CSC 311: Introduction to Machine Learning

Lecture 2 - Decision Trees & Ensembles

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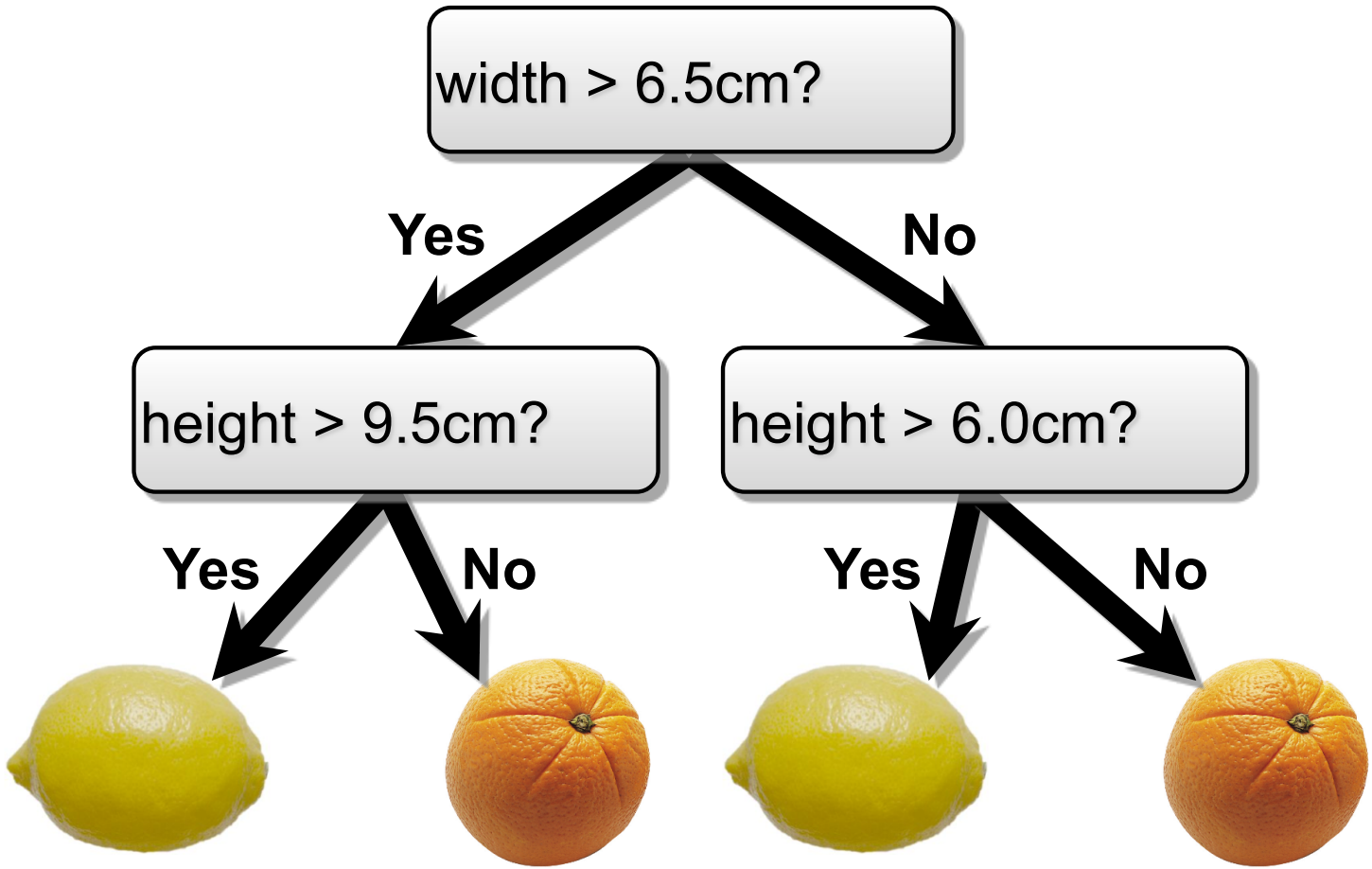
Today

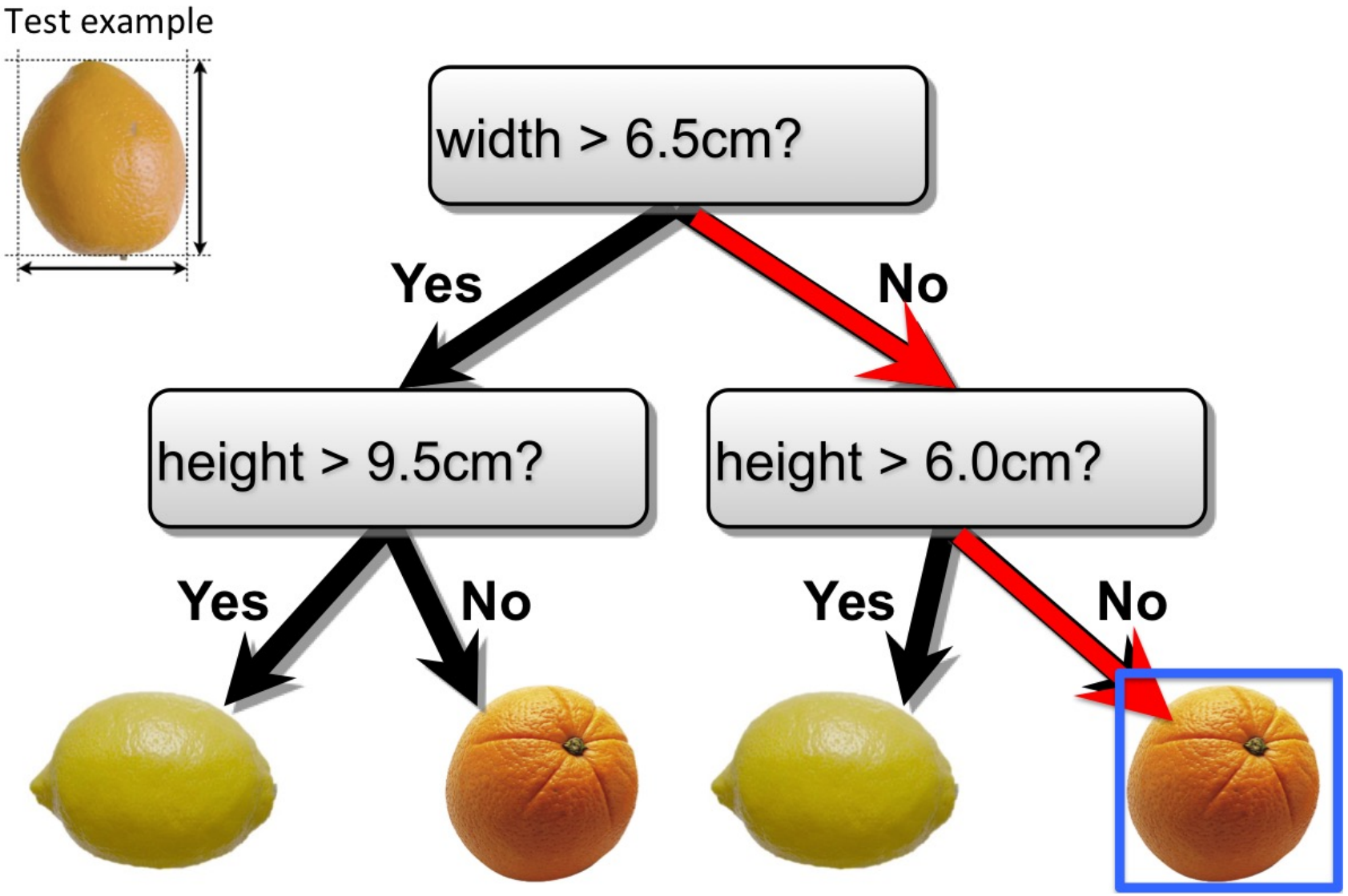
- **Decision Trees**
  - Simple but powerful learning algorithm
  - One of the most widely used learning algorithms in Kaggle competitions
- Lets us introduce ensembles, a key idea in ML
- Useful information theoretic concepts (entropy, mutual information, etc.)

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

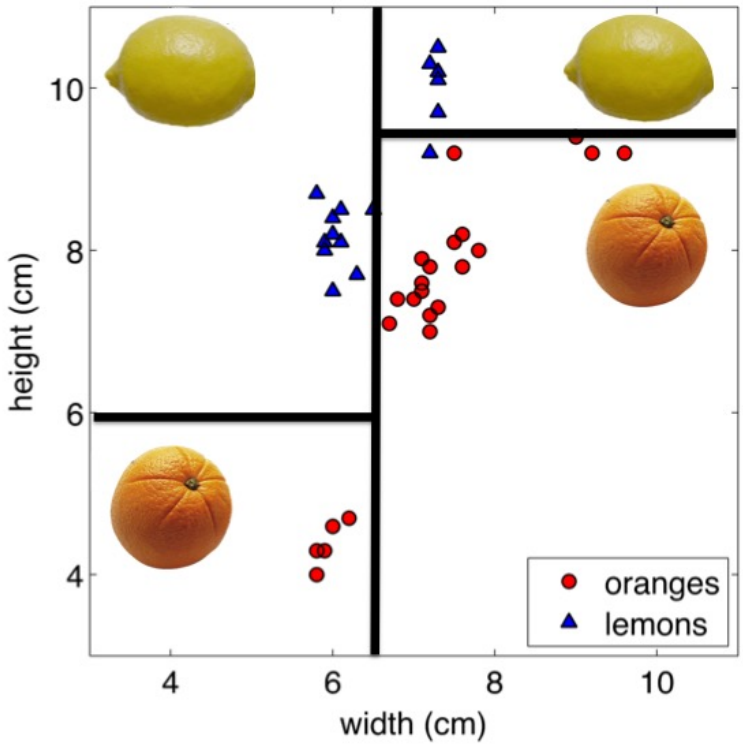


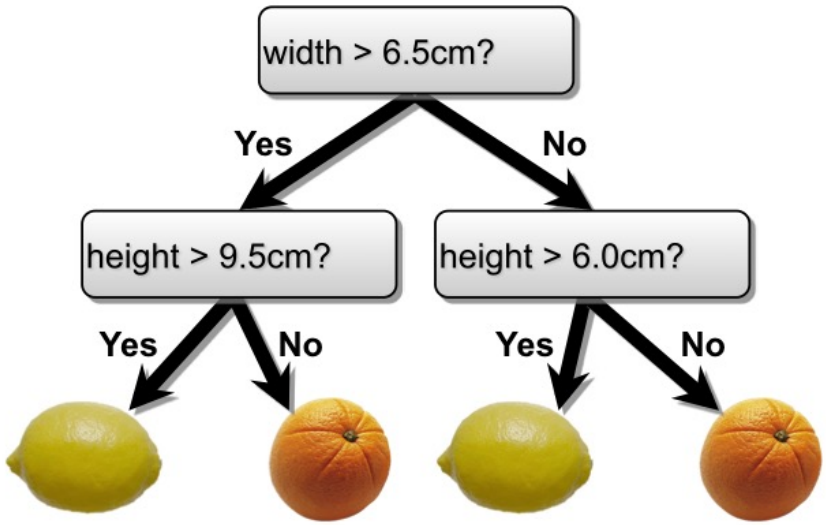
Decision Trees



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





Example with Discrete Inputs

- What if the attributes are discrete?

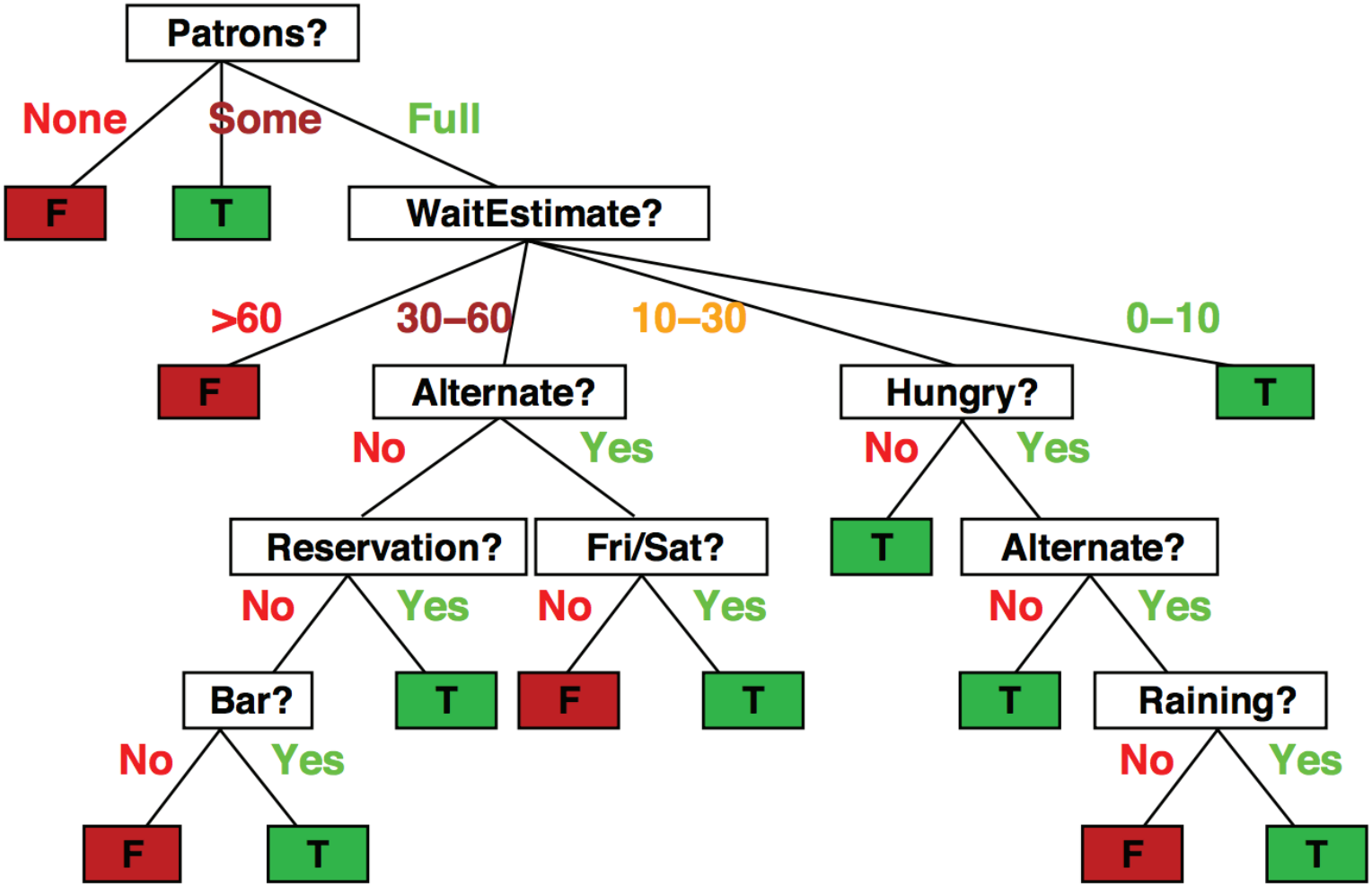
Example	Input Attributes										Goal
	Alt	*Bar*	*Fri*	*Hun*	*Pat*	*Price*	*Rain*	*Res*	*Type*	*Est*	*WillWait*
$\mathbf{x}_1$	*Yes*	*No*	*No*	*Yes*	*Some*	*$$$*	*No*	*Yes*	*French*	*0–10*	$y_1 =$ *Yes*
$\mathbf{x}_2$	*Yes*	*No*	*No*	*Yes*	*Full*	*$*	*No*	*No*	*Thai*	*30–60*	$y_2 =$ *No*
$\mathbf{x}_3$	*No*	*Yes*	*No*	*No*	*Some*	*$*	*No*	*No*	*Burger*	*0–10*	$y_3 =$ *Yes*
$\mathbf{x}_4$	*Yes*	*No*	*Yes*	*Yes*	*Full*	*$*	*Yes*	*No*	*Thai*	*10–30*	$y_4 =$ *Yes*
$\mathbf{x}_5$	*Yes*	*No*	*Yes*	*No*	*Full*	*$$$*	*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:

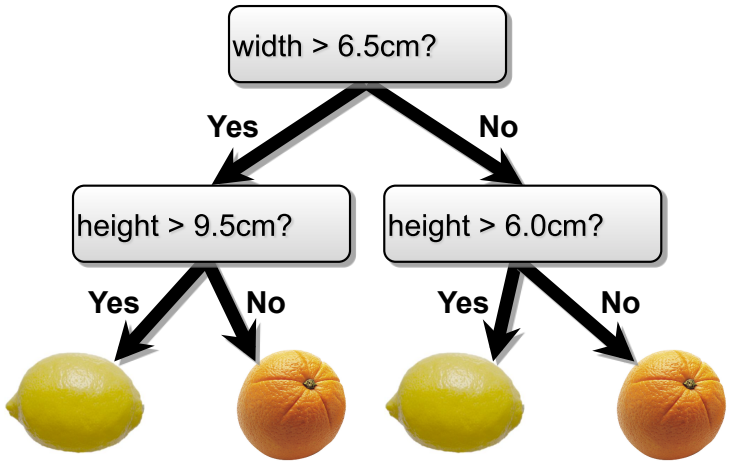
1. Alternate: whether there is a suitable alternative restaurant nearby.
2. Bar: whether the restaurant has a comfortable bar area to wait in.
3. Fri/Sat: true on Fridays and Saturdays.
4. Hungry: whether we are hungry.
5. Patrons: how many people are in the restaurant (values are None, Some, and Full).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

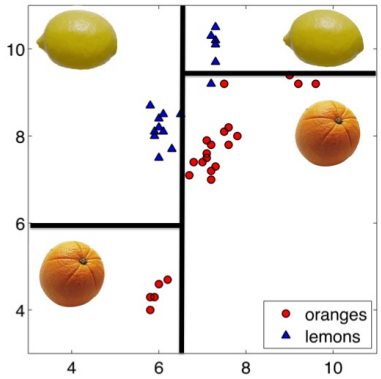


Decision Trees



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

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
- **Classification tree**:
  - discrete output
  - leaf value y^m typically set to the most common value in $\{t^{(m_1)}, \ldots, t^{(m_k)}\}$
- **Regression tree**:
  - continuous output
  - 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?

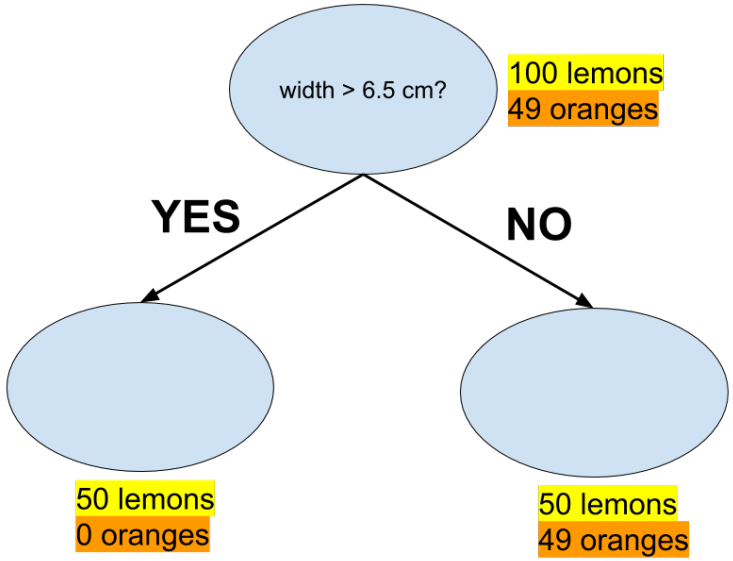
Learning Decision Trees

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

- Resort to a **greedy heuristic**! Start with empty decision tree and complete training set
  - Split on the "best" attribute, i.e. partition dataset
  - Recurse on subpartitions
- When should we stop?
- Which attribute is the "best" (and where should we split, if continuous)?
  - Choose based on accuracy?
  - Say region R is split in R_1 and R_2 based on loss $L(R)$.
  - Accuracy gain is $L(R) - \frac{|R_1|L(R_1)+|R_2|L(R_2)}{|R_1|+|R_2|}$

Choosing a Good Split

- Why isn't accuracy a good measure?
- Classify by the majority, loss is misclassification rate.



- Is this split good? Zero accuracy gain

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

- But we've reduced our uncertainty about whether a fruit is a lemon

Choosing a Good Split

- How can we quantify uncertainty in prediction for a given leaf node?
  - All examples in leaf have same class: good, low uncertainty
  - Each class has same amount of examples in leaf: bad, high uncertainty
- **Idea:** Use counts at leaves to define probability distributions, and use information theory to measure uncertainty

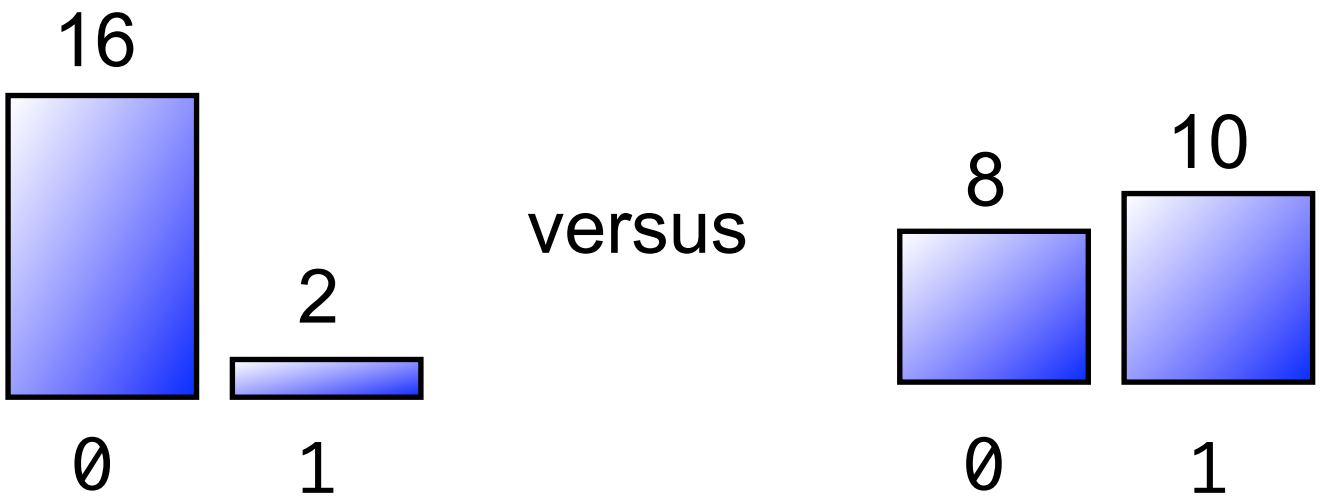
We Flip Two Different Coins

Sequence 1:

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

Sequence 2:

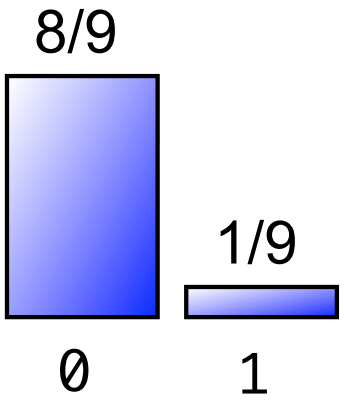
0 1 0 1 0 1 1 1 0 1 0 0 1 1 0 1 0 1 ... ?

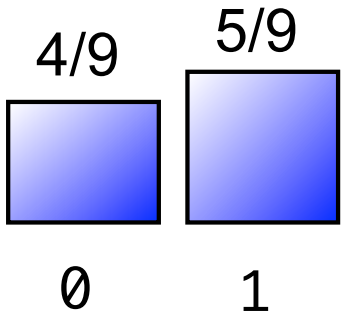


Quantifying Uncertainty

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

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





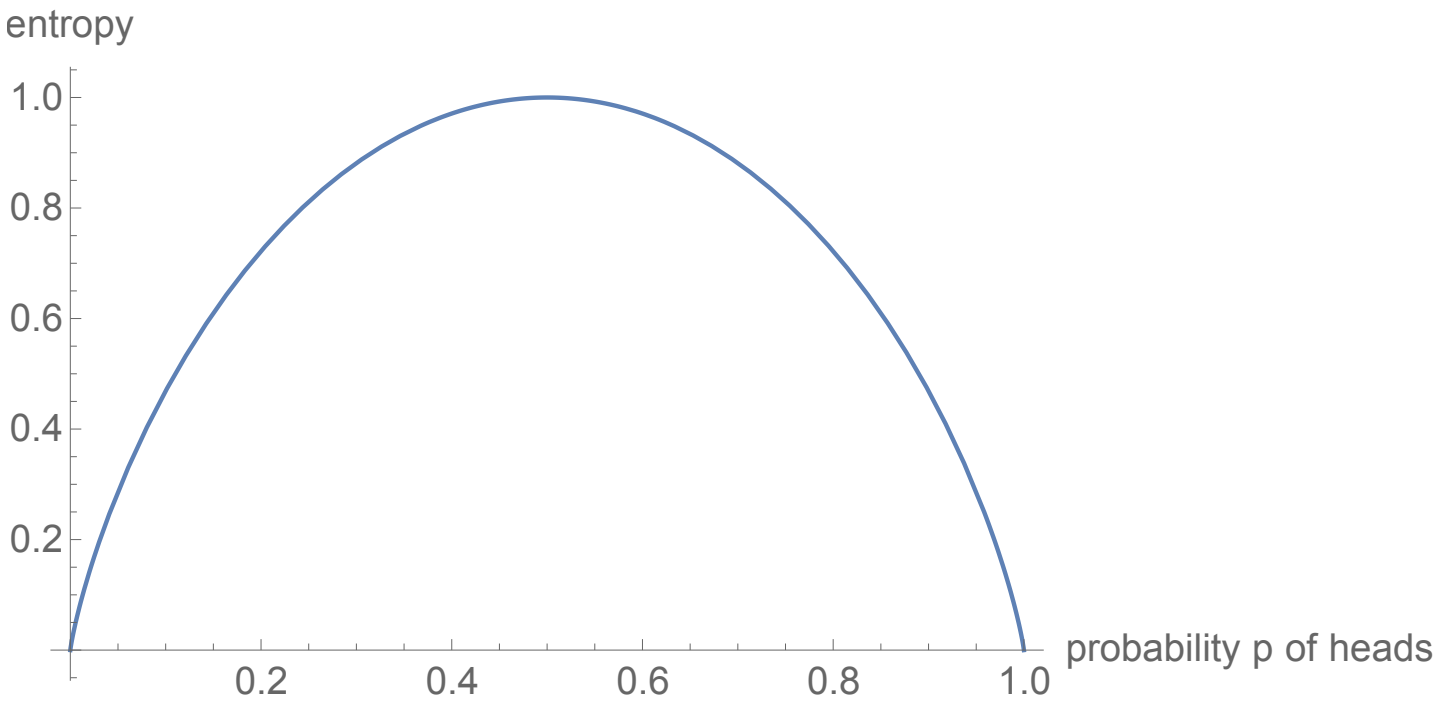
$$-\frac{8}{9}\log_2\frac{8}{9} - \frac{1}{9}\log_2\frac{1}{9} \approx \frac{1}{2}$$

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

- Averages over information content of each observation
- Unit = **bits** (based on the base of $\log_2$)
- A fair coin flip has 1 bit of entropy

Quantifying Uncertainty

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



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

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

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

Specific Conditional Entropy

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

	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**?

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

- 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:

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

Conditional Entropy

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

	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?

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

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

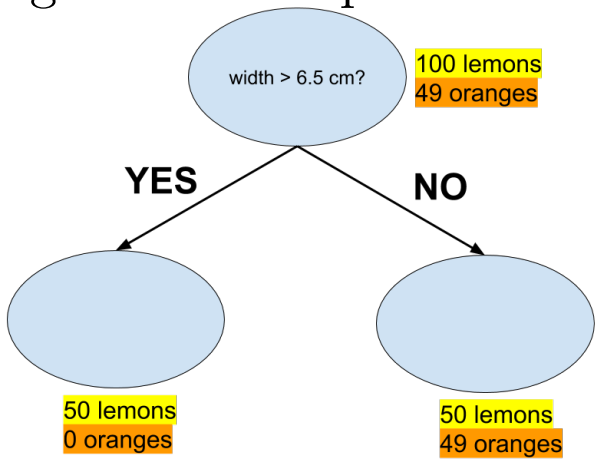
- How much information about cloudiness do we get by discovering whether it is raining?

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

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

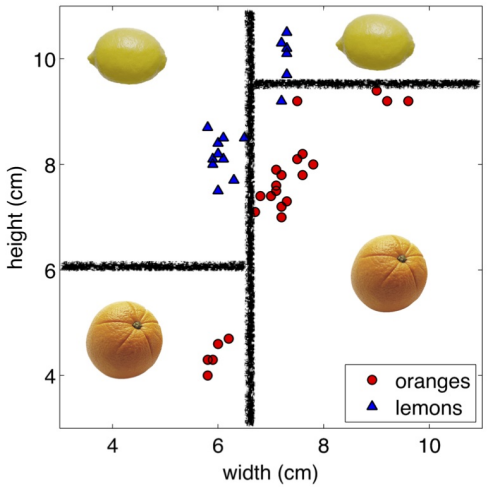
Revisiting Our Original Example

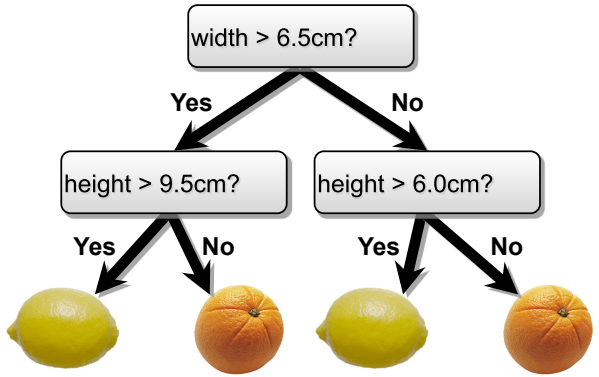
- Information gain measures the informativeness of a variable, which is exactly what we desire in a decision tree attribute!
- What is the information gain of this split?



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

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 **best** 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

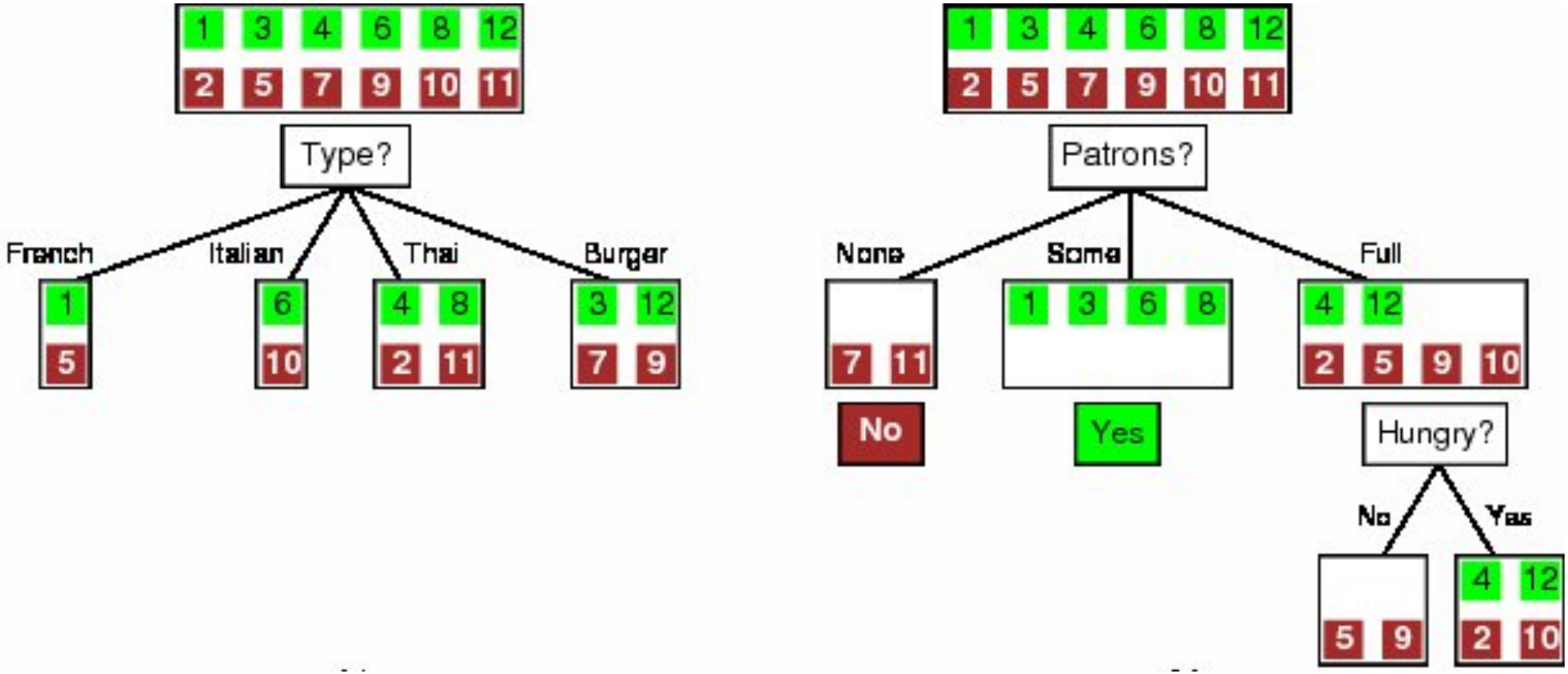
Example	Input Attributes										Goal
	Alt	*Bar*	*Fri*	*Hun*	*Pat*	*Price*	*Rain*	*Res*	*Type*	*Est*	*WillWait*
$\mathbf{x}_1$	*Yes*	*No*	*No*	*Yes*	*Some*	*$$$*	*No*	*Yes*	*French*	*0–10*	$y_1 = Yes$
$\mathbf{x}_2$	*Yes*	*No*	*No*	*Yes*	*Full*	*$*	*No*	*No*	*Thai*	*30–60*	$y_2 = No$
$\mathbf{x}_3$	*No*	*Yes*	*No*	*No*	*Some*	*$*	*No*	*No*	*Burger*	*0–10*	$y_3 = Yes$
$\mathbf{x}_4$	*Yes*	*No*	*Yes*	*Yes*	*Full*	*$*	*Yes*	*No*	*Thai*	*10–30*	$y_4 = Yes$
$\mathbf{x}_5$	*Yes*	*No*	*Yes*	*No*	*Full*	*$$$*	*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

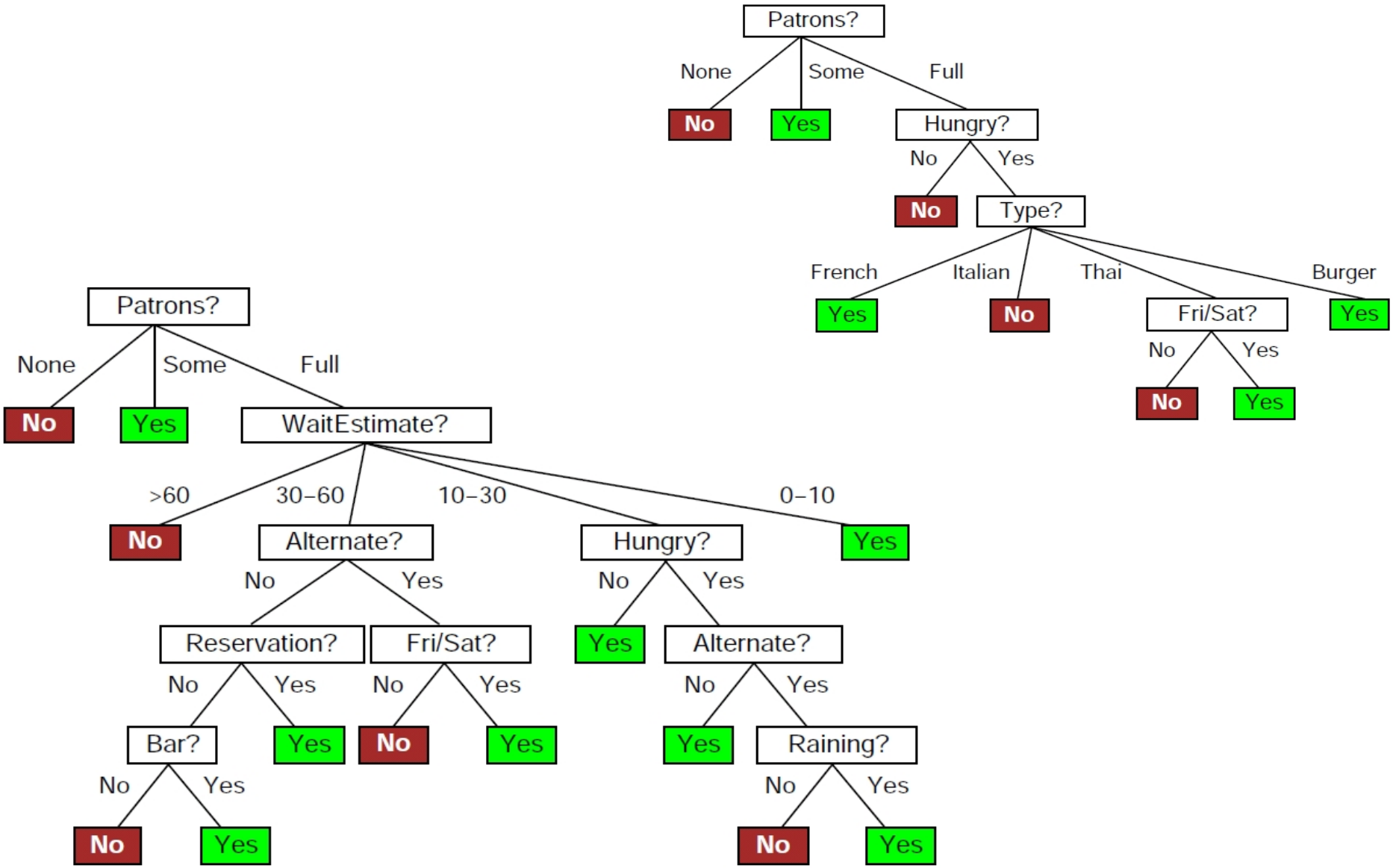


$$IG(Y) = H(Y) - H(Y|X)$$

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

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

Which Tree is Better?



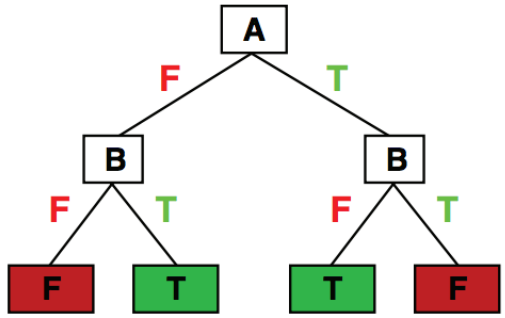
What Makes a Good Tree?

- Not too small: need to handle important but possibly subtle distinctions in data
- Not too big:
  - 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

Expressiveness

- **Discrete-input, discrete-output case**:
  - Decision trees can express any function of the input attributes
  - E.g., for Boolean functions, truth table row → 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]

Decision Tree Miscellany

- 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
  - Mistakes at top-level propagate down tree
- 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.

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
- 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 (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.

Overview

- We've seen two particular learning algorithms: k-NN and decision trees
- Next: **combine multiple models into an ensemble** which performs better than the individual members
  - Generic class of techniques that can be applied to almost any learning algorithms...
  - ... but are particularly well suited to decision trees
  - Understanding generalization using the **bias/variance decomposition**
  - Reducing variance using bagging
- Next lecture
  - Making a weak classifier stronger (i.e. reducing bias) using boosting

Ensemble methods: Overview

- An **ensemble** of predictors is a set of predictors whose individual decisions are combined in some way to predict new examples
  - E.g., (possibly weighted) majority vote
- For this to be nontrivial, the learned hypotheses must differ somehow, e.g.
  - Different algorithm
  - Different choice of hyperparameters
  - Trained on different data
  - Trained with different weighting of the training examples
- Ensembles are usually easy to implement. The hard part is deciding what kind of ensemble you want, based on your goals.

Agenda

- This lecture: **bagging**
  - Train classifiers independently on random subsets of the training data.
- Next lecture: **boosting**
  - Train classifiers sequentially, each time focusing on training examples that the previous ones got wrong.
- Bagging and boosting serve very different purposes. To understand this, we need to take a detour to understand the bias and variance of a learning algorithm.

Loss Functions

- A **loss function** $L(y, t)$ defines how bad it is if, for some example x, the algorithm predicts y, but the target is actually t.
- Example: **0-1 loss** for classification

$$L_{0-1}(y, t) = \begin{cases} 0 & \text{if } y = t \\ 1 & \text{if } y \neq t \end{cases}$$

  - Averaging the 0-1 loss over the training set gives the **training error rate**, and averaging over the test set gives the **test error rate**.

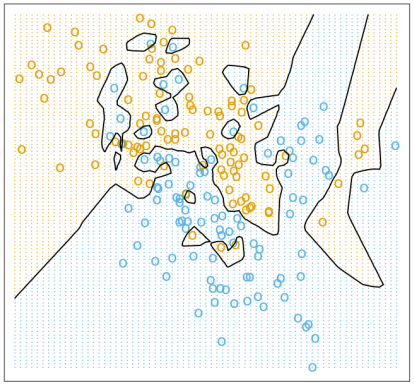
- Example: **squared error loss** for regression

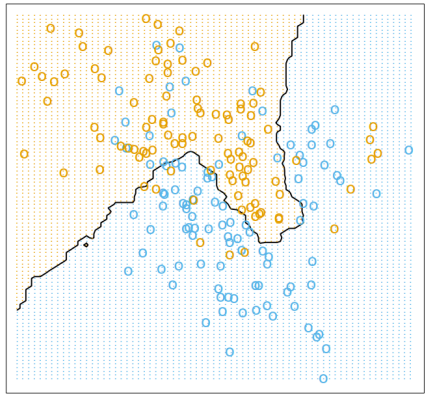
$$L_{\text{SE}}(y, t) = \frac{1}{2}(y - t)^2$$

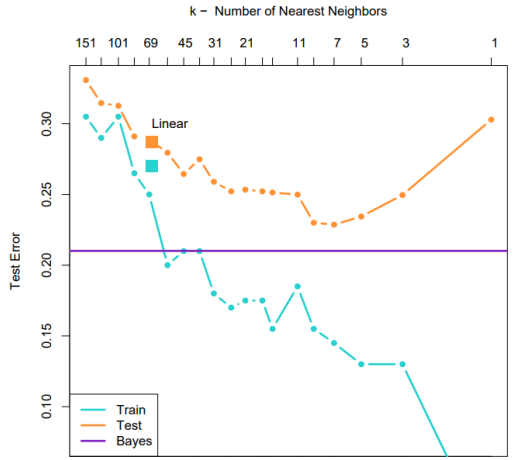
  - The average squared error loss is called **mean squared error (MSE)**.

Bias-Variance Decomposition

- Recall that overly simple models underfit the data, and overly complex models overfit.



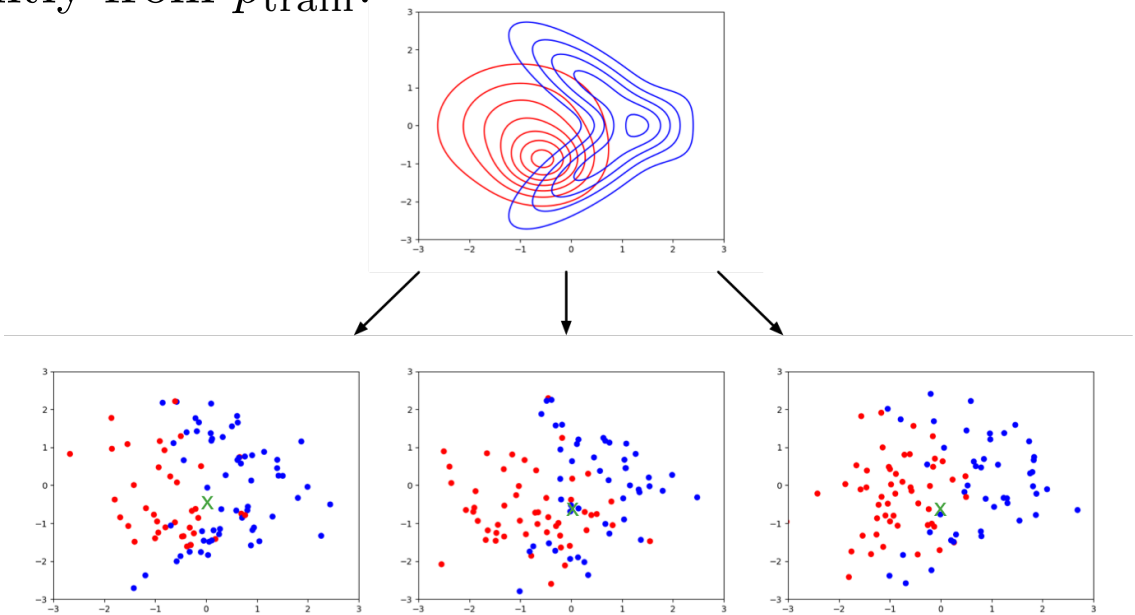




- We can quantify this effect in terms of the **bias/variance decomposition**.
- Bias and variance of what?

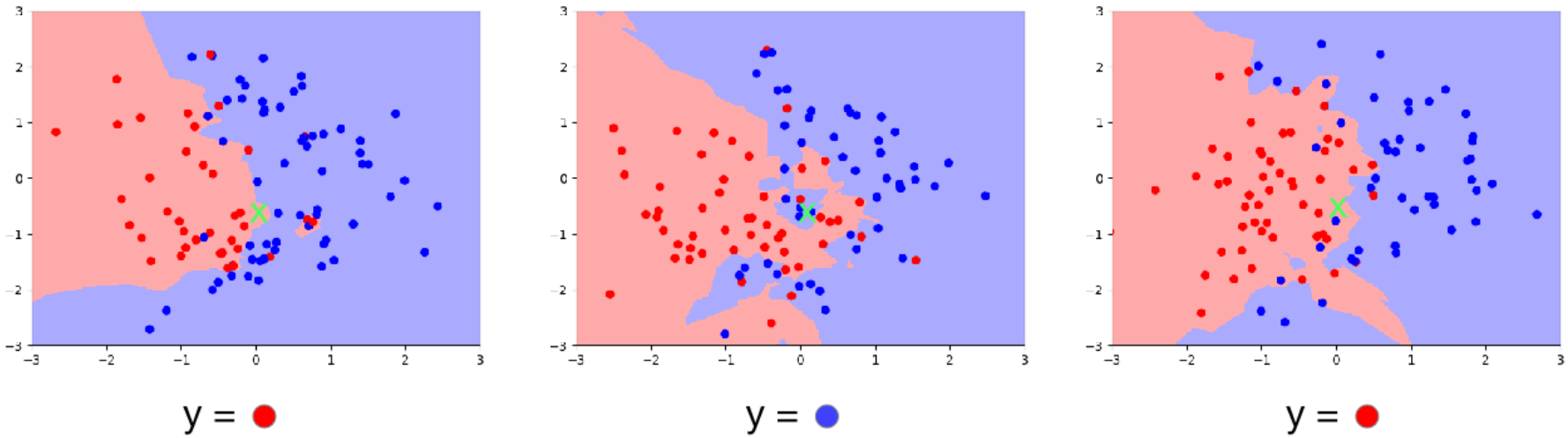
Bias-Variance Decomposition: Basic Setup

- Suppose the training set $\mathcal{D}$ consists of N pairs $(\mathbf{x}^{(i)}, t^{(i)})$ sampled **independent and identically distributed (i.i.d.)** from a single **data generating distribution** p_{data}.
  - Let p_{train} denote the induced distribution over training sets
- Pick a fixed query point $\mathbf{x}$ (denoted with a green x).
- Consider an experiment where we sample lots of training sets independently from p_{train}.



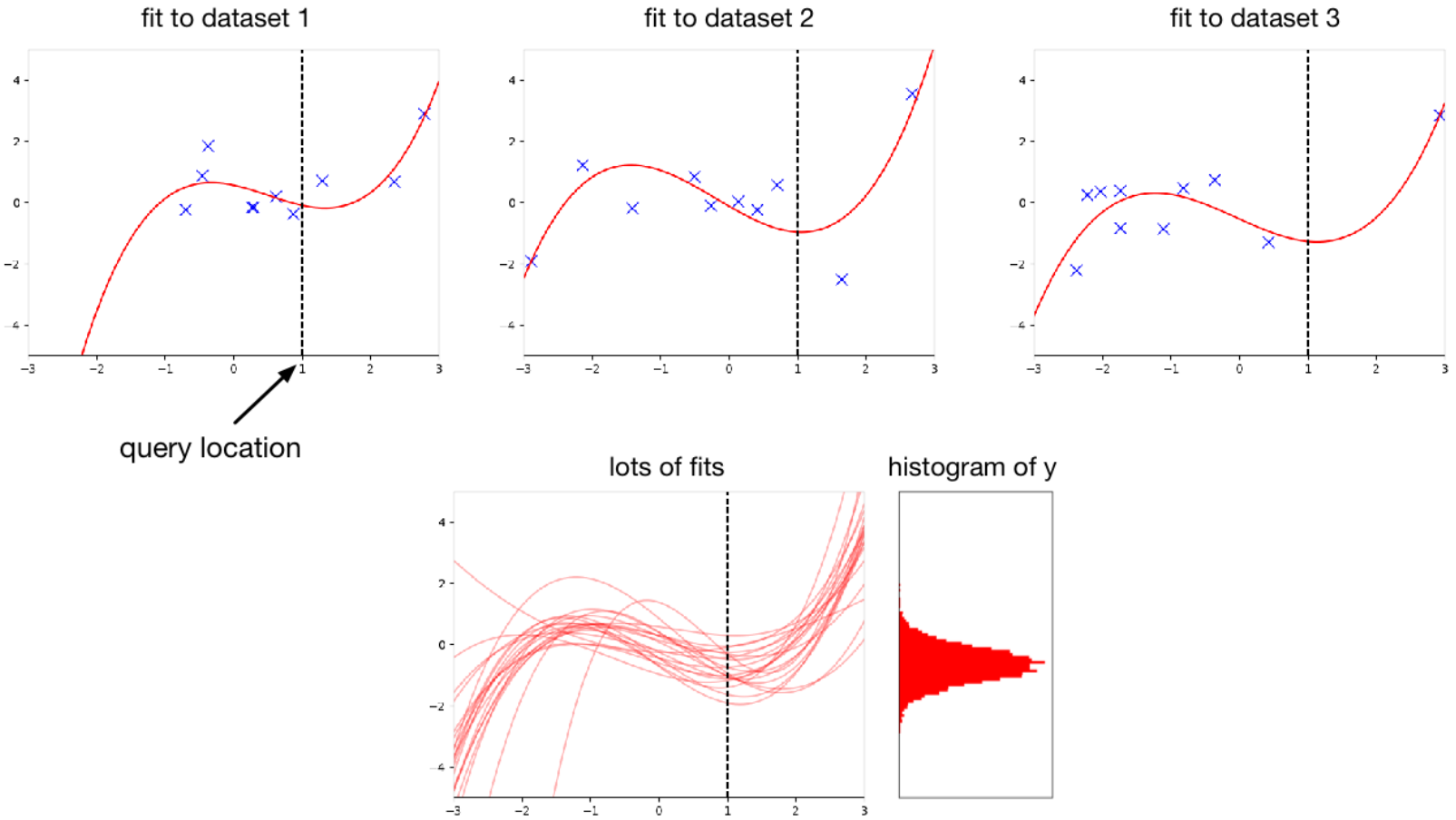
Bias-Variance Decomposition: Basic Setup

- Let's run our learning algorithm on each training set $\mathcal{D}$, producing a classifier $h_{\mathcal{D}}$
- We can compute each classifier's prediction $h_{\mathcal{D}}(\mathbf{x}) = y$ at the query point $\mathbf{x}$.
- y is a random variable, where the **randomness comes from the choice of training set**
  - $\mathcal{D}$ is random $\implies$ $h_{\mathcal{D}}$ is random $\implies$ $h_{\mathcal{D}}(\mathbf{x})$ is random



Bias-Variance Decomposition: Basic Setup

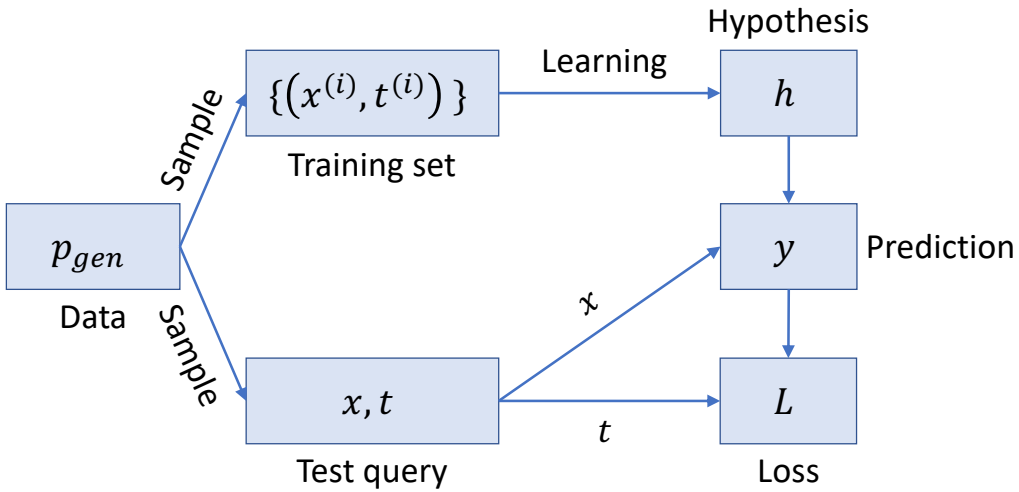
Here is the analogous setup for regression:



Since $y = h_{\mathcal{D}}(\mathbf{x})$ is a random variable, we can talk about its expectation, variance, etc. over the distribution of training sets p_{train}

Bias-Variance Decomposition: Basic Setup

- Recap of basic setup:



- Assume (for the moment) that t is deterministic given x
- There is a distribution over the loss at $\mathbf{x}$, with expectation $\mathbb{E}_{\mathcal{D} \sim p_{\text{train}}}[L(h_{\mathcal{D}}(\mathbf{x}), t)]$.
- For each query point $\mathbf{x}$, the expected loss is different. We are interested in quantifying how well our classifier does over the distribution p_{data}, averaging over training sets: $\mathbb{E}_{\mathbf{x} \sim p_{\text{data}}, \mathcal{D} \sim p_{\text{train}}}[L(h_{\mathcal{D}}(\mathbf{x}), t)]$.

Bias-Variance Decomposition

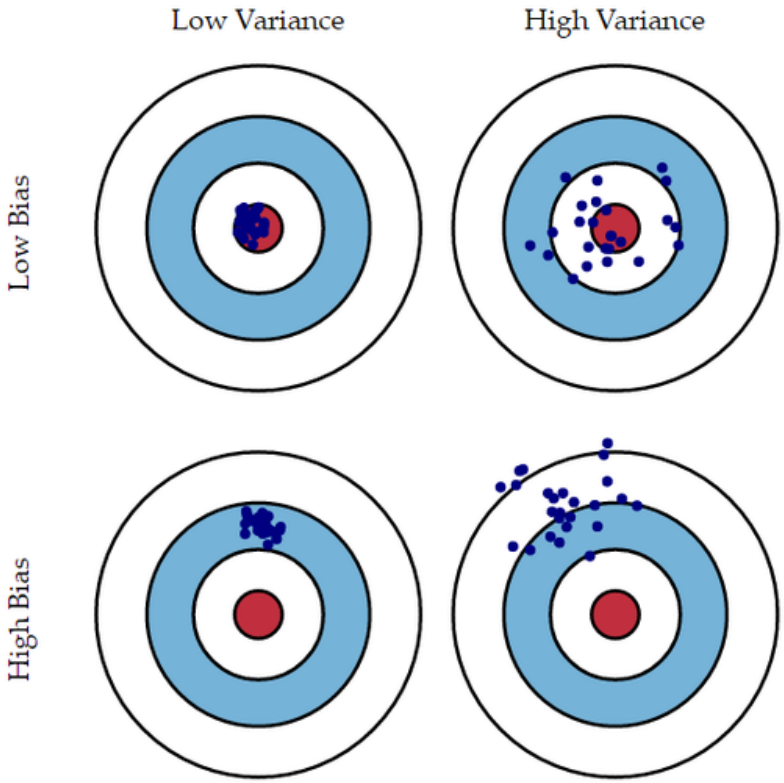
- For now, focus on squared error loss, $L(y,t) = \frac{1}{2}(y-t)^2$.
- We can decompose the expected loss (suppressing distributions $\mathbf{x}$, $\mathcal{D}$ drawn from for compactness):

$$\begin{aligned}
\mathbb{E}_{\mathbf{x},\mathcal{D}}[(h_{\mathcal{D}}(\mathbf{x}) - t)^2] &= \mathbb{E}_{\mathbf{x},\mathcal{D}}[(h_{\mathcal{D}}(\mathbf{x}) - \mathbb{E}_{\mathcal{D}}[h_{\mathcal{D}}(\mathbf{x})] + \mathbb{E}_{\mathcal{D}}[h_{\mathcal{D}}(\mathbf{x})] - t)^2] \\
&= \mathbb{E}_{\mathbf{x},\mathcal{D}}[(h_{\mathcal{D}}(\mathbf{x}) - \mathbb{E}_{\mathcal{D}}[h_{\mathcal{D}}(\mathbf{x})])^2 + (\mathbb{E}_{\mathcal{D}}[h_{\mathcal{D}}(\mathbf{x})] - t)^2 + \\
&\qquad 2(h_{\mathcal{D}}(\mathbf{x}) - \mathbb{E}_{\mathcal{D}}[h_{\mathcal{D}}(\mathbf{x})])(\mathbb{E}_{\mathcal{D}}[h_{\mathcal{D}}(\mathbf{x})] - t)] \\
&= \underbrace{\mathbb{E}_{\mathbf{x},\mathcal{D}}[(h_{\mathcal{D}}(\mathbf{x}) - \mathbb{E}_{\mathcal{D}}[h_{\mathcal{D}}(\mathbf{x})])^2]}_{\text{variance}} + \underbrace{\mathbb{E}_{\mathbf{x}}[(\mathbb{E}_{\mathcal{D}}[h_{\mathcal{D}}(\mathbf{x})] - t)^2]}_{\text{bias}}
\end{aligned}$$

- Bias: On average, how close is our classifier to true target? (corresponds to underfitting)
- Variance: How widely dispersed are our predictions as we generate new datasets? (corresponds to overfitting)

Bias and Variance

- Throwing darts = predictions for each draw of a dataset



- What doesn't this capture?
- We average over points $\mathbf{x}$ from the data distribution

Bagging

Now, back to bagging!

Bagging: Motivation

- Suppose we could somehow sample m independent training sets $\{\mathcal{D}_i\}_{i=1}^m$ from p_{train}.
- We could then learn a predictor $h_i := h_{\mathcal{D}_i}$ based on each one, and take the average $h = \frac{1}{m}\sum_{i=1}^m h_i$.
- How does this affect the terms of the expected loss?
  - **Bias: unchanged**, since the averaged prediction has the same expectation

$$\mathbb{E}_{\mathcal{D}_1,\ldots,\mathcal{D}_m \overset{iid}{\sim} p_{\text{train}}}[h(\mathbf{x})] = \frac{1}{m}\sum_{i=1}^m \mathbb{E}_{\mathcal{D}_i \sim p_{\text{train}}}[h_i(\mathbf{x})] = \mathbb{E}_{\mathcal{D}\sim p_{\text{train}}}[h_{\mathcal{D}}(\mathbf{x})]$$

  - **Variance: reduced**, since we're averaging over independent samples

$$\operatorname*{Var}_{\mathcal{D}_1,\ldots,\mathcal{D}_m}[h(\mathbf{x})] = \frac{1}{m^2}\sum_{i=1}^m \operatorname*{Var}_{\mathcal{D}_i}[h_i(\mathbf{x})] = \frac{1}{m}\operatorname*{Var}_{\mathcal{D}}[h_{\mathcal{D}}(\mathbf{x})].$$

Bagging: The Idea

- In practice, we don't have access to the underlying data generating distribution p_{data}.
- It is expensive to independently collect many datasets.
- Solution: **bootstrap aggregation**, or **bagging**.
  - Take a single dataset $\mathcal{D}$ with n examples.
  - Generate m new datasets, each by sampling n training examples from $\mathcal{D}$, with replacement.
  - Average the predictions of models trained on each of these datasets.

Bagging: The Idea

- Problem: the datasets are not independent, so we don't get the $1/m$ variance reduction.
  - Possible to show that if the sampled predictions have variance σ^2 and correlation ρ, then

$$\text{Var}\left(\frac{1}{m}\sum_{i=1}^{m} h_i(\mathbf{x})\right) = \frac{1}{m}(1-\rho)\sigma^2 + \rho\sigma^2.$$

- Ironically, it can be advantageous to introduce *additional* variability into your algorithm, as long as it reduces the correlation between samples.
  - Intuition: you want to invest in a diversified portfolio, not just one stock.
  - Can help to use average over multiple algorithms, or multiple configurations of the same algorithm.

Random Forests

- **Random forests** = bagged decision trees, with one extra trick to decorrelate the predictions
- When choosing each node of the decision tree, choose a random set of d input features, and only consider splits on those features
- Random forests are probably the best black-box machine learning algorithm — they often work well with no tuning whatsoever.
  - one of the most widely used algorithms in Kaggle competitions

Bayes Optimality

- Let's return to quantifying expected loss and make the situation slightly more complicated (and realistic): what if t is not deterministic given $\mathbf{x}$? i.e. have $p(t|\mathbf{x})$
- Can no longer measure bias as expected distance from true target, since there's a distribution over targets!
- Instead, we'll measure distance from $y_*(\mathbf{x}) = \mathbb{E}[t \,|\, \mathbf{x}]$
  - This is the best possible prediction, in the sense that it minimizes the expected loss

Bayes Optimality

- **Proof:** Start by fixing $\mathbf{x}$. Want to show:
  $\text{argmin}_y \mathbb{E}_t[(y-t)^2] = y_* = \mathbb{E}_t[t]$ (Distribution of t is $p(t|\mathbf{x})$)

$$\begin{aligned}
\mathbb{E}_t[(y-t)^2] &= \mathbb{E}_t[y^2 - 2yt + t^2] \\
&= y^2 - 2y\mathbb{E}_t[t] + \mathbb{E}_t[t^2] \\
&= y^2 - 2y\mathbb{E}_t[t] + \mathbb{E}_t[t]^2 + \text{Var}[t \,|\, \mathbf{x}] \\
&= y^2 - 2yy_* + y_*^2 + \text{Var}[t \,|\, \mathbf{x}] \\
&= (y - y_*)^2 + \text{Var}[t \,|\, \mathbf{x}]
\end{aligned}$$

- The first term is nonnegative, and can be made 0 by setting $y = y_*$.
- The second term doesn't depend on y! Corresponds to the inherent unpredictability, or **noise**, of the targets, and is called the **Bayes error**.
  - This is the best we can ever hope to do with any learning algorithm. An algorithm that achieves it is **Bayes optimal**.

Bayes Optimality

- We can again decompose the expected loss, this time including t in our expectation (check this!):

$$\mathbb{E}_{\mathbf{x},\mathcal{D},t}[(h_{\mathcal{D}}(\mathbf{x}) - t)^2] = \underbrace{\mathbb{E}_{\mathbf{x}}[(\mathbb{E}_{\mathcal{D}}[h_{\mathcal{D}}(\mathbf{x})] - y_*(\mathbf{x}))^2]}_{\text{bias}} + \underbrace{\mathbb{E}_{\mathbf{x},\mathcal{D}}[(h_{\mathcal{D}}(\mathbf{x}) - \mathbb{E}_{\mathcal{D}}[h_{\mathcal{D}}(\mathbf{x})])^2]}_{\text{variance}} + \underbrace{\text{Var}[t \mid \mathbf{x}]}_{\text{Bayes}}$$

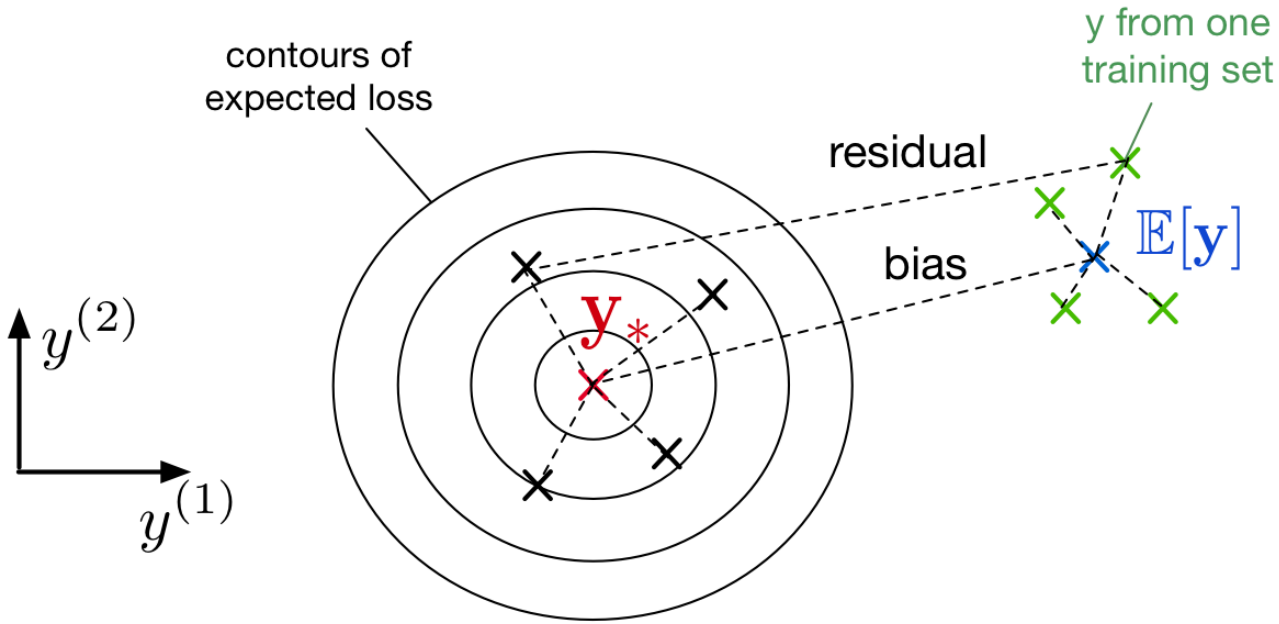
- Contrast if t is not random:

$$\underbrace{\mathbb{E}_{\mathbf{x}}[(\mathbb{E}_{\mathcal{D}}[h_{\mathcal{D}}(\mathbf{x})] - t)^2]}_{\text{bias}} + \underbrace{\mathbb{E}_{\mathbf{x},\mathcal{D}}[(h_{\mathcal{D}}(\mathbf{x}) - \mathbb{E}_{\mathcal{D}}[h_{\mathcal{D}}(\mathbf{x})])^2]}_{\text{variance}}$$

- We have no control over the Bayes error! In particular, bagging/boosting do not help

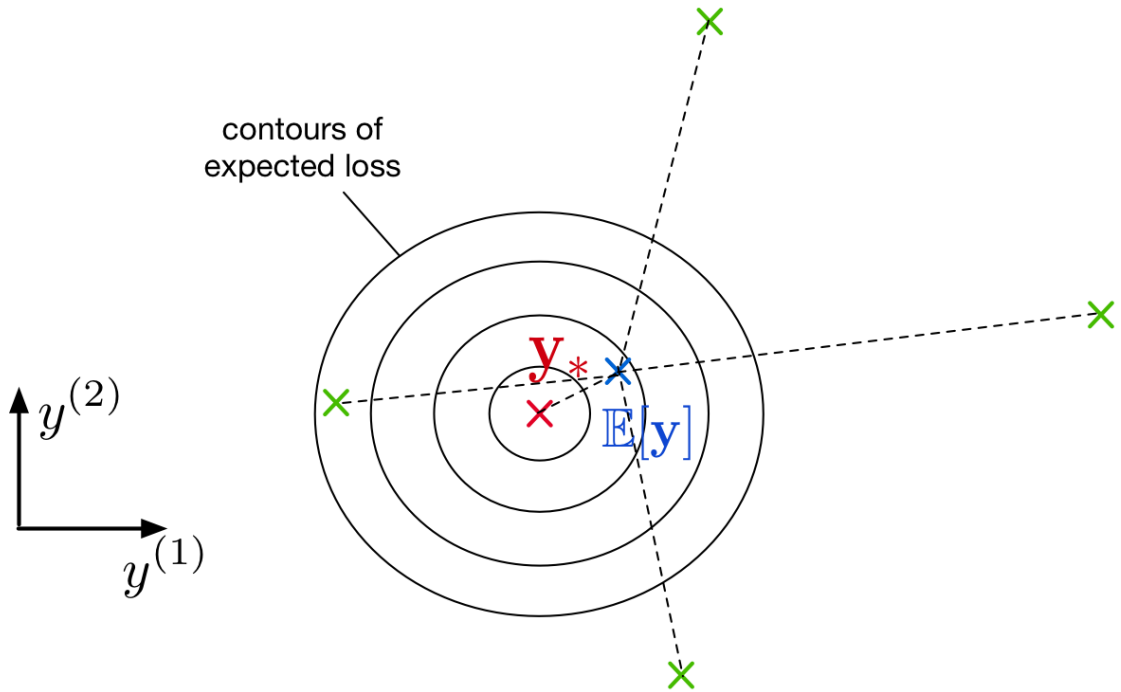
Bias/Variance Decomposition: Another Visualization

- We can visualize this decomposition in **output space**, where the axes correspond to predictions on the test examples.
- If we have an overly simple model (e.g. k-NN with large k), it might have
  - high bias (because it's too simplistic to capture the structure in the data)
  - low variance (because there's enough data to get a stable estimate of the decision boundary)



Bias/Variance Decomposition: Another Visualization

- If you have an overly complex model (e.g. k-NN with $k = 1$), it might have
  - low bias (since it learns all the relevant structure)
  - high variance (it fits the quirks of the data you happened to sample)



Summary

- Bagging reduces overfitting by averaging predictions.
- Used in most competition winners
  - Even if a single model is great, a small ensemble usually helps.
- Limitations:
  - Does not reduce bias.
  - There is still correlation between classifiers.
- Random forest solution: Add more randomness.