CSC 311: Introduction to Machine Learning

Lecture 2 - Decision Trees and Bias-Variance

Michael Zhang   Chandra Gummaluru

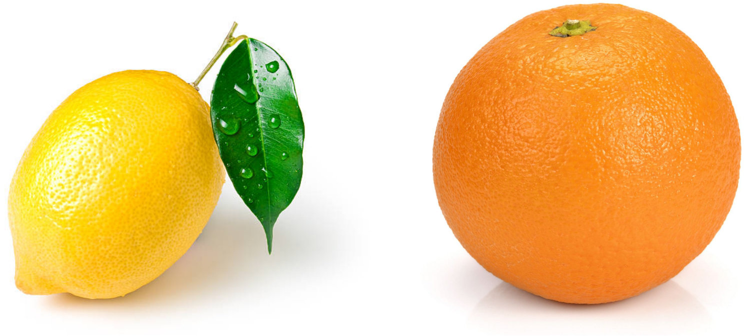
University of Toronto, Winter 2023

Outline

Today

- Announcement: Math diagnostic due Friday, HW1 released soon
- Decision Trees
  - Simple but powerful learning algorithm
  - Used widely in Kaggle competitions
  - Lets us motivate concepts from information theory (entropy, mutual information, etc.)
- Bias-variance decomposition
  - Concept to motivate combining different classifiers.
- Ideas we will need in today's lecture
  - Trees [from algorithms]
  - Expectations, marginalization, chain rule [from probability]

Lemons or Oranges

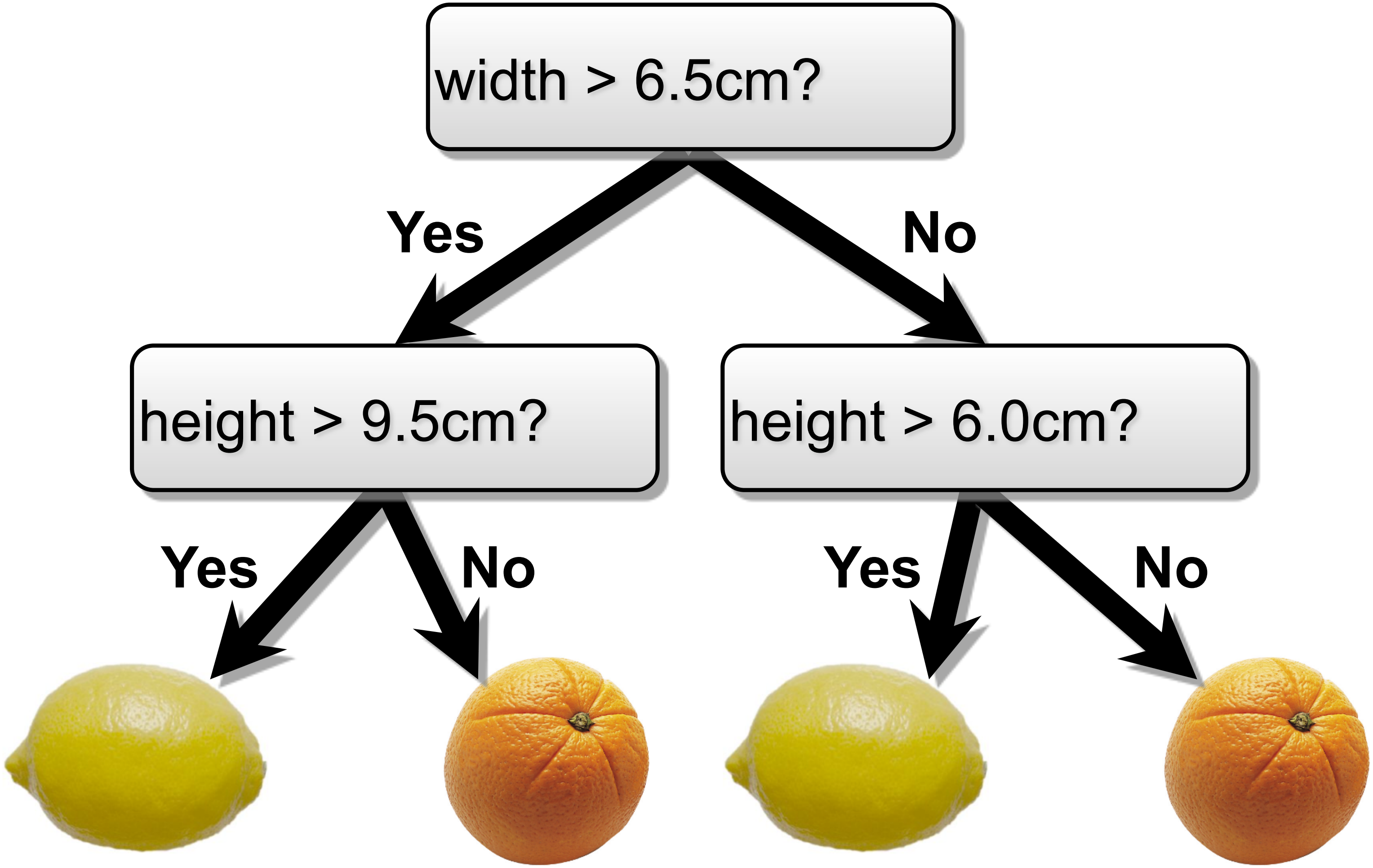


Scenario: You run a sorting facility for citrus fruits

- Binary classification: lemons or oranges
- Features measured by sensor on conveyor belt: height and width

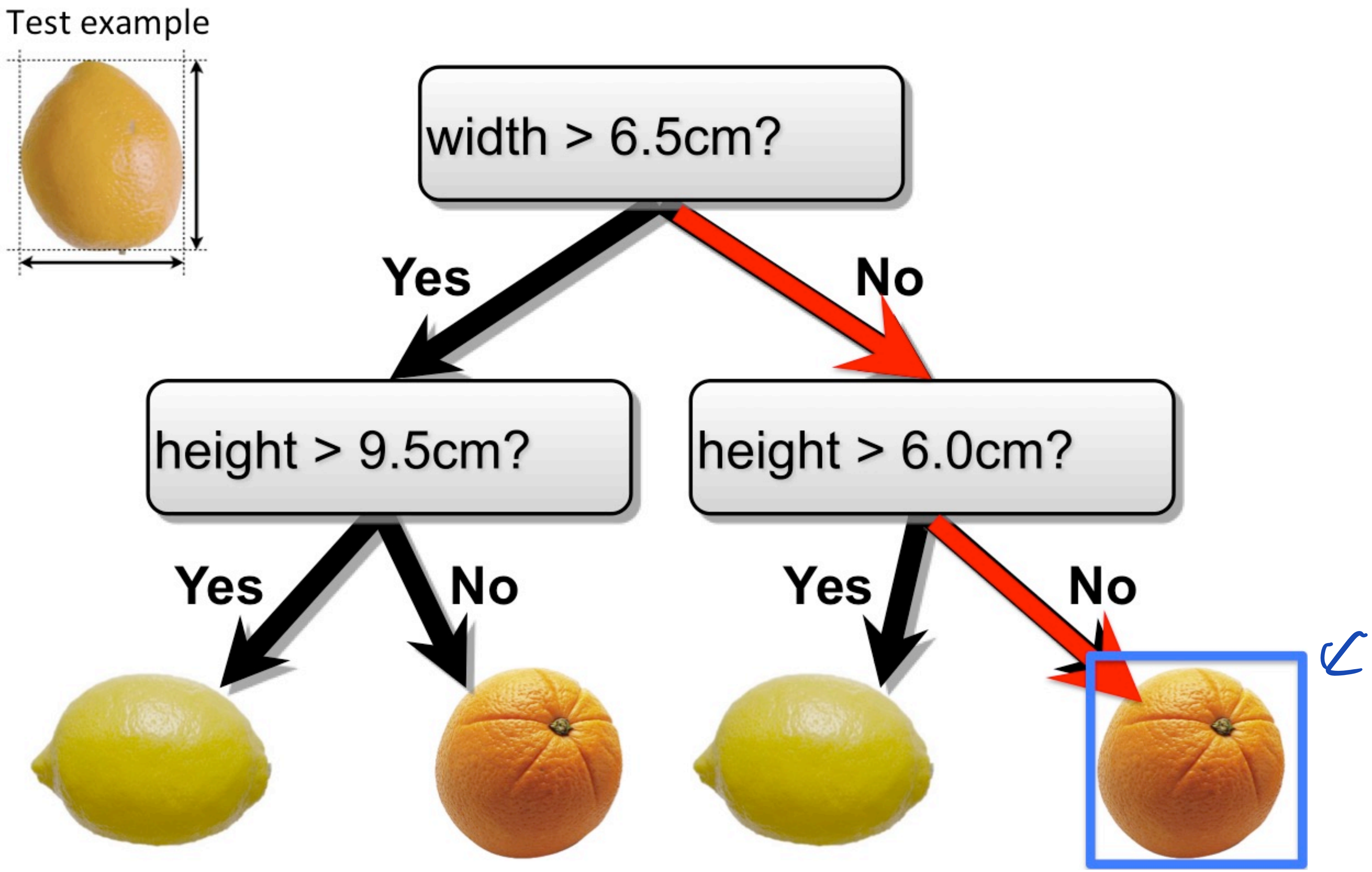
Decision Trees

- Make predictions by splitting on features according to a tree structure.



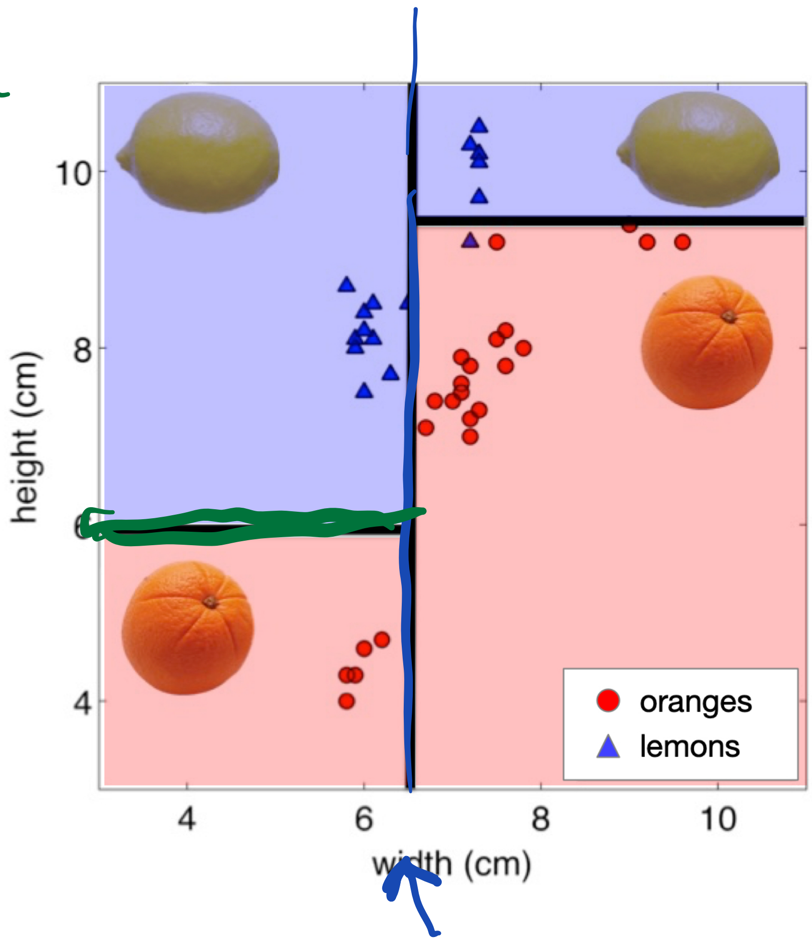
Decision Trees

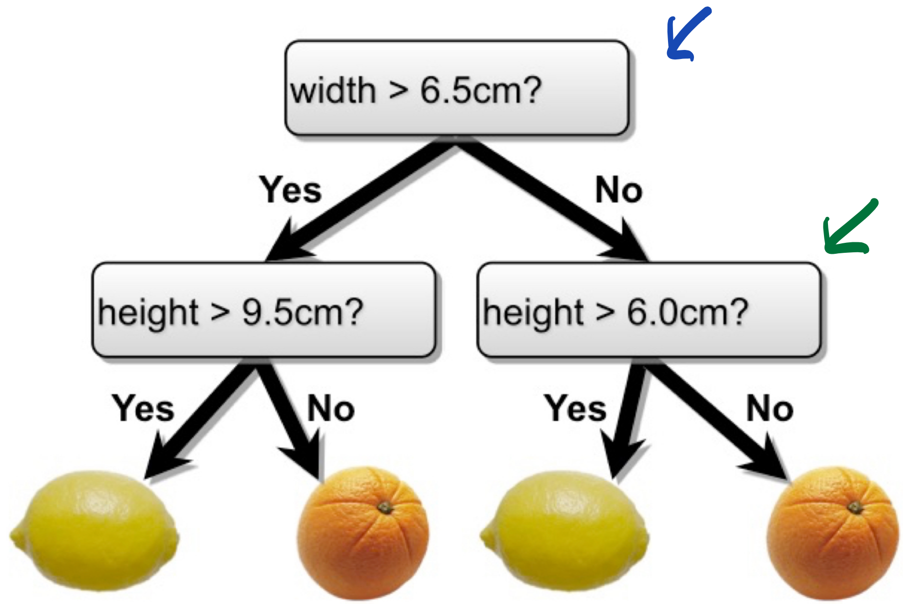
- Make predictions by splitting on features according to a tree structure.



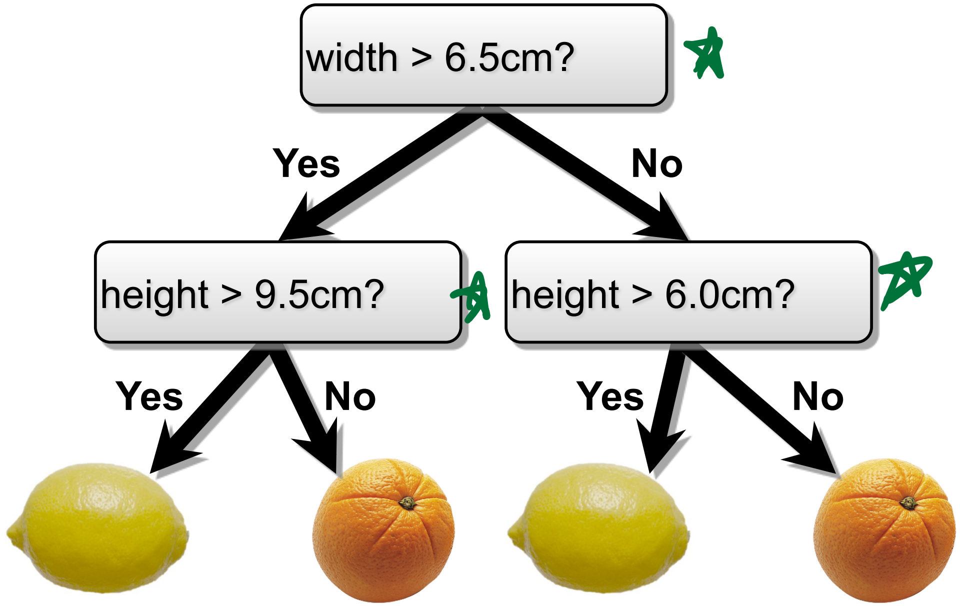
Decision Trees—Continuous Features

- Split *continuous features* by checking whether that feature is greater than or less than some threshold.
- Decision boundary is made up of axis-aligned planes.





Decision Trees



- Internal nodes test a feature
- Branching is determined by the feature value
- Leaf nodes are outputs (predictions)

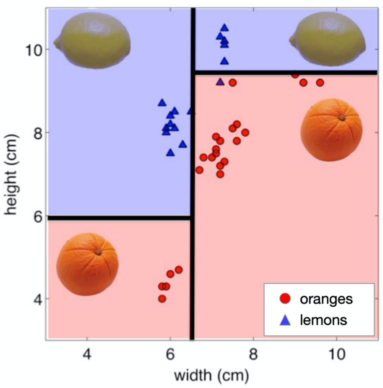
Question: What are the hyperparameters of this model?

maximum depth

# of nodes

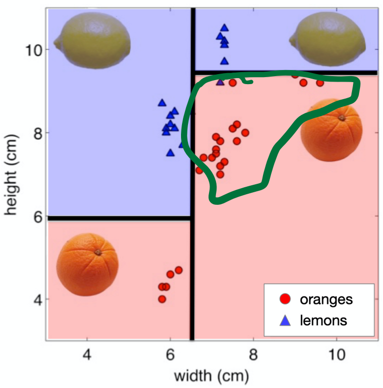
Decision Trees—Classification and Regression

- 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
- $m = 4$ on the right and k is the same across each region



Decision Trees—Classification and Regression

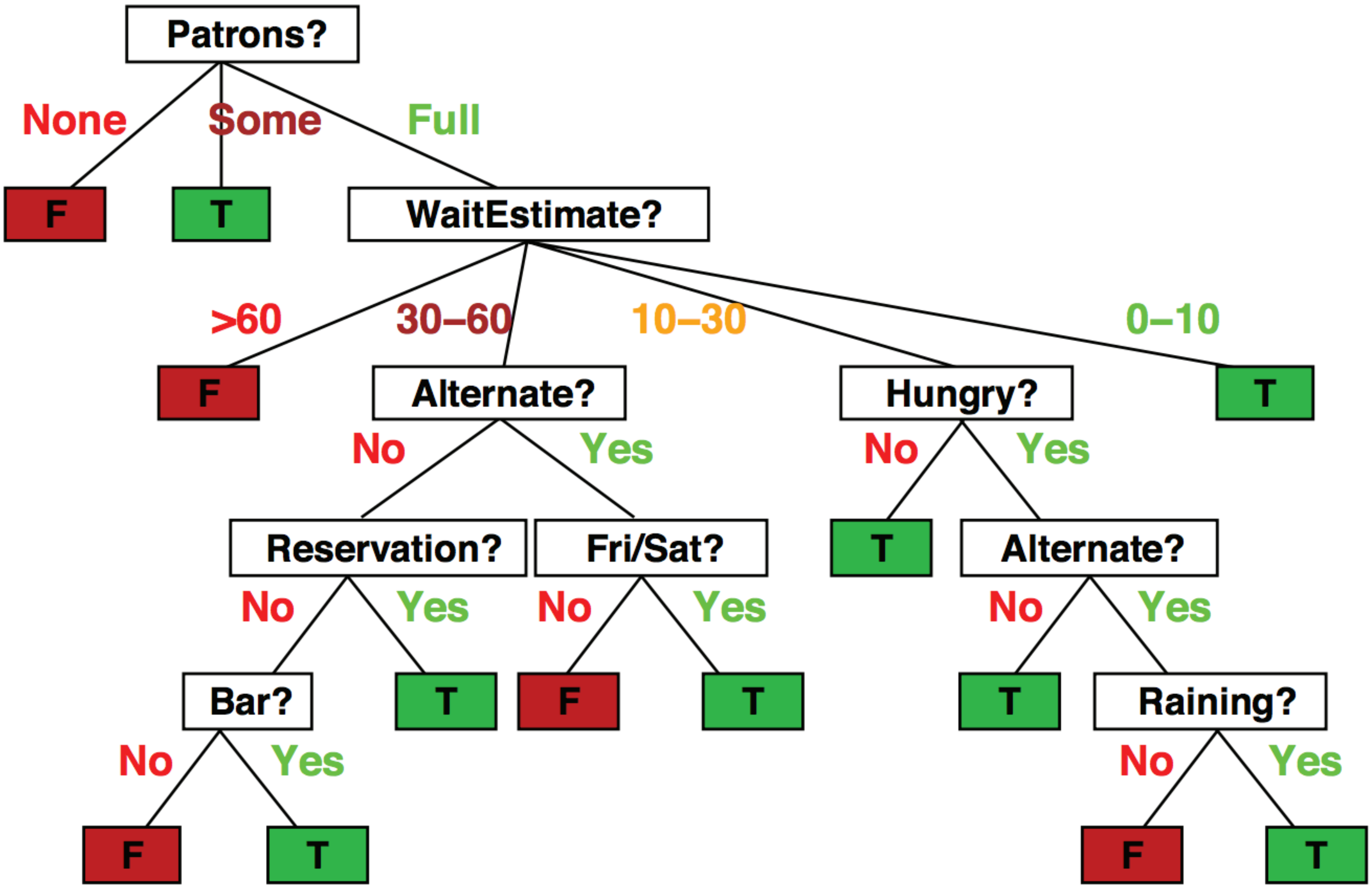
- Each path from root to a leaf defines a region R_m of input space
- Let $\{(x^{(m_1)}, t^{(m_1)}), \ldots, (x^{(m_k)}, t^{(m_k)})\}$ be the training examples that fall into R_m
- $m = 4$ on the right and k is the same across each region



- Regression tree: (house price)
  - continuous output
  - leaf value y^m typically set to the mean value in $\{t^{(m_1)}, \ldots, t^{(m_k)}\}$
- Classification tree (we will focus on this):
  - discrete output
  - leaf value y^m typically set to the most common value in $\{t^{(m_1)}, \ldots, t^{(m_k)}\}$

Decision Trees—Discrete Features

- Will I eat at this restaurant?



Decision Trees—Discrete Features

- Split *discrete features* into a partition of possible values.

data

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

labels

Features:

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).

Learning Decision Trees

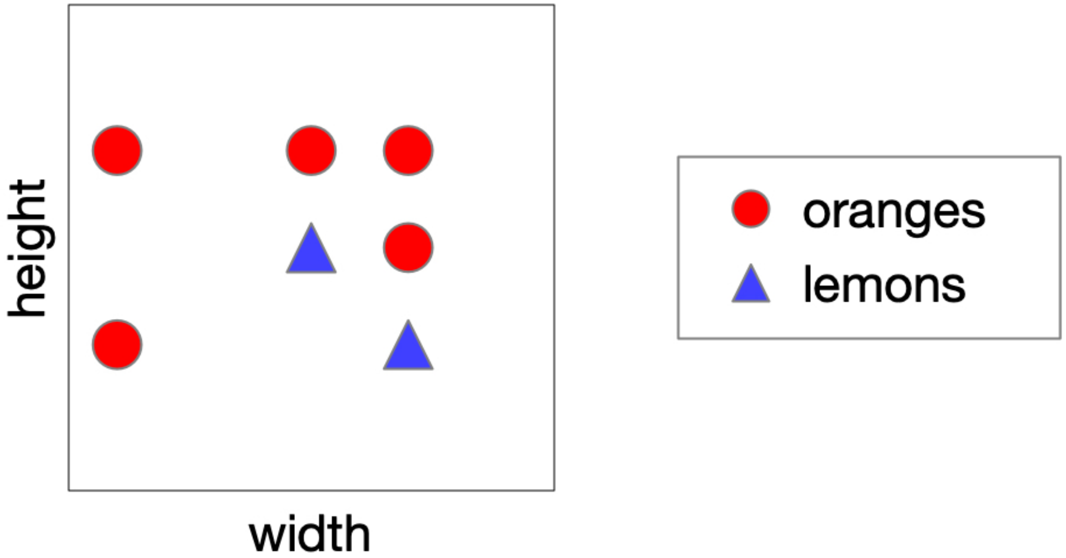
- Decision trees are universal function approximators.
  - For any training set we can construct a decision tree that has exactly the one leaf for every training point, but it probably won't generalize.
  - Example - If all D features were binary, and we had $N = 2^D$ unique training examples, a **Full Binary Tree** would have one leaf per example.
- Finding the smallest decision tree that correctly classifies a training set is NP complete. (hard problem)
  - If you are interested, check: Hyafil & Rivest'76.
- So, how do we construct a useful decision tree?

Learning Decision Trees

- Resort to a greedy heuristic:
  - Start with the whole training set and an empty decision tree.
  - Pick a feature and candidate split that would most reduce a loss
  - Split on that feature and recurse on subpartitions.
- What is a loss? metric to measure performance
  - When learning a model, we use a scalar number to assess whether we're on track
  - Scalar value: low is good, high is bad
- Which loss should we use?

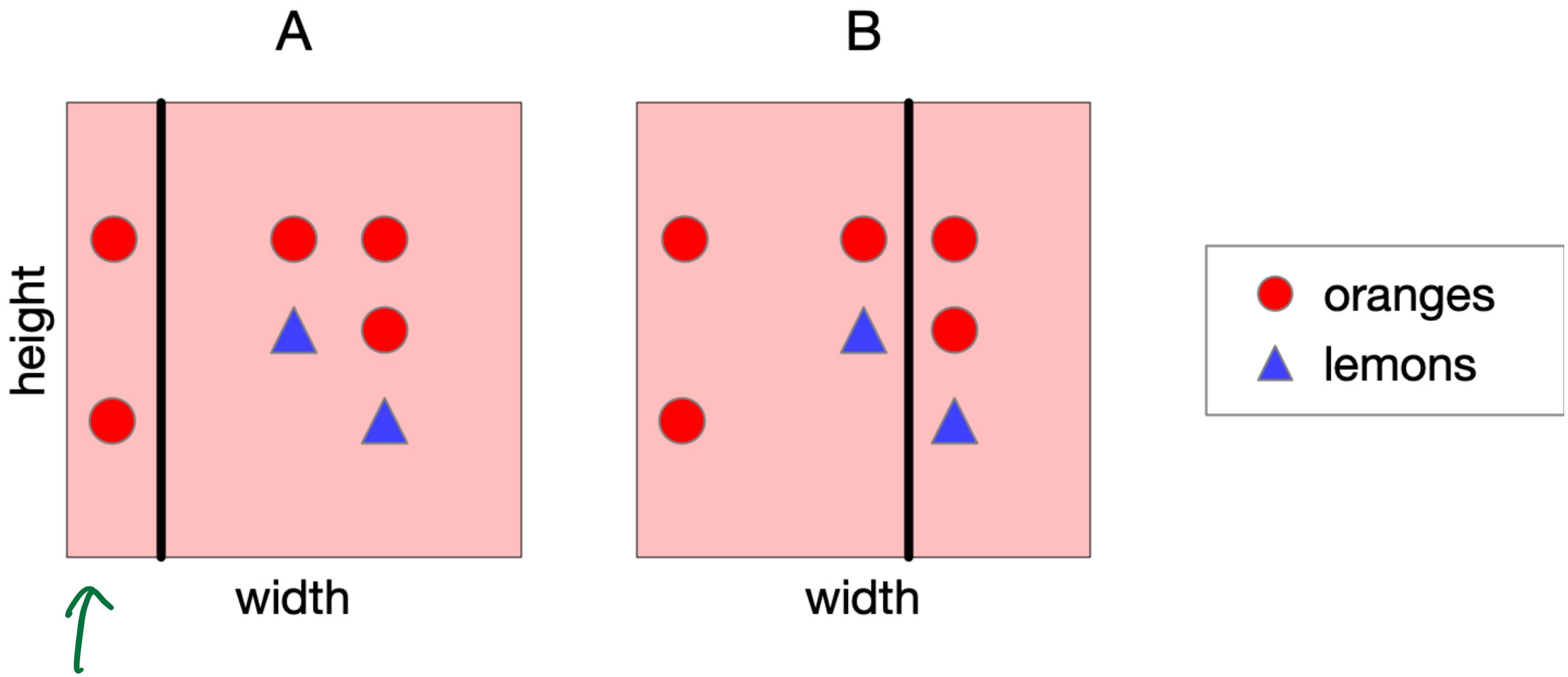
Choosing a Good Split

- Consider the following data. Let's split on width.
- Classify by majority.



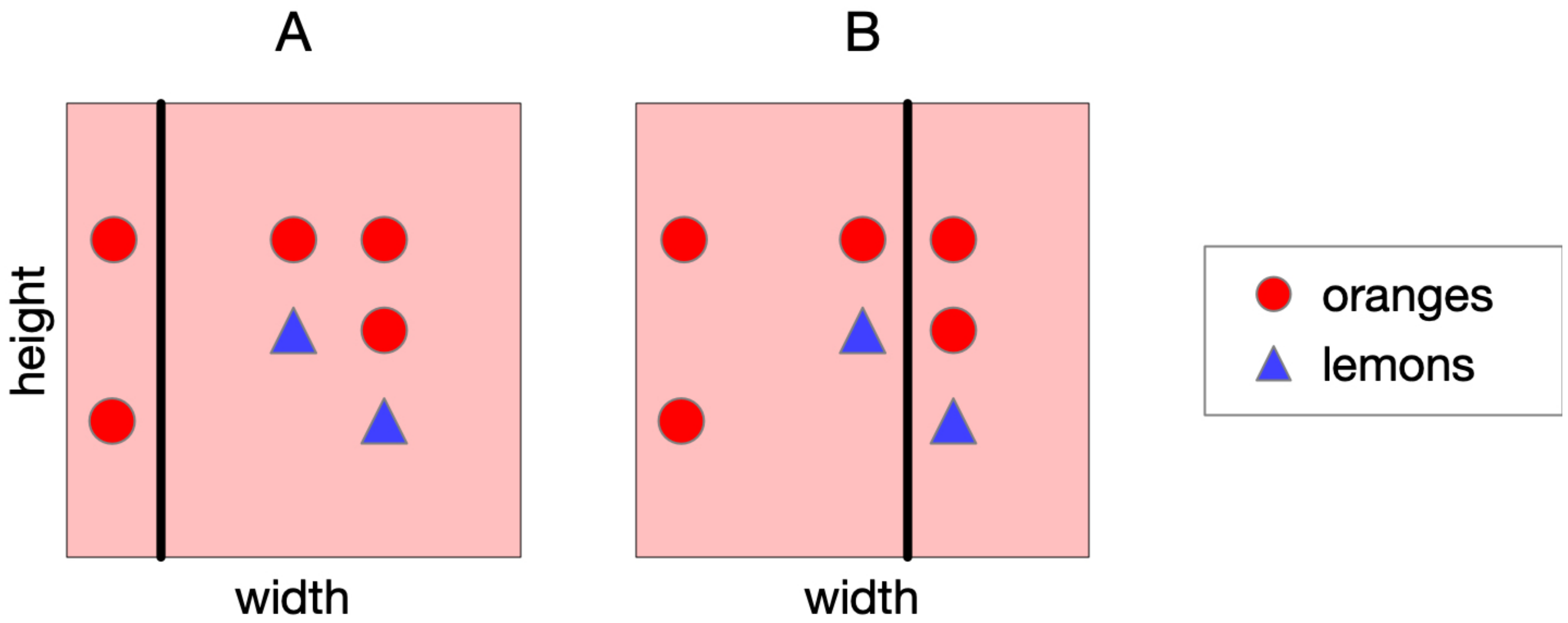
Choosing a Good Split

- Which is the best split? Vote!



Choosing a Good Split

- A feels like a better split, because the left-hand region is very certain about whether the fruit is an orange.
- Can we quantify this?



Choosing a Good Split

- How can we quantify uncertainty in prediction for a given leaf node?
  - If all examples in leaf have same class: good, low uncertainty
  - If each class has same amount of examples in leaf: bad, high uncertainty
- **Idea:** Use counts at leaves to define probability distributions; use a probabilistic notion of uncertainty to decide splits.
- There are different ways to evaluate a split. We will focus on a common way: **entropy**.
- A brief detour through information theory...

Entropy - Quantifying uncertainty

- You may have encountered the term entropy quantifying the state of chaos in chemical and physical systems,
- In statistics, it is a property of a random variable,
- The entropy of a discrete random variable is a number that quantifies the uncertainty inherent in its possible outcomes.
- The mathematical definition of entropy that we give in a few slides may seem arbitrary, but it can be motivated axiomatically.
    - If you're interested, check: *Information Theory* by Robert Ash or Elements of Information Theory by Cover and Thomas.
- To explain entropy, consider flipping two different coins...

We Flip Two Different Coins

Each coin is a binary random variable with outcomes 1 or 0:

Sequence 1:
0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 1 0 0 ... ?

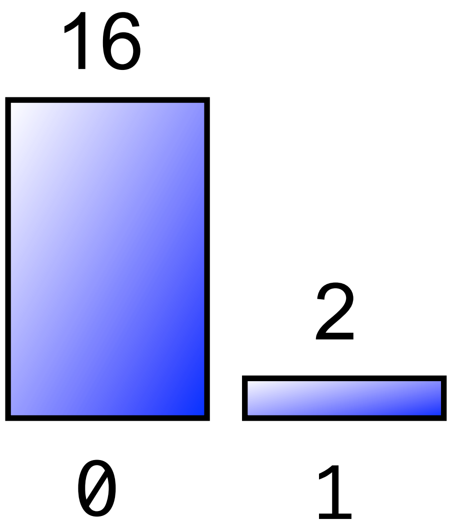
Sequence 2:
0 1 0 1 0 1 1 1 0 1 0 0 1 1 0 1 0 1 ... ?

We Flip Two Different Coins

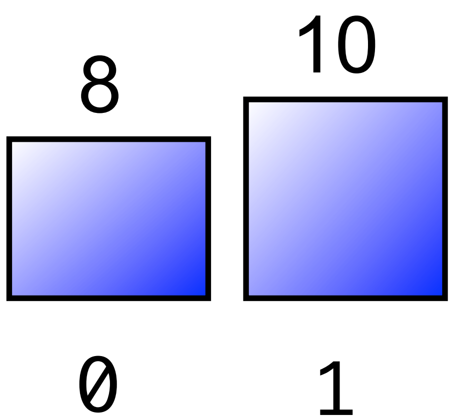
Each coin is a binary random variable with outcomes 1 or 0:

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



1 has less uncertainty

Quantifying Uncertainty

$= \sum_i -p(i) \log p(i)$

- The entropy of a loaded coin with probability p of heads is given by

$$-p \log_2(p) - (1-p)\log_2(1-p)$$

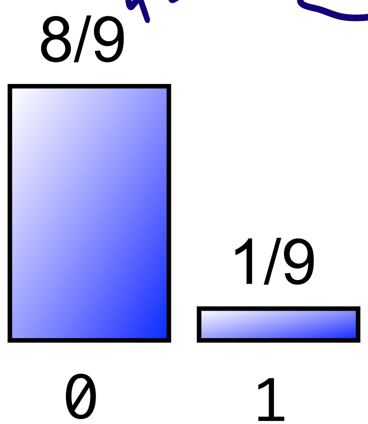
$\sum_i p(i) \log \frac{1}{p(i)}$

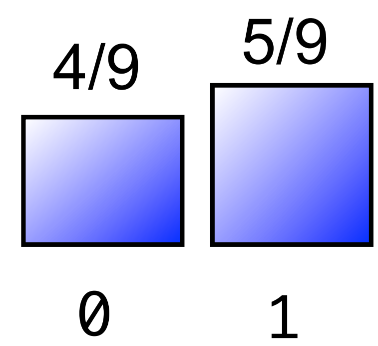
A	$\frac{1}{2}$	1
B	$\frac{1}{4}$	01
C	$\frac{1}{4}$	00

$\frac{1}{2}\cdot 1 + \frac{1}{4}\cdot 2 + \frac{1}{4}\cdot 2$

ACBC

1000100

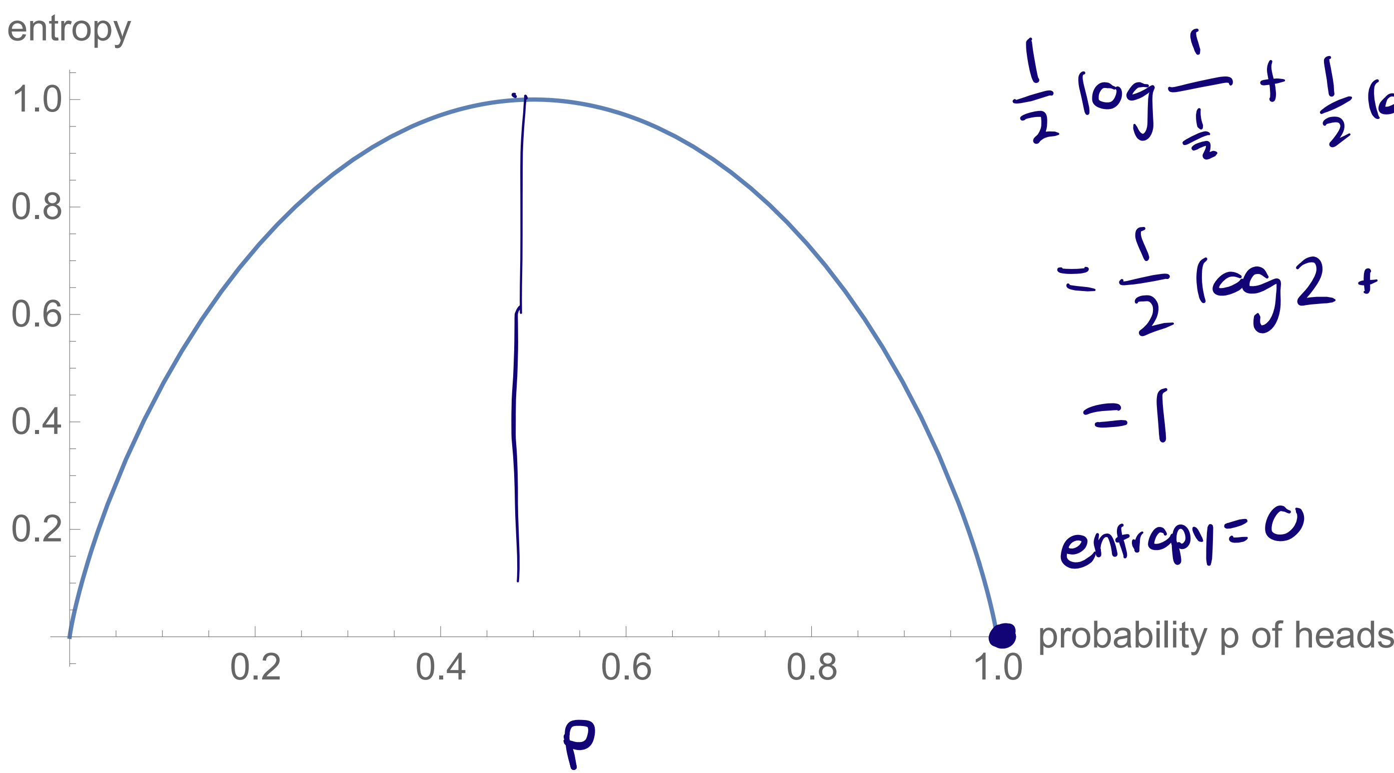




$$-\frac{8}{9}\log_2\frac{8}{9} - \frac{1}{9}\log_2\frac{1}{9} \approx \frac{1}{2} \qquad -\frac{4}{9}\log_2\frac{4}{9} - \frac{5}{9}\log_2\frac{5}{9} \approx 0.99$$

- Notice: the coin whose outcomes are more certain has a lower entropy.
- In the extreme case $p = 0$ or $p = 1$, we were certain of the outcome before observing. So, we gained no certainty by observing it, i.e., entropy is 0.

- Can also think of entropy as the expected information content of a random draw from a probability distribution.



$$\frac{1}{2}\log\frac{1}{\frac{1}{2}} + \frac{1}{2}\log\frac{1}{\frac{1}{2}}$$

$$= \frac{1}{2}\log 2 + \frac{1}{2}\log 2$$

$$= 1$$

entropy = 0

- Claude Shannon showed: you cannot store the outcome of a random draw using fewer expected bits than the entropy without losing information.
- So units of entropy are bits; a fair coin flip has 1 bit of entropy.

Entropy

- More generally, the entropy of a discrete random variable Y is given by

$$H(Y) = -\sum_{y \in Y} p(y) \log_2 p(y)$$

- **"High Entropy"**:
  - Variable has a uniform like distribution over many outcomes
  - Flat histogram
  - Values sampled from it are less predictable

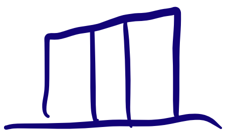
[Slide credit: Vibhav Gogate]

Entropy

- More generally, the entropy of a discrete random variable Y is given by

$$H(Y) = -\sum_{y \in Y} p(y) \log_2 p(y)$$

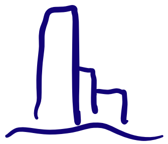
- **"High Entropy"**:



  - Variable has a uniform like distribution over many outcomes
  - Flat histogram
  - Values sampled from it are less predictable

- **"Low Entropy"**

  - Distribution is concentrated on only a few outcomes
  - Histogram is concentrated in a few areas
  - Values sampled from it are more predictable



[Slide credit: Vibhav Gogate]

Entropy

- Suppose we observe partial information X about a random variable Y
  - For example, $X = \text{sign}(Y)$.
- We want to work towards a definition of the expected amount of information that will be conveyed about Y by observing X.
  - Or equivalently, the expected reduction in our uncertainty about Y after observing X.

(split we consider)

(initial dist. of labels)

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

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

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

$p(\text{cloudy} \mid \text{raining})$

$= \dfrac{p(\text{cloudy} \cap \text{raining})}{p(\text{raining})}$

$= \dfrac{\frac{24}{100}}{\frac{25}{100}}$

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

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

$-\sum_i p(i) \log p(i)$

$= \begin{bmatrix} \frac{24}{25} \\ \frac{1}{25} \end{bmatrix}$ not cloudy

- 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:

$$\sum_x p(X=x)\,H(Y|X=x)$$

$$= \sum_x p(X=x) \sum_y - p(Y=y|X=x) \log p(Y=y|X=x)$$

$$p(X=x, Y=y)$$

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

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

$\frac{1}{4} = \frac{24}{100} + \frac{1}{100}$

$\frac{3}{4}$

- 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 does not affect our uncertainty about Y: $H(Y|X) = H(Y)$
  - But knowing Y makes our knowledge of Y certain: $H(Y|Y) = 0$
  - 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 more certain am I about whether it's cloudy if I'm told whether it is raining? My uncertainty in Y minus my expected uncertainty that would remain in Y after seeing X.
- This is called the information gain $IG(Y|X)$ in Y due to X, or the mutual information of Y and X

$$IG(Y|X) = H(Y) - H(Y|X) \geq 0 \tag{1}$$

- If X is completely uninformative about Y: $IG(Y|X) = 0$
- If X is completely informative about Y: $IG(Y|X) = H(Y)$

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

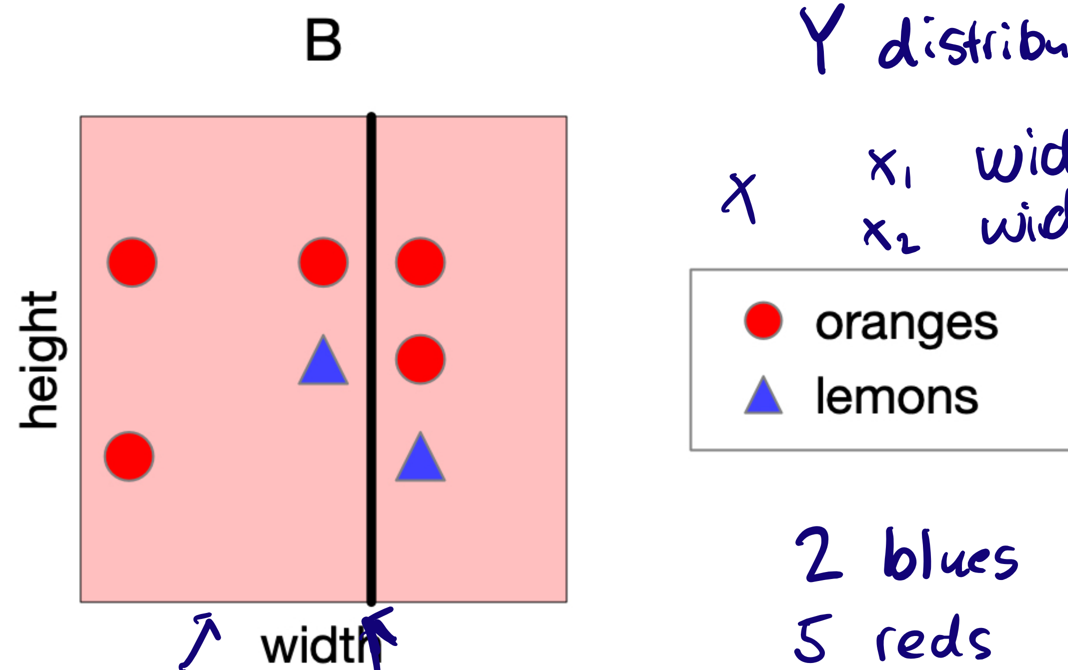
Revisiting Our Original Example

$H(Y|X) = 0$

- Information gain measures the informativeness of a variable, which is exactly what we desire in a decision tree split!
- The information gain of a split: how much information (over the training set) about the class label Y is gained by knowing which side of a split you're on.

Information Gain of Split B

- What is the information gain of split B? Not terribly informative...



Y distribution of labels

X $\quad x_1$ width > 10 left
$\quad x_2$ width ≤ 10 right

2 blues
5 reds

$\frac{4}{7}$ 1 blue 3 red

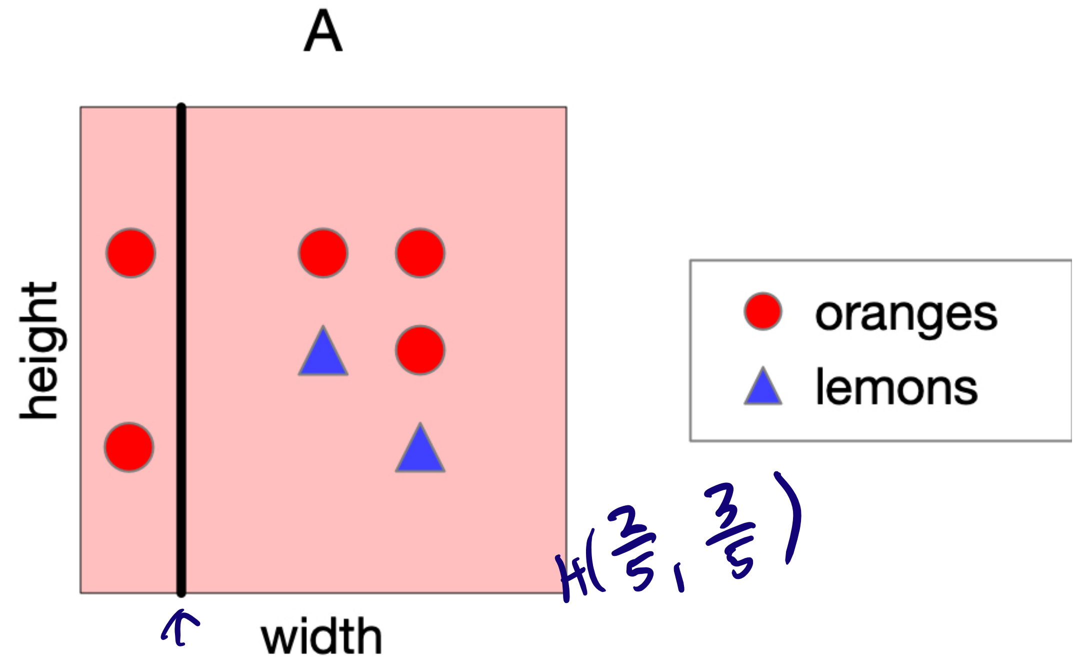
$\frac{3}{7}$ 1 blue 2 reds

- Entropy of class outcome before split:
$H(Y) = -\frac{2}{7}\log_2(\frac{2}{7}) - \frac{5}{7}\log_2(\frac{5}{7}) \approx 0.86$
- Conditional entropy of class outcome after split:
$H(Y|left) \approx 0.81$, $H(Y|right) \approx 0.92$
- $IG(split) \approx 0.86 - (\frac{4}{7} \cdot 0.81 + \frac{3}{7} \cdot 0.92) \approx 0.006$

$\frac{4}{7} \underbrace{H(\frac{1}{4}, \frac{3}{4})}_{0.81} + \frac{3}{7} \underbrace{H(\frac{1}{3}, \frac{2}{3})}_{0.92}$

Information Gain of Split A

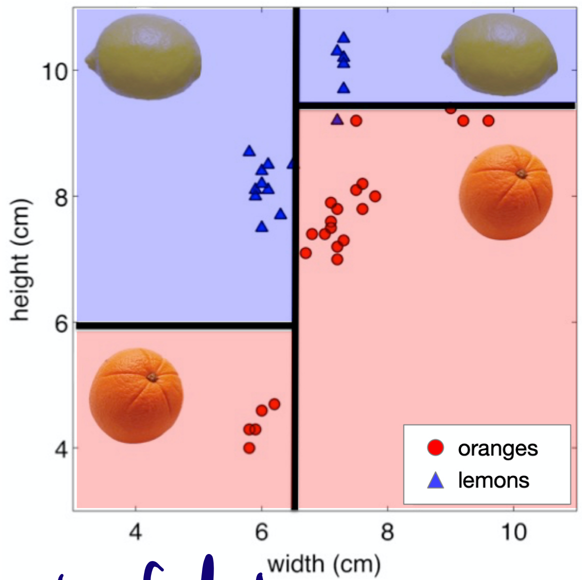
- What is the information gain of split A? Very informative!



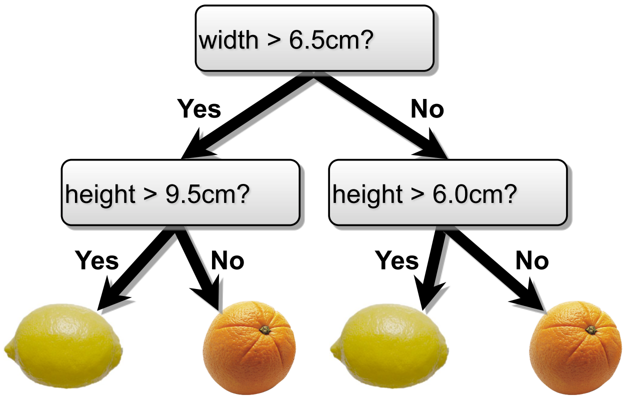
$H(\frac{2}{5}, \frac{3}{5})$

- Entropy of class outcome before split:
  $H(Y) = -\frac{2}{7}\log_2(\frac{2}{7}) - \frac{5}{7}\log_2(\frac{5}{7}) \approx 0.86$ same
- Conditional entropy of class outcome after split:
  $H(Y|left) = 0$, $H(Y|right) \approx 0.97$
- $IG(split) \approx 0.86 - (\frac{2}{7} \cdot 0 + \frac{5}{7} \cdot 0.97) \approx 0.17!!$

Constructing Decision Trees



Given a bunch of data



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

Decision Tree Construction Algorithm

1 2 3

f_1 : 2, 2, 3, 5, 6, 8

- Simple, greedy, recursive approach, builds up tree node-by-node
  1. pick a feature to split at a non-terminal node
  2. split examples into groups based on feature 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
- Terminates when all leaves contain only examples in the same class or are empty.
- Questions for discussion:
  - How do you choose the feature to split on?
  - How do you choose the threshold for each feature?

Back to Our Example

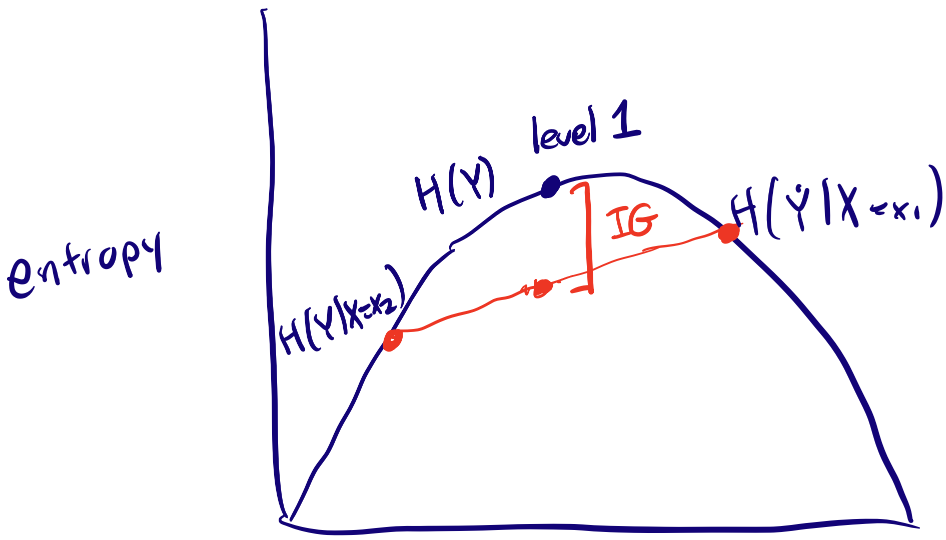
Example	Input Attributes										Goal
	Alt	*Bar*	*Fri*	*Hun*	*Pat*	*Price*	*Rain*	*Res*	*Type*	*Est*	*WillWait*
$\mathbf{x}_1$	Yes	No	No	Yes	Some	$$$	No	Yes	French	0–10	$y_1 =$ Yes
$\mathbf{x}_2$	Yes	No	No	Yes	Full	$	No	No	Thai	30–60	$y_2 =$ No
$\mathbf{x}_3$	No	Yes	No	No	Some	$	No	No	Burger	0–10	$y_3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

Features:

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]

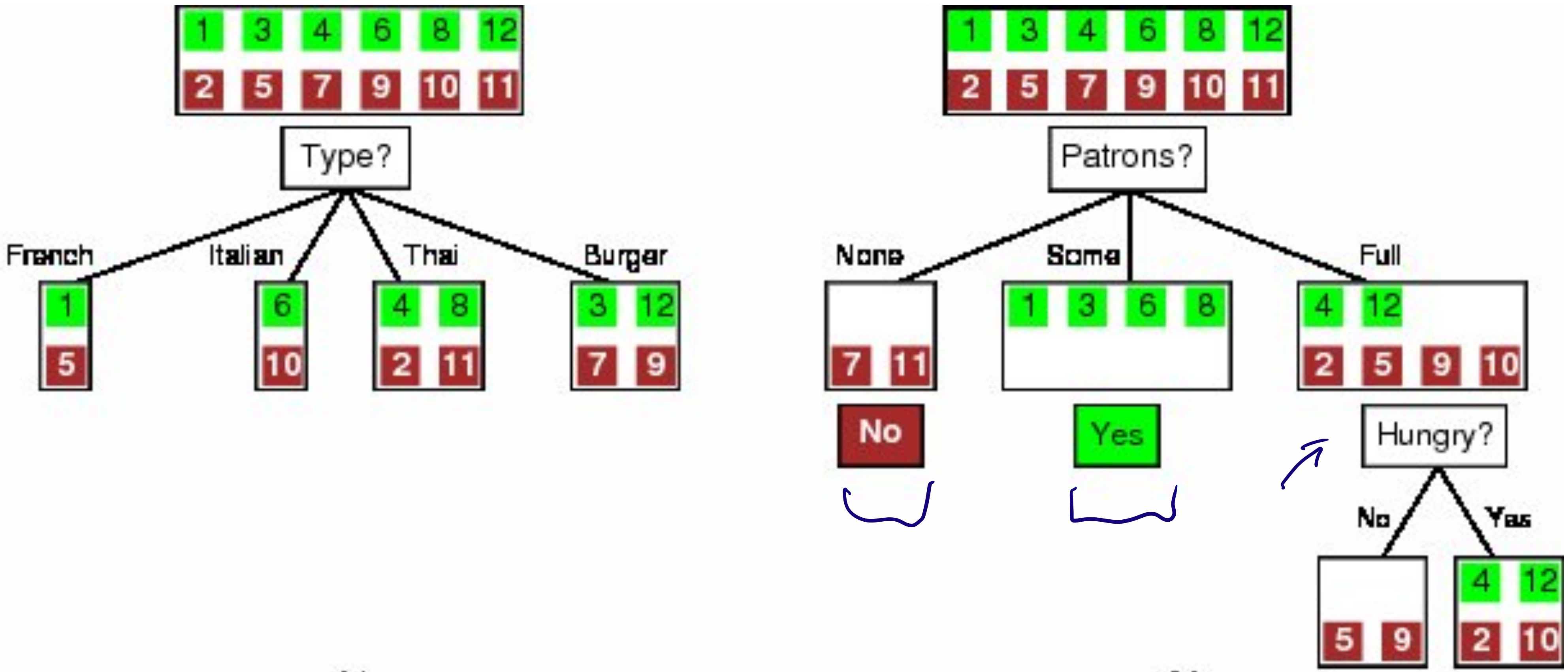
Visualizing information gain



function is <u>concave</u>

(line below curve)

Feature Selection

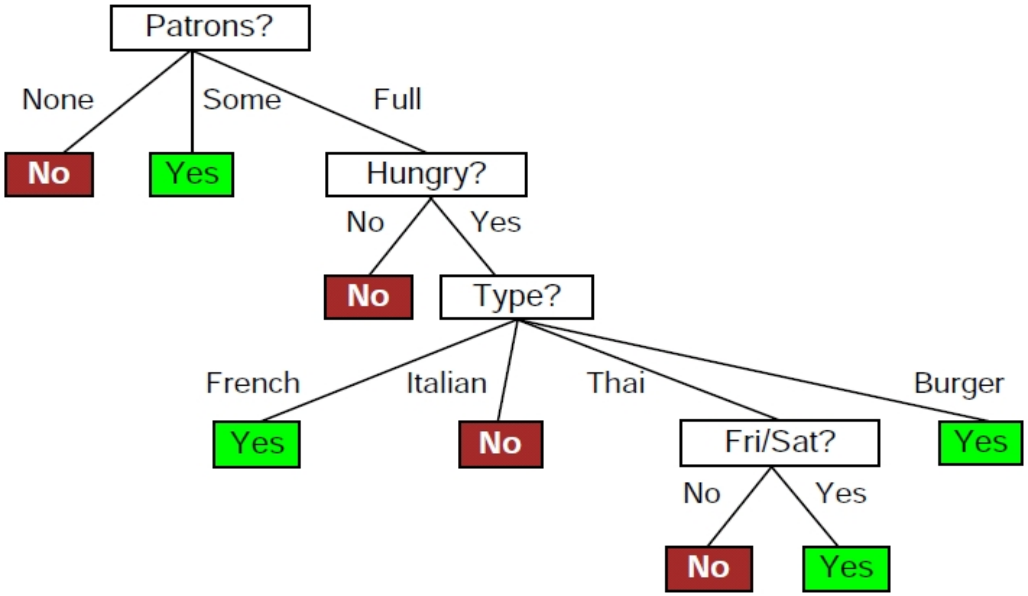


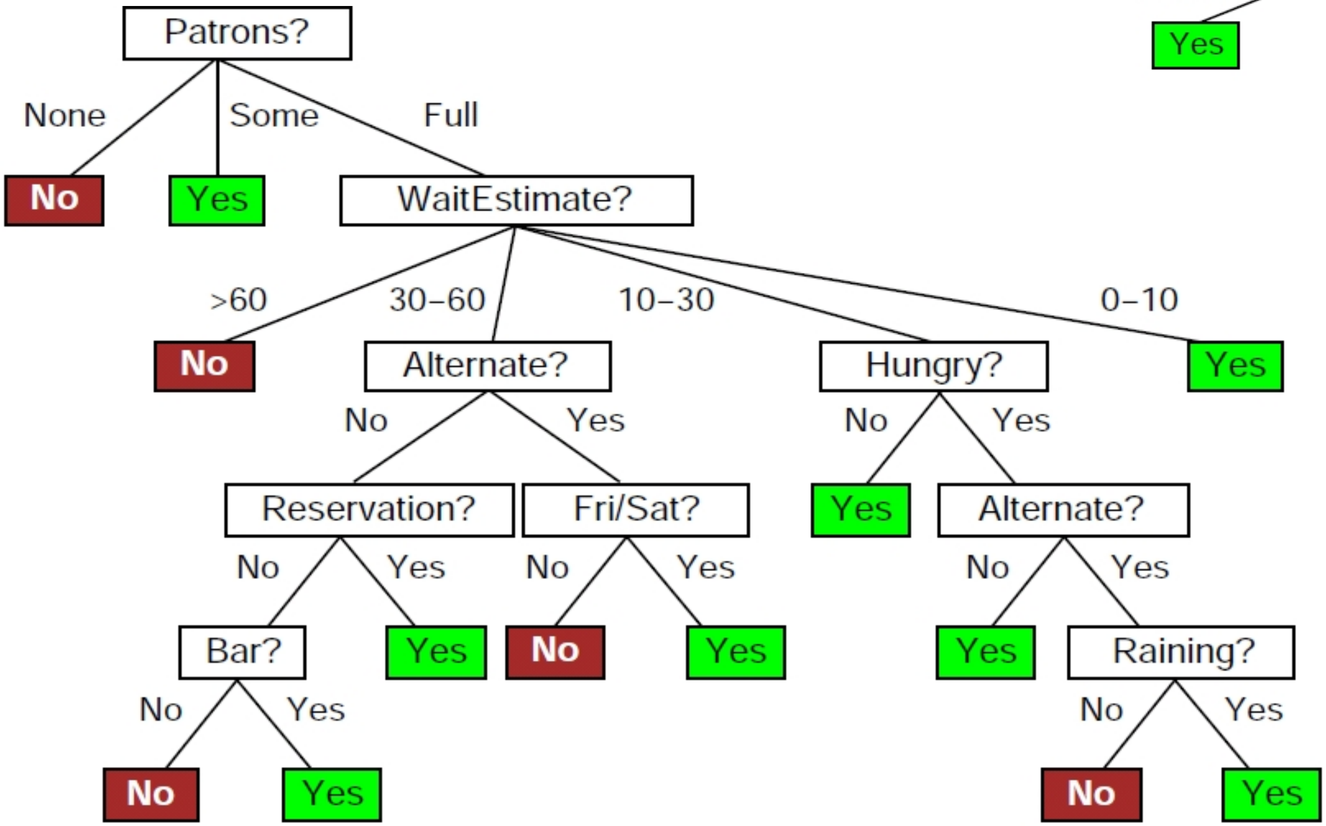
$$IG(Y) = H(Y) - H(Y|X)$$

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

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

Which Tree is Better? Vote!





What Makes a Good Tree?

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

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

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"

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

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

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
- Handling continuous attributes

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
- Handling continuous attributes
  - Split based on a threshold, chosen to maximize information gain

Decision Tree Miscellany

−100 −50 10 30

decision tree treats them the same

−10 −5 1 3

- 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.

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
- 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.

KNN versus Decision Trees

Advantages of decision trees over KNNs

KNN versus Decision Trees

Advantages of decision trees over KNNs

- Simple to deal with discrete features, missing values, and poorly scaled data
- Fast at test time (why?)
- More interpretable

KNNs - look at all training examples

number of levels of trees

KNN versus Decision Trees

Advantages of decision trees over KNNs

- Simple to deal with discrete features, missing values, and poorly scaled data
- Fast at test time (why?)
- More interpretable

Advantages of KNNs over decision trees

KNN versus Decision Trees

Advantages of decision trees over KNNs

- Simple to deal with discrete features, missing values, and poorly scaled data
- Fast at test time (why?)
- More interpretable

Advantages of KNNs over decision trees

- Few hyperparameters
- Can incorporate interesting distance measures (e.g. shape contexts)

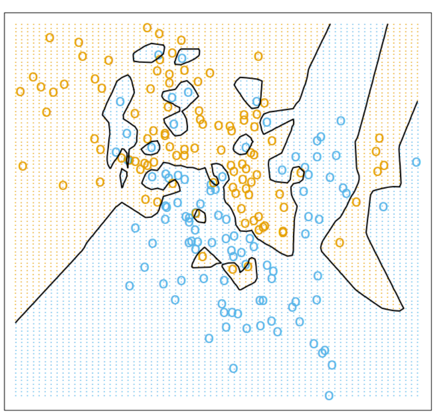
Ensembling

- We can combine multiple classifiers into an ensemble, which is a set of predictors whose individual decisions are combined in some way to classify new examples
  - Leverages "wisdom of the crowd"
  - 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
- Next lecture, we will study some specific ensembling techniques.

- Today, we deepen our understanding of generalization through a bias-variance decomposition.
  - This will help us understand ensembling methods.
- What is generalization?
  - Ability of a model to correctly classify/predict from unseen examples (from the same distribution that the training data was drawn from).
  - **Why does this matter?** Gives us confidence that the model has correctly captured the right patterns in the training data and will work when deployed.

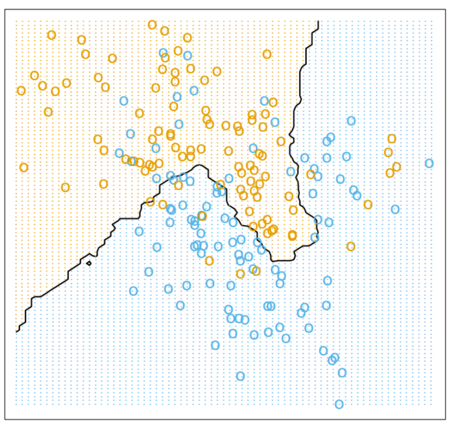
Bias-Variance Decomposition

- Overly simple models underfit the data, and overly complex models overfit.
- We can quantify underfitting and overfitting in terms of the bias/variance decomposition.

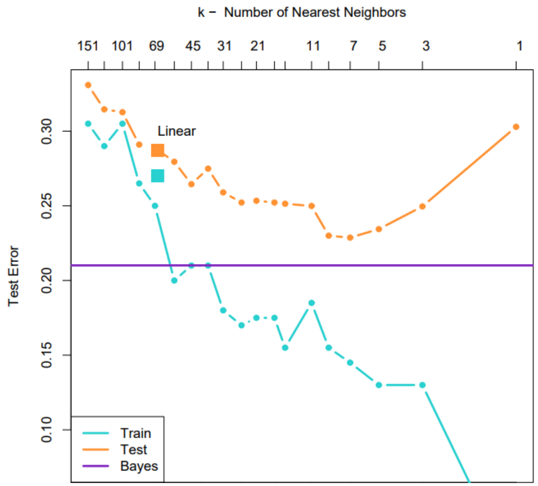


A

k=1
NN can overfit



B

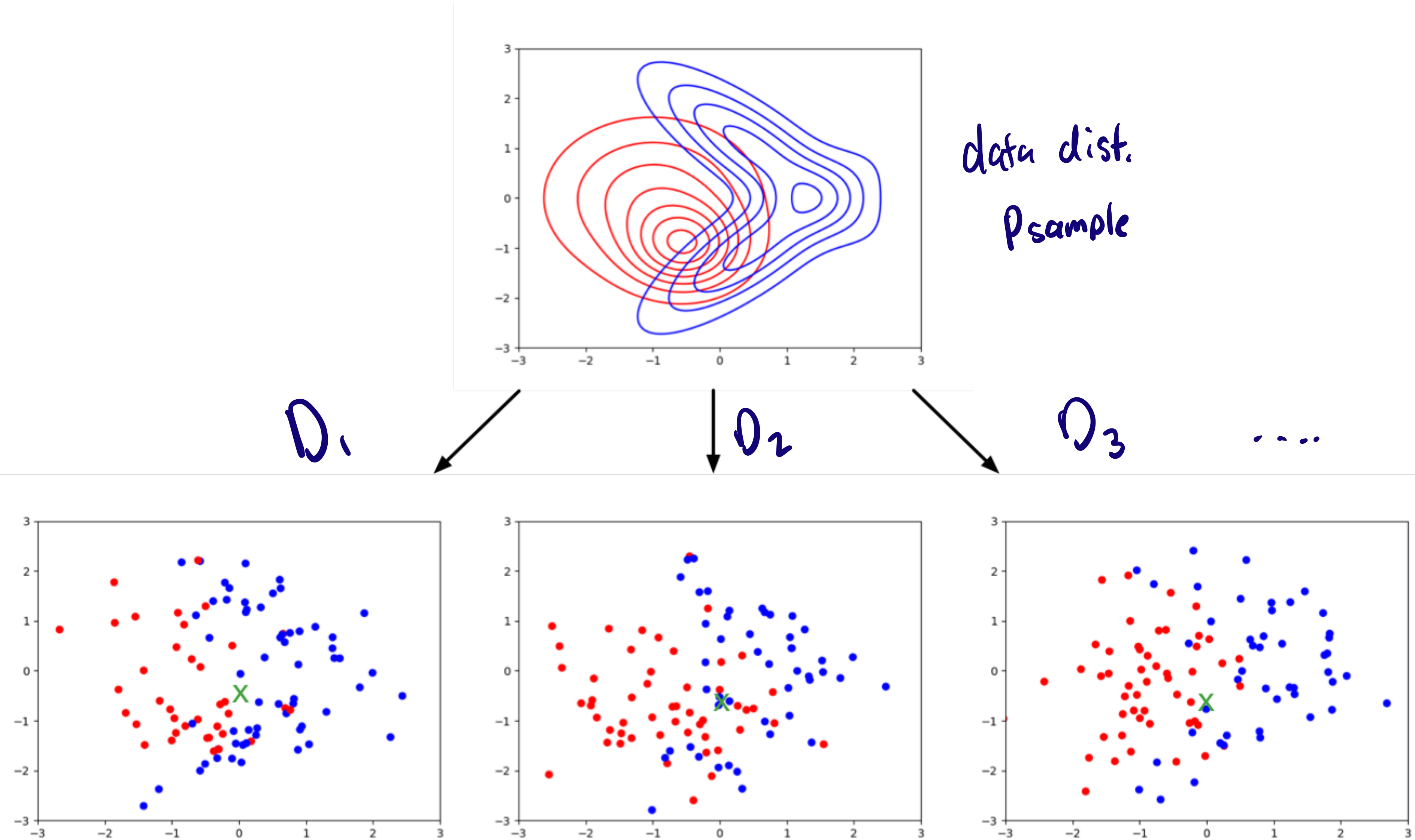


Basic Setup for Classification

thought experiment

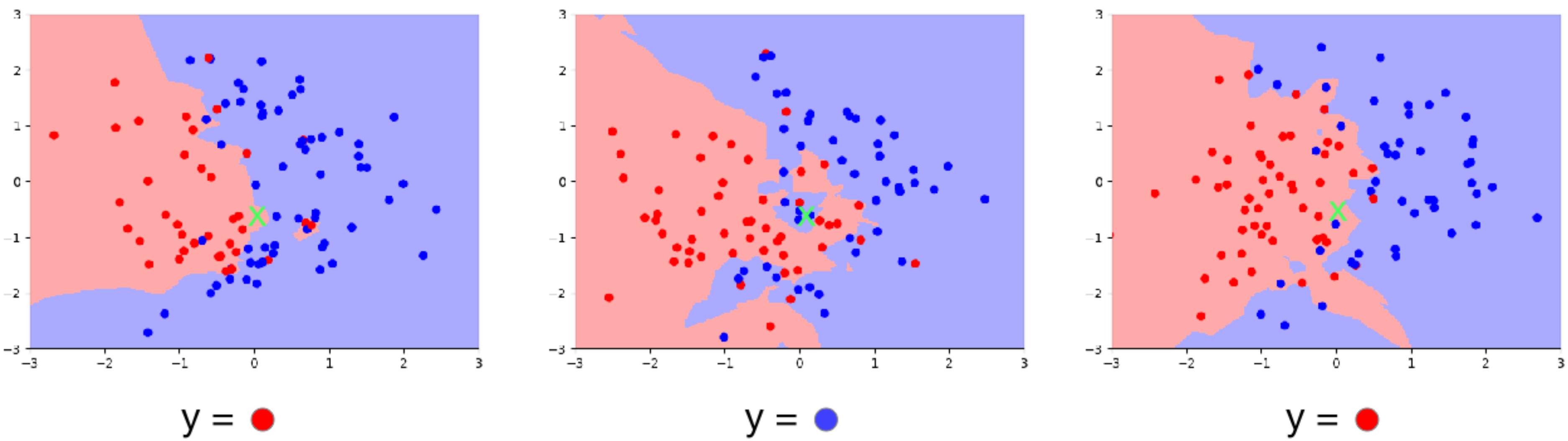
- p_{sample} is a data generating distribution.
  For lemons and oranges, p_{sample} characterizes heights and widths.
- Pick a fixed query point $\mathbf{x}$ (denoted with a green x).
  We want to get a prediction y at $\mathbf{x}$.
- A training set $\mathcal{D}$ consists of pairs $(\mathbf{x}_i, t_i)$ sampled independent and identically distributed (i.i.d.) from p_{sample}.
- We can sample lots of training sets independently from p_{sample}.

Basic Setup for Classification

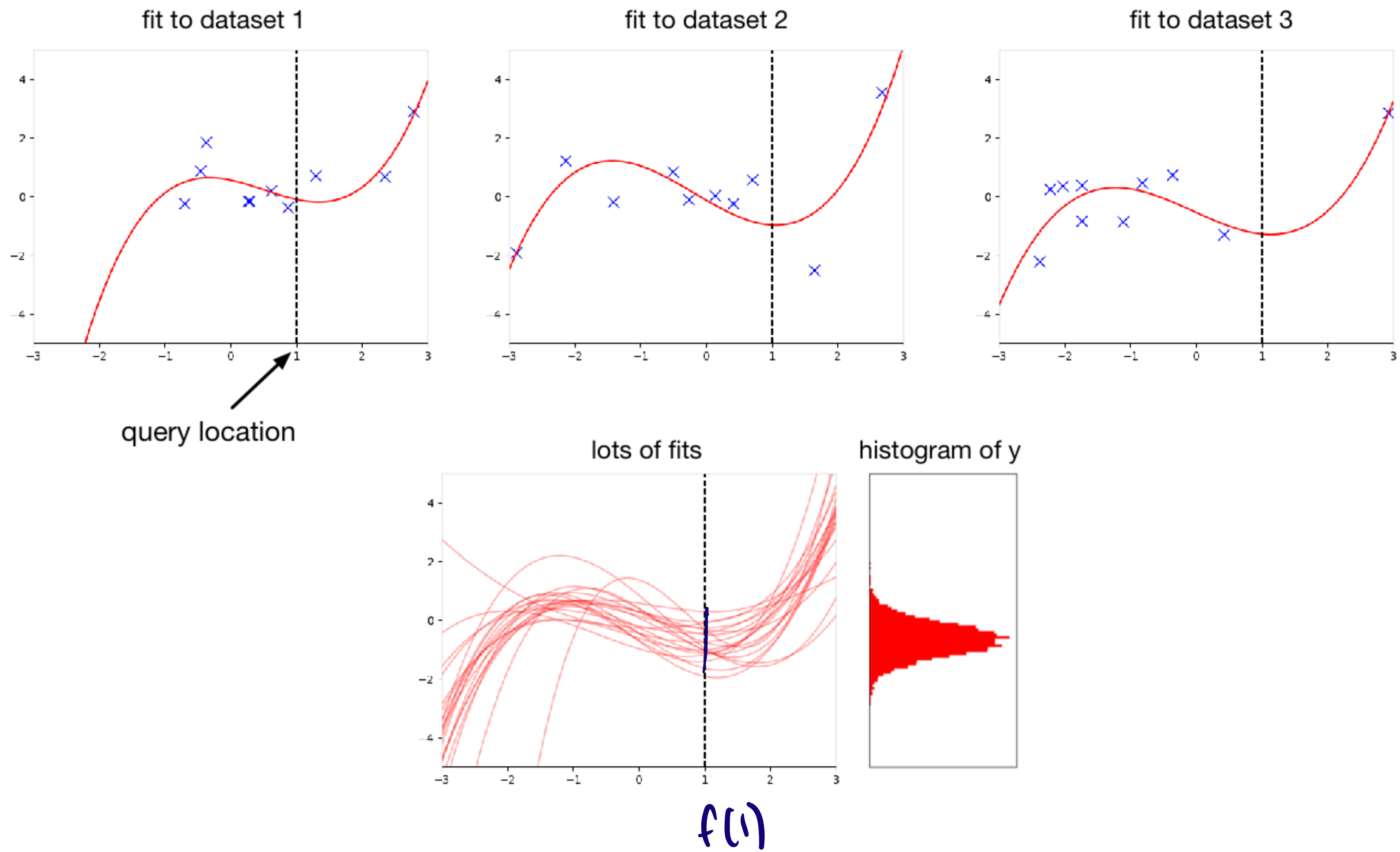


Basic Setup for Classification

- 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.
- Since y is a random variable, we can compute its expectation, variance, etc.



Basic Setup for Regression



Basic Setup

features, target
D_1 x, t (outputs)
D_2
⋮
D_n

- Fix a query point $\mathbf{x}$.
- Repeat:
  - Sample a random training dataset $\mathcal{D}$ i.i.d. from the data generating distribution p_{sample}.
  - Run the learning algorithm on $\mathcal{D}$ to get a prediction y at $\mathbf{x}$.
  - Sample the (true) target from the conditional distribution $p(t|\mathbf{x})$.
  - Compute the loss $L(y, t)$.

Comments:

- Notice: y is independent of t. (Why?)

We just see the samples

Basic Setup

- Fix a query point $\mathbf{x}$.
- Repeat:
  - Sample a random training dataset $\mathcal{D}$ i.i.d. from the data generating distribution p_{sample}.
  - Run the learning algorithm on $\mathcal{D}$ to get a prediction y at $\mathbf{x}$.
  - Sample the (true) target from the conditional distribution $p(t|\mathbf{x})$.
  - Compute the loss $L(y, t)$.

Comments:

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

Choosing a prediction y

- Consider squared error loss, $L(y, t) = \frac{1}{2}(y - t)^2$.
- Suppose that we knew the conditional distribution $p(t \mid \mathbf{x})$. What value of y should we predict?
  - Treat t as a random variable and choose y.

$\mathrm{var}(u) = E[u^2] - E[u]^2$

$E[u^2] = \mathrm{var}(u) + E[u]^2$

Loss for a choice of y:

$$
\begin{aligned}
&\mathbb{E}[(y-t)^2 \mid x] \\
&= E[y^2 - 2yt + t^2 \mid x] \\
&= E[y^2 \mid x] - E[2yt \mid x] + E[t^2 \mid x] \\
&= y^2 - 2y\,E[t \mid x] + E[t^2 \mid x] \\
&= y^2 - 2y\,E[t \mid x] + \mathrm{var}(t \mid x) + E[t \mid x]^2 \\
&= (y - E[t \mid x])^2 + \underbrace{\mathrm{var}(t \mid x)}_{\geq 0}
\end{aligned}
$$

$y^* = E[t \mid x]$

Choosing a prediction y

- Consider squared error loss, $L(y, t) = \frac{1}{2}(y - t)^2$.
- Suppose that we knew the conditional distribution $p(t \,|\, \mathbf{x})$. What value of y should we predict?
  - Treat t as a random variable and choose y.
- **Claim:** $y_* = \mathbb{E}[t \,|\, \mathbf{x}]$ is the best possible prediction.
- **Proof:**

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

Bayes Optimality

if you knew p_{sample}, $y = \mathbb{E}[t|x]$

$(x, t) \sim$ true dist.

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

mean squared error

Bayes error

- The first term is nonnegative, and can be made 0 by setting $y = y_*$.
- The second term is the Bayes error, or the noise or inherent unpredictability of the target t.
  - An algorithm that achieves it is Bayes optimal.
  - This term doesn't depend on y.
  - Best we can ever hope to do with any learning algorithm.
- This process of choosing a single value y_* based on $p(t \mid \mathbf{x})$ is an example of decision theory.

Decomposition Continued

- Now let's treat y as a random variable (where the randomness comes from the choice of dataset).
- We can decompose the expected loss further (suppressing the conditioning on $\mathbf{x}$ for clarity):

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

y

Bayes Optimality

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

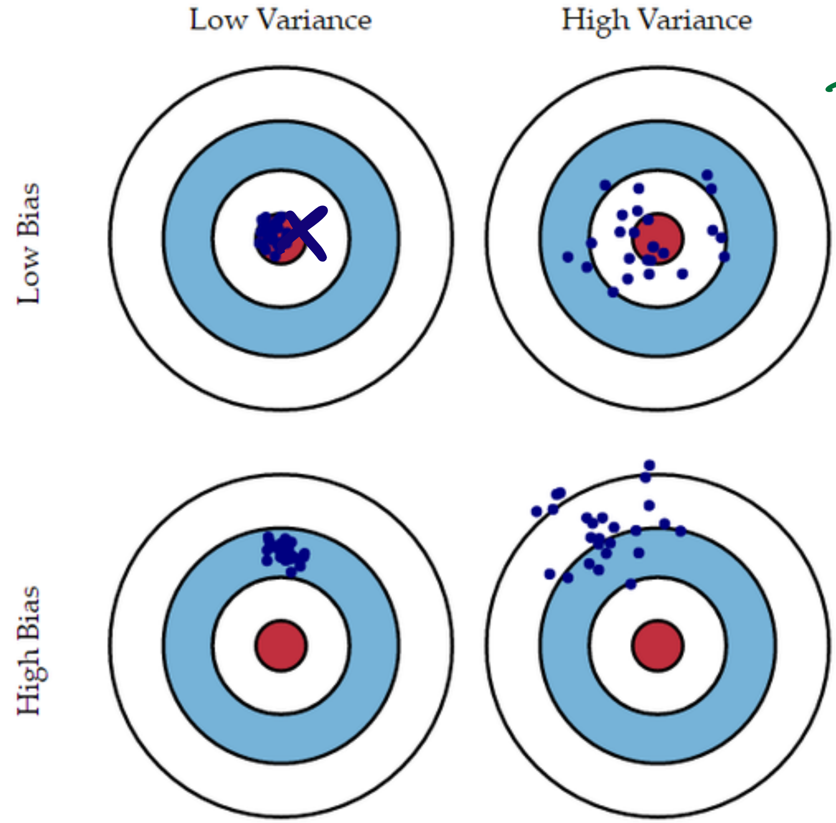
We split the expected loss into three terms:

mean squared error

- 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

Bias and Variance

- Throwing darts = predictions for each draw of a dataset



averaging helps

- Be careful, what doesn't this capture?
  - We average over points $\mathbf{x}$ from the data distribution.