

# CSC 2515 Lecture 2: Decision Trees and Ensembles

Roger Grosse

University of Toronto

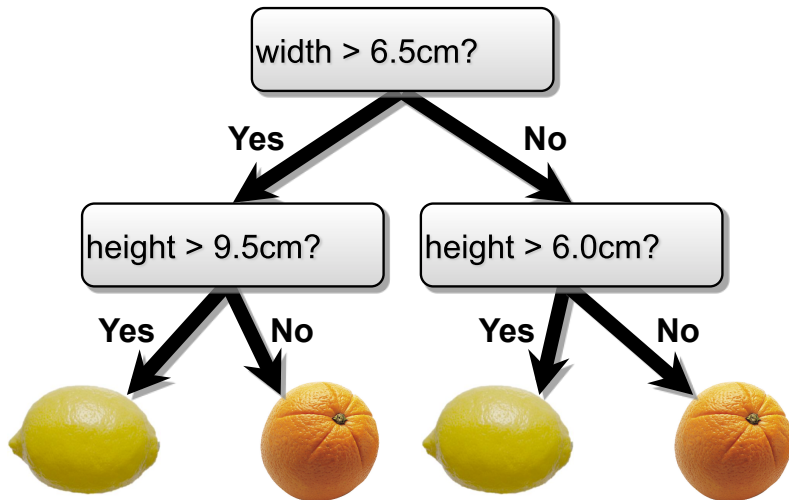
- Decision Trees

- ▶ Simple but powerful learning algorithm
- ▶ One of the most widely used learning algorithms in Kaggle competitions

- Lets us introduce ensembles, a key idea in ML more broadly

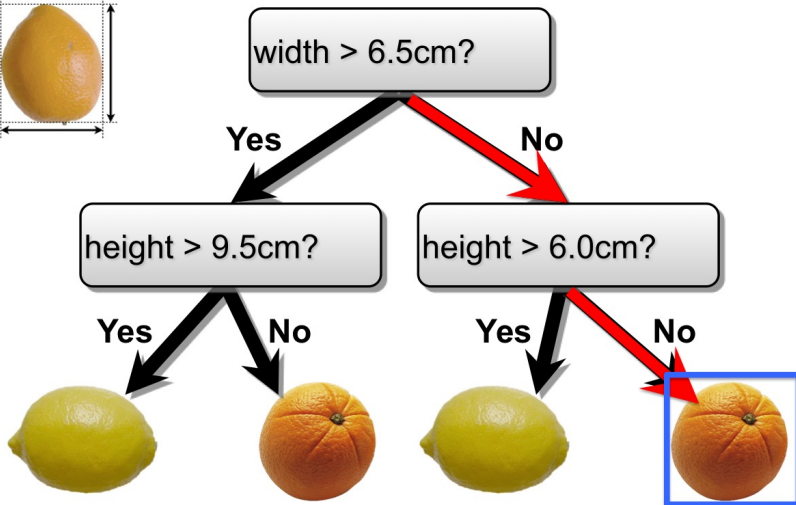
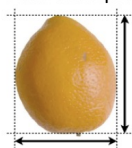
- Useful information theoretic concepts (entropy, mutual information, etc.)

# Decision Trees



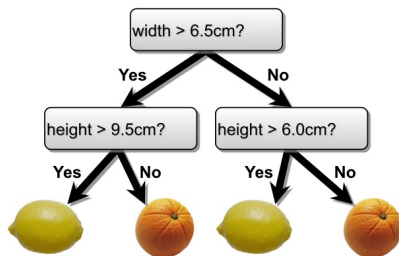
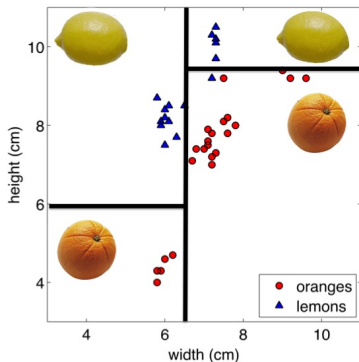
# Decision Trees

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?

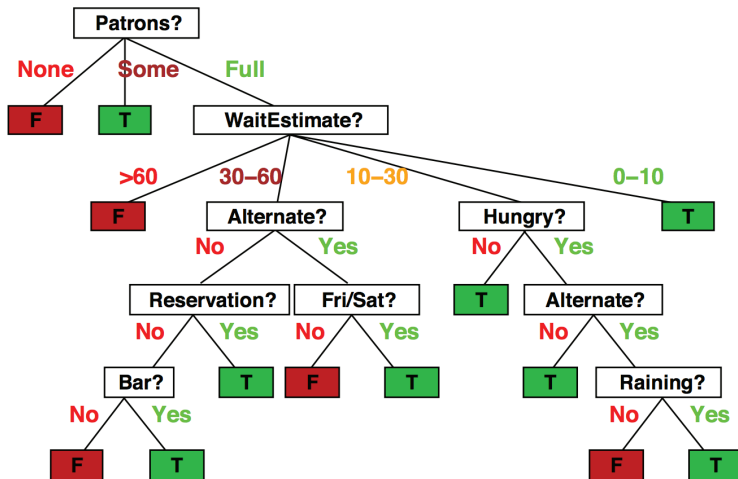
Example	Input Attributes										Goal
	<i>Alt</i>	<i>Bar</i>	<i>Fri</i>	<i>Hun</i>	<i>Pat</i>	<i>Price</i>	<i>Rain</i>	<i>Res</i>	<i>Type</i>	<i>Est</i>	<i>WillWait</i>
<b>x<sub>1</sub></b>	Yes	No	No	Yes	Some	\$\$\$	No	Yes	French	0-10	<i>y<sub>1</sub> = Yes</i>
<b>x<sub>2</sub></b>	Yes	No	No	Yes	Full	\$	No	No	Thai	30-60	<i>y<sub>2</sub> = No</i>
<b>x<sub>3</sub></b>	No	Yes	No	No	Some	\$	No	No	Burger	0-10	<i>y<sub>3</sub> = Yes</i>
<b>x<sub>4</sub></b>	Yes	No	Yes	Yes	Full	\$	Yes	No	Thai	10-30	<i>y<sub>4</sub> = Yes</i>
<b>x<sub>5</sub></b>	Yes	No	Yes	No	Full	\$\$\$	No	Yes	French	>60	<i>y<sub>5</sub> = No</i>
<b>x<sub>6</sub></b>	No	Yes	No	Yes	Some	\$\$	Yes	Yes	Italian	0-10	<i>y<sub>6</sub> = Yes</i>
<b>x<sub>7</sub></b>	No	Yes	No	No	None	\$	Yes	No	Burger	0-10	<i>y<sub>7</sub> = No</i>
<b>x<sub>8</sub></b>	No	No	No	Yes	Some	\$\$	Yes	Yes	Thai	0-10	<i>y<sub>8</sub> = Yes</i>
<b>x<sub>9</sub></b>	No	Yes	Yes	No	Full	\$	Yes	No	Burger	>60	<i>y<sub>9</sub> = No</i>
<b>x<sub>10</sub></b>	Yes	Yes	Yes	Yes	Full	\$\$\$	No	Yes	Italian	10-30	<i>y<sub>10</sub> = No</i>
<b>x<sub>11</sub></b>	No	No	No	No	None	\$	No	No	Thai	0-10	<i>y<sub>11</sub> = No</i>
<b>x<sub>12</sub></b>	Yes	Yes	Yes	Yes	Full	\$	No	No	Burger	30-60	<i>y<sub>12</sub> = Yes</i>

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).

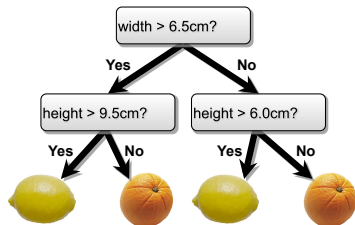
Attributes:

# 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

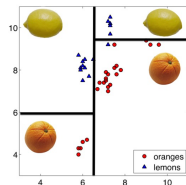
- Each path from root to a leaf defines a region  $R_m$  of input space
- Let  $\{(x^{(m_1)}, t^{(m_1)}), \dots, (x^{(m_k)}, t^{(m_k)})\}$  be the training examples that fall into  $R_m$

- **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  $\{t^{(m_1)}, \dots, t^{(m_k)}\}$



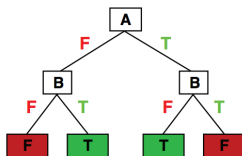
Note: We will focus on classification

[Slide credit: S. Russell]

- **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?

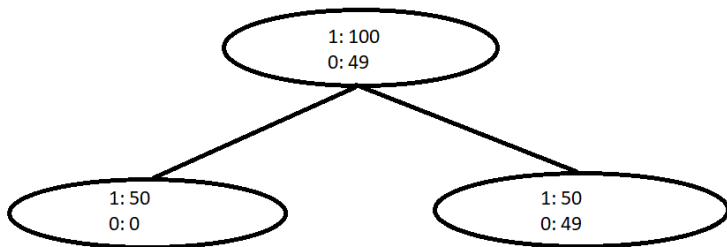
# Learning Decision Trees

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]

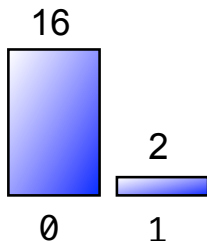
# We Flip Two Different Coins

Sequence 1:

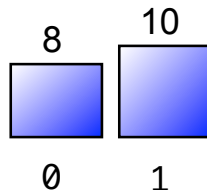
0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 1 0 0 ... ?

Sequence 2:

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



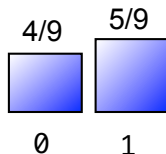
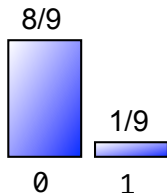
versus



# Quantifying Uncertainty

Entropy is a measure of expected “surprise”:

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



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

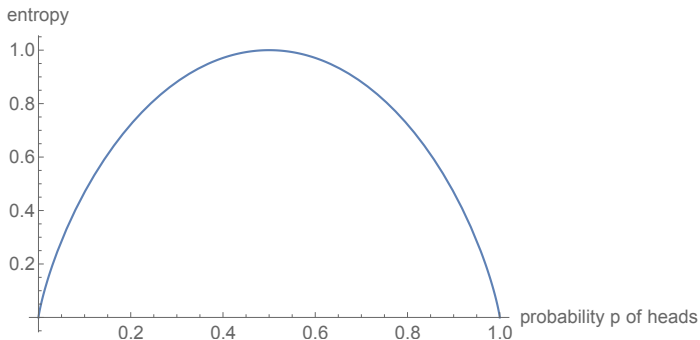
$$-\frac{4}{9} \log_2 \frac{4}{9} - \frac{5}{9} \log_2 \frac{5}{9} \approx 0.99$$

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

	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?**

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

- 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?

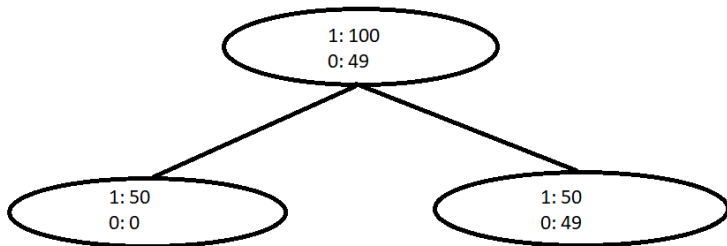
$$\begin{aligned}IG(Y|X) &= H(Y) - H(Y|X) \\ &\approx 0.25 \text{ bits}\end{aligned}$$

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



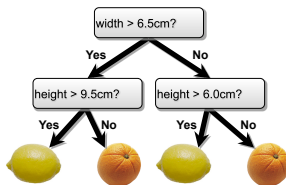
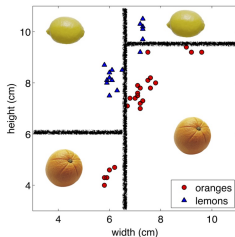
# Revisiting Our Original Example

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

# 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 highest 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

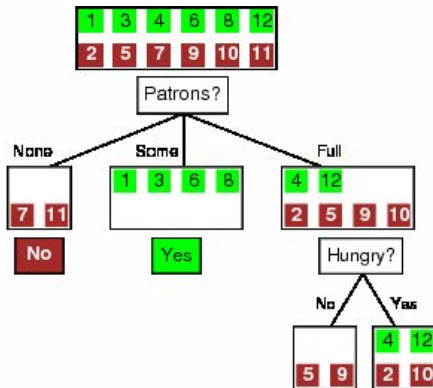
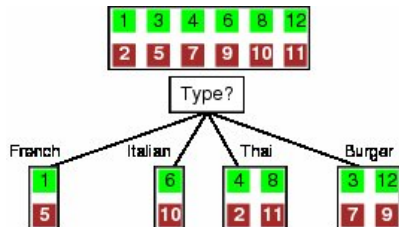
Example	Input Attributes										Goal
	<i>Alt</i>	<i>Bar</i>	<i>Fri</i>	<i>Hun</i>	<i>Pat</i>	<i>Price</i>	<i>Rain</i>	<i>Res</i>	<i>Type</i>	<i>Est</i>	<i>WillWait</i>
$x_1$	Yes	No	No	Yes	Some	\$\$\$	No	Yes	French	0-10	$y_1 = \text{Yes}$
$x_2$	Yes	No	No	Yes	Full	\$	No	No	Thai	30-60	$y_2 = \text{No}$
$x_3$	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).

[from: Russell & Norvig]

Attributes:

# Attribute Selection

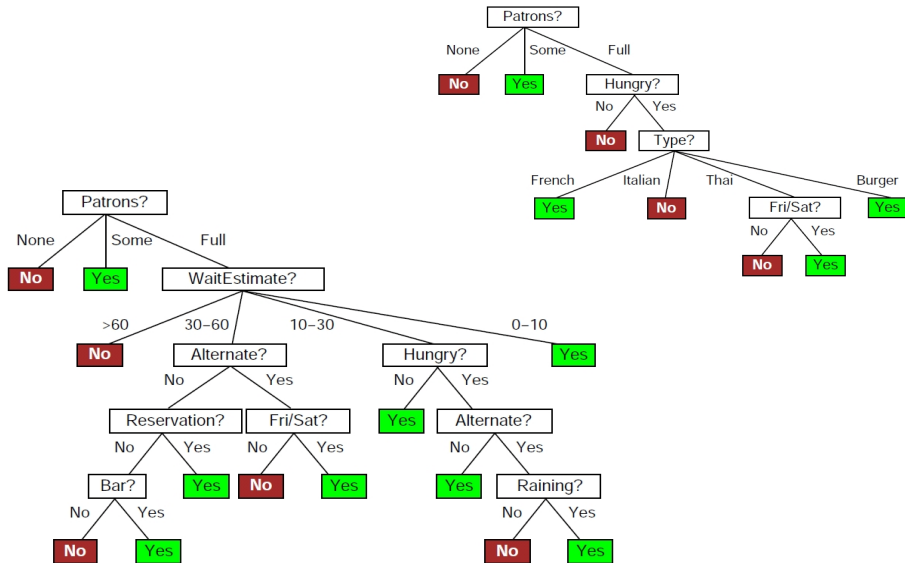


$$IG(Y) = H(Y) - H(Y|X)$$

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

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

# 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.



# Comparison to k-NN

## 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

## 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.

## Ensembles and Bagging

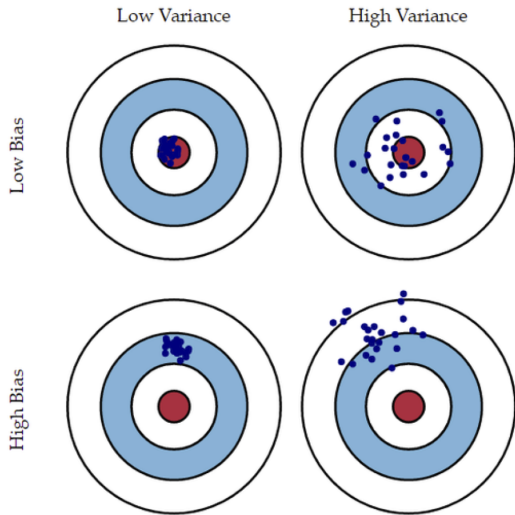
# Ensemble methods: Overview

- An **ensemble** of predictors is a set of predictors whose individual decisions are combined in some way to classify new examples
  - ▶ E.g., (possibly weighted) majority vote
- For this to be nontrivial, the classifiers 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 trivial to implement. The hard part is deciding what kind of ensemble you want, based on your goals.

# Ensemble methods: Overview

- This lecture: [bagging](#)
  - ▶ Train classifiers independently on random subsets of the training data.
- Later 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.

# Bias and Variance



# Loss Functions

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

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

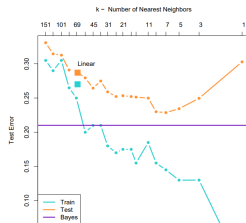
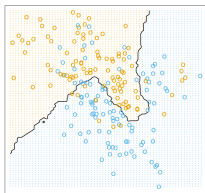
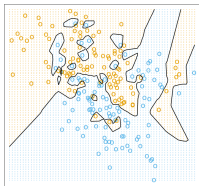
- ▶ Averaging the 0-1 loss over the training set gives the **training error rate**, and averaging over the test set gives the **test error rate**.
- Example: **squared error loss** for regression

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

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

# Bias-Variance Decomposition

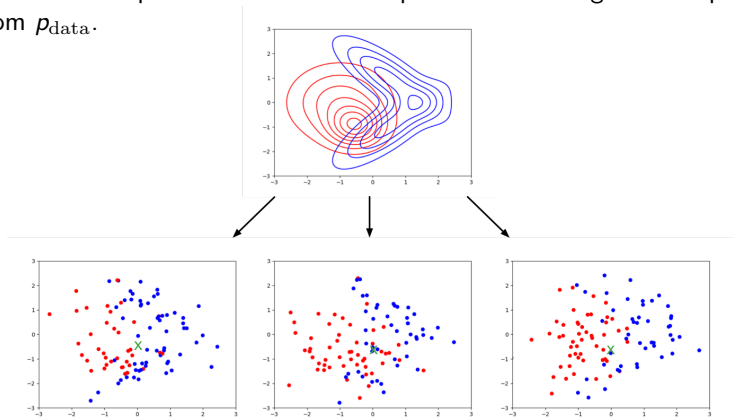
- Recall that overly simple models underfit the data, and overly complex models overfit.



- We can quantify this effect in terms of the [bias/variance decomposition](#).
  - Bias and variance of what?

# Bias-Variance Decomposition: Basic Setup

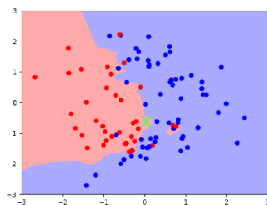
- Suppose the training set  $\mathcal{D}$  consists of pairs  $(\mathbf{x}_i, t_i)$  sampled **independent and identically distributed (i.i.d.)** from a single **data generating distribution**  $p_{\text{data}}$ .
- Pick a fixed query point  $\mathbf{x}$  (denoted with a green x).
- Consider an experiment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



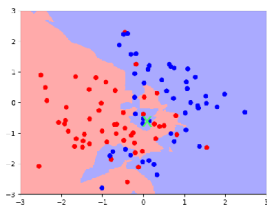


# Bias-Variance Decomposition: Basic Setup

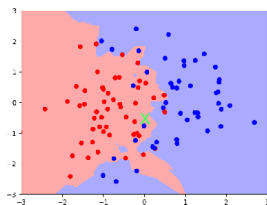
- Let's run our learning algorithm on each training set, and compute its prediction  $y$  at the query point  $\mathbf{x}$ .
- We can view  $y$  as a random variable, where the randomness comes from the choice of training set.
- The classification accuracy is determined by the distribution of  $y$ .



$y = \bullet$



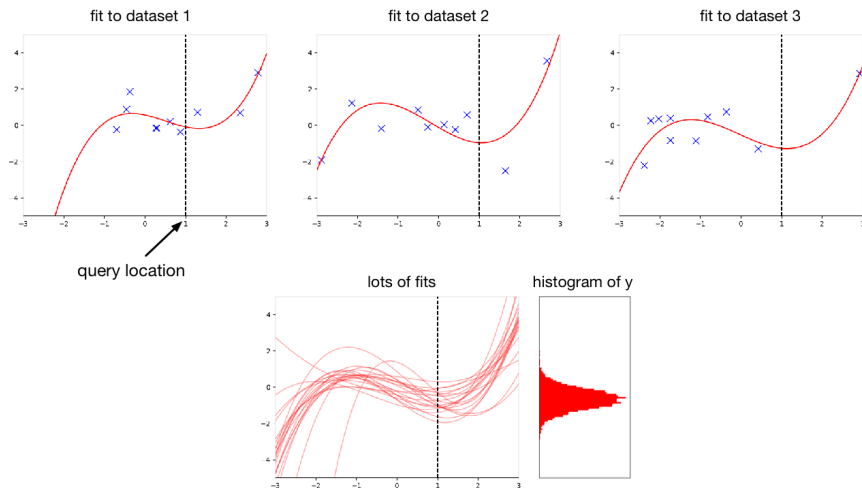
$y = \bullet$



$y = \bullet$

# Bias-Variance Decomposition: Basic Setup

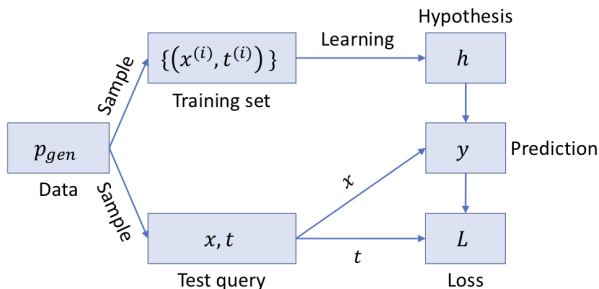
Here is the analogous setup for regression:



Since  $y$  is a random variable, we can talk about its expectation, variance, etc.

# Bias-Variance Decomposition: Basic Setup

- Recap of basic setup:



- Notice:  $y$  is independent of  $t$ . (Why?)
- This gives a distribution over the loss at  $\mathbf{x}$ , with expectation  $\mathbb{E}[L(y, t) | \mathbf{x}]$ .
- For each query point  $\mathbf{x}$ , the expected loss is different. We are interested in minimizing the expectation of this with respect to  $\mathbf{x} \sim p_{data}$ .

# Bayes Optimality

- For now, focus on squared error loss,  $L(y, t) = \frac{1}{2}(y - t)^2$ .
- A first step: suppose we knew the conditional distribution  $p(t | \mathbf{x})$ . What value  $y$  should we predict?
  - ▶ Here, we are treating  $t$  as a random variable and choosing  $y$ .
- **Claim:**  $y_* = \mathbb{E}[t | \mathbf{x}]$  is the best possible prediction.
- **Proof:**

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

$$\mathbb{E}[(y - t)^2 | \mathbf{x}] = (y - y_*)^2 + \text{Var}[t | \mathbf{x}]$$

- The first term is nonnegative, and can be made 0 by setting  $y = y_*$ .
- The second term 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**.
  - ▶ Notice that this term doesn't depend on  $y$ .
- This process of choosing a single value  $y_*$  based on  $p(t | \mathbf{x})$  is an example of **decision theory**.

- Now return to treating  $y$  as a random variable (where the randomness comes from the choice of dataset).
- We can decompose out the expected loss (suppressing the conditioning on  $\mathbf{x}$  for clarity):

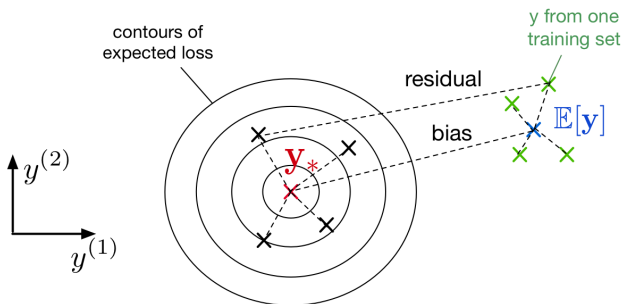
$$\begin{aligned}\mathbb{E}[(y - t)^2] &= \mathbb{E}[(y - y_*)^2] + \text{Var}(t) \\ &= \mathbb{E}[y_*^2 - 2y_*y + y^2] + \text{Var}(t) \\ &= y_*^2 - 2y_*\mathbb{E}[y] + \mathbb{E}[y^2] + \text{Var}(t) \\ &= y_*^2 - 2y_*\mathbb{E}[y] + \mathbb{E}[y]^2 + \text{Var}(y) + \text{Var}(t) \\ &= \underbrace{(y_* - \mathbb{E}[y])^2}_{\text{bias}} + \underbrace{\text{Var}(y)}_{\text{variance}} + \underbrace{\text{Var}(t)}_{\text{Bayes error}}\end{aligned}$$

$$\mathbb{E}[(y - t)^2] = \underbrace{(y_* - \mathbb{E}[y])^2}_{\text{bias}} + \underbrace{\text{Var}(y)}_{\text{variance}} + \underbrace{\text{Var}(t)}_{\text{Bayes error}}$$

- We just split the expected loss into three terms:
  - ▶ **bias**: how wrong the expected prediction is (corresponds to underfitting)
  - ▶ **variance**: the amount of variability in the predictions (corresponds to overfitting)
  - ▶ Bayes error: the inherent unpredictability of the targets
- Even though this analysis only applies to squared error, we often loosely use “bias” and “variance” as synonyms for “underfitting” and “overfitting”.

# Bias/Variance Decomposition: Another Visualization

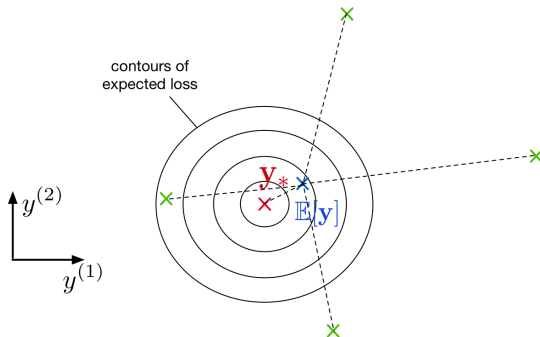
- We can visualize this decomposition in **output space**, where the axes correspond to predictions on the test examples.
- If we have an overly simple model (e.g. KNN with large  $k$ ), it might have
  - ▶ high bias (because it's too simplistic to capture the structure in the data)
  - ▶ low variance (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. KNN 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)



# Bagging

Now, back to bagging!

# Bagging: Motivation

- Suppose we could somehow sample  $m$  independent training sets from  $p_{\text{data}}$ .
- We could then compute the prediction  $y_i$  based on each one, and take the average  $y = \frac{1}{m} \sum_{i=1}^m y_i$ .
- How does this affect the three terms of the expected loss?
  - ▶ **Bayes error: unchanged**, since we have no control over it
  - ▶ **Bias: unchanged**, since the averaged prediction has the same expectation

$$\mathbb{E}[y] = \mathbb{E}\left[\frac{1}{m} \sum_{i=1}^m y_i\right] = \mathbb{E}[y_i]$$

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

$$\text{Var}[y] = \text{Var}\left[\frac{1}{m} \sum_{i=1}^m y_i\right] = \frac{1}{m^2} \sum_{i=1}^m \text{Var}[y_i] = \frac{1}{m} \text{Var}[y_i].$$

# Bagging: The Idea

- In practice, running an algorithm separately on independently sampled datasets is very wasteful!
- 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.
- The bootstrap is one of the most important ideas in all of statistics!

# 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  $\sigma^2$  and correlation  $\rho$ , then

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

- 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** = 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

# 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.