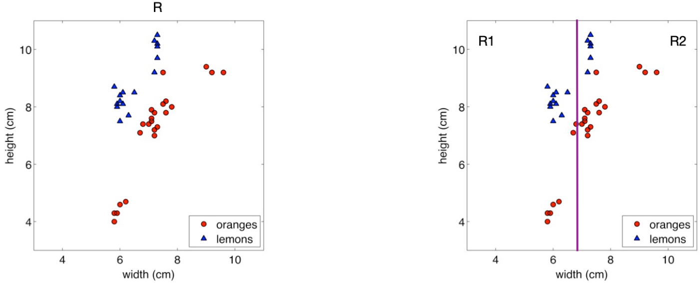
Learning the simplest (smallest) decision tree which correctly classifies training set is an NP complete problem (see Hyafil & Rivest'76).

- Resort to a greedy heuristic!
- Start with empty decision tree and complete training set
  - Split (i.e., partition dataset) on the "best" attribute.
  - Recurse on subpartitions

- When should we stop?
- Which attribute is the "best"?
  - We define a notion of gain of a split
  - Gain is defined based on change in some criteria before and after a split.
    - Various notions of gain

Which attribute is the “best”?

- Let us choose the accuracy (i.e., misclassification error L – the number of incorrect classifications) as the criteria, and define the accuracy gain.
- Let us define accuracy gain:
  - Suppose that we have region R. Denote the loss of that region as $L(R)$.
  - We split R to two regions R_1 and R_2.
  - What is the accuracy of the split regions?



Learning Decision Trees

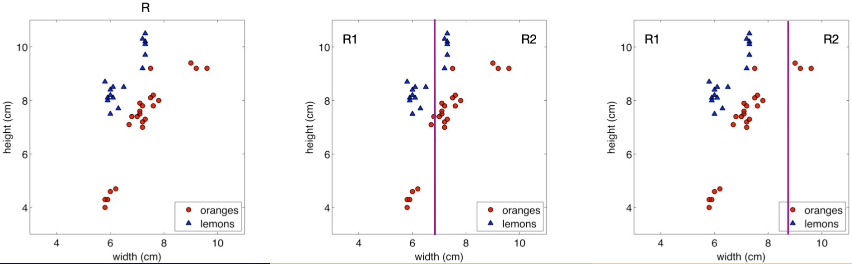
- Misclassification loss before the split: $L(R)$
- Misclassification loss after the split:

$$\frac{|R_1|}{|R|}L(R_1) + \frac{|R_2|}{|R|}L(R_2)$$

- Accuracy gain is

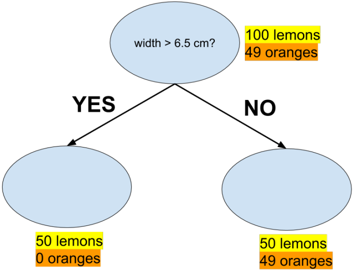
$$L(R) - \frac{|R_1|L(R_1) + |R_2|L(R_2)}{|R|}$$

- Note: Different splits lead to different accuracy gains.



Choosing a Good Split

- Accuracy is not always a good measure to decide the split. Why?



- Is this split good? Accuracy gain is

$$L(R) - \frac{|R_1|L(R_1) + |R_2|L(R_2)}{|R_1| + |R_2|} = \frac{49}{149} - \frac{50 \times 0 + 99 \times \frac{49}{99}}{149} = 0$$

- But we have reduced our uncertainty about whether a fruit is a lemon!

Choosing a Good Split

- We can use uncertainty as the criteria, and use gain in the certainty (or gain in the reduction of uncertainty) to decide the split
- How can we quantify uncertainty in prediction for a given leaf node?
  - All examples in leaf have the same class: good (low uncertainty)
  - Each class has the same number of examples in leaf: bad (high uncertainty)
- Idea: Use counts at leaves to define probability distributions, and use information theory to measure uncertainty

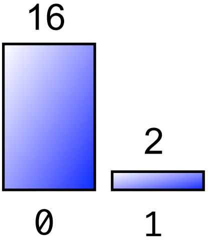
Basics of Information Theory

Flipping Two Different Coins

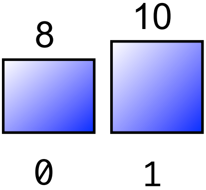
Q: Which coin is more uncertain?

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 ... ?



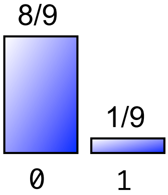
versus

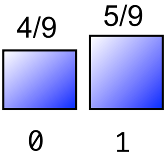


Quantifying Uncertainty

Entropy is a measure of expected "surprise": How uncertain are we of the value of a draw from this distribution?

$$H(X) = -\mathbb{E}_{X\sim p}[\log_2 p(X)] = -\sum_{x \in X} p(x)\log_2 p(x)$$





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

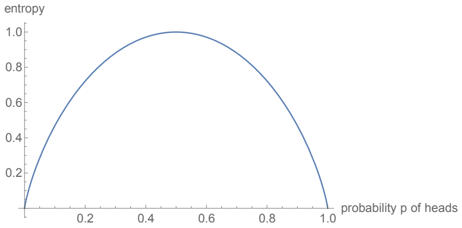
$$-\frac{4}{9}\log_2\frac{4}{9} - \frac{5}{9}\log_2\frac{5}{9} \approx 0.99$$

- Averages over information content of each observation
- Unit = **bits** (based on the base of logarithm)
- A fair coin flip has 1 bit of entropy

Entropy

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

- Q: What is the entropy of a uniform distribution over $\mathcal{X} = \{1, \ldots, N\}$?
- Q: What is the entropy of a distribution concentrated on one of the outcomes (that is, $p = (1, 0, 0, \ldots, 0)$)?
- Q: What is the entropy of a Bernoulli random variable with probability of 1 being p (and $1 - p$ for 0)?



Entropy

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

[Slide credit: Vibhav Gogate]

Entropy of a Joint Distribution

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

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

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

Q: What weather condition has 2 bits of information?

Specific Conditional Entropy

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

	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**?

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

- 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:

$$\begin{aligned} H(Y|X) &= \mathbb{E}_{X\sim p(x)}[H(Y|X)] \\ &= \sum_{x\in\mathcal{X}} p(x)H(Y|X=x) \\ &= -\sum_{x\in\mathcal{X}}\sum_{y\in\mathcal{Y}} p(x,y)\log_2 p(y|x) \\ &= -\mathbb{E}_{(X,Y)\sim p(x,y)}[\log_2 p(Y|X)] \end{aligned} \tag{1}$$

Conditional Entropy

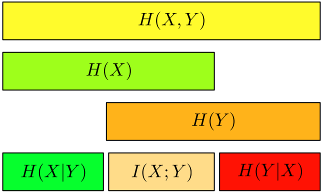
- Example: $\mathcal{X} = \{\text{Raining, Not raining}\}$, $\mathcal{Y} = \{\text{Cloudy, Not cloudy}\}$

	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?

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

Conditional Entropy



- Some useful properties for the discrete case:
  - 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 does not tell us anything about Y: $H(Y|X) = H(Y)$.
  - If X and Y independent, then $H(X, Y) = H(X) + H(Y)$.
  - But Y tells us everything about Y: $H(Y|Y) = 0$.
  - By knowing X, we can only decrease uncertainty about Y: $H(Y|X) \leq H(Y)$.

Exercise: Verify these!

The figure is reproduced from Fig 8.1 of MacKay, Information Theory, Inference, and ... .

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?

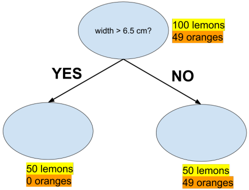
$$\begin{aligned} I(X;Y) = IG(Y|X) &= H(Y) - H(Y|X) \\ &\approx 0.25 \text{ bits} \end{aligned}$$

- 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: $IG(Y|X) = H(Y)$
- Information gain measures the informativeness of a variable, which is exactly what we desire in a decision tree attribute!

Back to Decision Trees

Revisiting Our Original Example

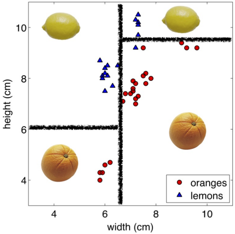
- What is the information gain of this split?

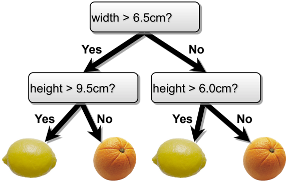


- Let Y be r.v. denoting lemon or orange, B be r.v. denoting whether left or right split taken, and treat counts as probabilities.
- Root entropy: $H(Y) = -\frac{49}{149}\log_2(\frac{49}{149}) - \frac{100}{149}\log_2(\frac{100}{149}) \approx 0.91$
- Leafs entropy: $H(Y|B = \text{left}) = 0$, $H(Y|B = \text{right}) \approx 1$.

$$
\begin{aligned}
IG(Y|B) &= H(Y) - H(Y|B) \\
&= H(Y) - \{H(Y|B{=}\text{left})\mathbb{P}(B{=}\text{left}) + H(Y|B{=}\text{right})\mathbb{P}(B{=}\text{right}) \\
&\approx 0.91 - (0 \cdot \frac{1}{3} + 1 \cdot \frac{2}{3}) \approx 0.24 > 0.
\end{aligned}
$$

Constructing Decision Trees





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

Decision Tree Construction Algorithm

- Simple, greedy, recursive approach, builds up tree node-by-node
- Start with empty decision tree and complete training set
  - Split on the most informative attribute, partitioning dataset
  - Recurse on subpartitions
- Possible termination condition: end if all examples in current subpartition share the same class

Back to Our Example

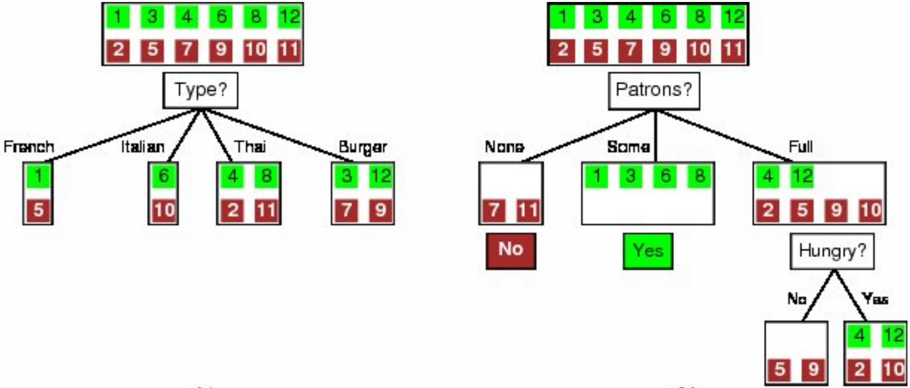
Example	Input Attributes										Goal
	Alt	*Bar*	*Fri*	*Hun*	*Pat*	*Price*	*Rain*	*Res*	*Type*	*Est*	*WillWait*
$\mathbf{x}_1$	Yes	No	No	Yes	Some	$$$	No	Yes	French	0–10	$y_1 =$ Yes
$\mathbf{x}_2$	Yes	No	No	Yes	Full	$	No	No	Thai	30–60	$y_2 =$ No
$\mathbf{x}_3$	No	Yes	No	No	Some	$	No	No	Burger	0–10	$y_3 =$ Yes
$\mathbf{x}_4$	Yes	No	Yes	Yes	Full	$	Yes	No	Thai	10–30	$y_4 =$ Yes
$\mathbf{x}_5$	Yes	No	Yes	No	Full	$$$	No	Yes	French	>60	$y_5 =$ No
$\mathbf{x}_6$	No	Yes	No	Yes	Some	$$	Yes	Yes	Italian	0–10	$y_6 =$ Yes
$\mathbf{x}_7$	No	Yes	No	No	None	$	Yes	No	Burger	0–10	$y_7 =$ No
$\mathbf{x}_8$	No	No	No	Yes	Some	$$	Yes	Yes	Thai	0–10	$y_8 =$ Yes
$\mathbf{x}_9$	No	Yes	Yes	No	Full	$	Yes	No	Burger	>60	$y_9 =$ No
$\mathbf{x}_{10}$	Yes	Yes	Yes	Yes	Full	$$$	No	Yes	Italian	10–30	$y_{10} =$ No
$\mathbf{x}_{11}$	No	No	No	No	None	$	No	No	Thai	0–10	$y_{11} =$ No
$\mathbf{x}_{12}$	Yes	Yes	Yes	Yes	Full	$	No	No	Burger	30–60	$y_{12} =$ Yes

Attributes:

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).

[from: Russell & Norvig]

Attribute Selection

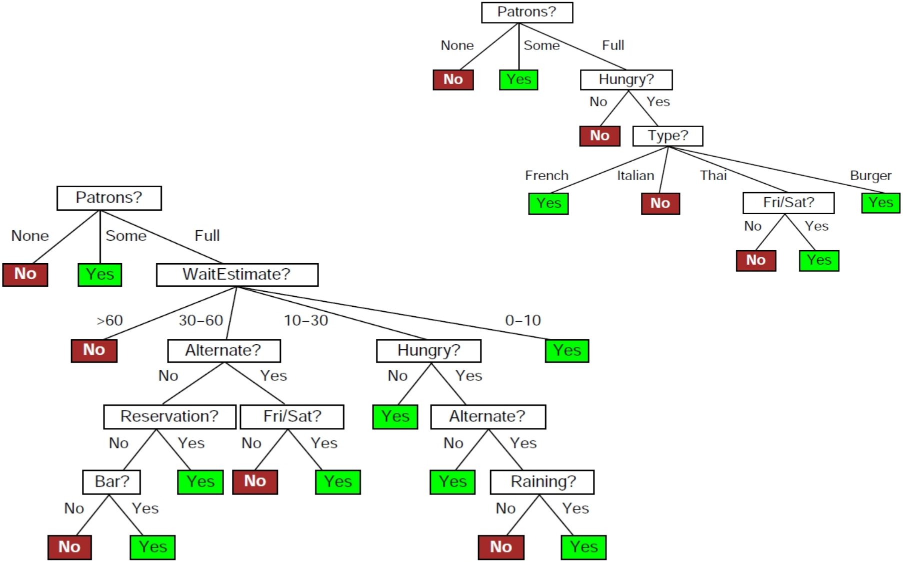


$$IG(Y) = H(Y) - H(Y|X)$$

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

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

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:
  - Avoid over-fitting training examples.
    - We need enough samples in each region to confidently determine the output.
  - Computational efficiency (avoid redundant, spurious attributes)
  - Human interpretability
- "Occam's Razor": find the simplest hypothesis that fits the observations
  - Useful principle, but not obvious how to formalize simplicity.
  - We shall encounter some other ways to formalize simplicity.
  - See Domingos, 1999, "The role of Occam's razor in knowledge discovery"
- We desire small trees with informative nodes near the root

Decision Tree Miscellany

- Problems:
  - You have exponentially less data at lower levels
  - A large tree can overfit the data
  - Greedy algorithms do not necessarily yield the global optimum
  - Mistakes at top-level propagate down tree
- Handling continuous attributes
  - Split based on a threshold, chosen to maximize information gain
- There are other criteria used to measure the quality of a split, e.g., Gini index
- Trees can be pruned in order to make them less complex
- Decision trees can also be used for regression on real-valued outputs. Choose splits to minimize squared error, rather than maximize information gain.

Comparison to K-NN

Advantages of decision trees over K-NN

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

Comparison to K-NN

Advantages of k-NN over decision trees

- Able to handle attributes/features that interact in complex ways
- Can incorporate interesting distance measures, e.g., shape contexts.

Summary

- There are ways to make Decisions Trees much more powerful (using a technique called Bagging (Bootstrap Aggregating), though at the cost of losing some useful properties such as interpretability. We get to them later.
- Next we get to more modular approaches to designing ML methods.