

CSC 311: Introduction to Machine Learning

Lecture 2 - Decision Trees & Bias-Variance Decomposition

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University of Toronto, Summer 2023

Outline

- 1 Introduction
- 2 Decision Trees
- 3 Bias-Variance Decomposition

Today



- 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

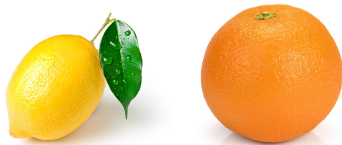
- ▶ Concept to motivate combining different classifiers.

- Ideas we will need in today's lecture

- ▶ Trees [from algorithms]
- ▶ Expectations, marginalization, chain rule [from probability]

- 1 Introduction
- 2 Decision Trees
- 3 Bias-Variance Decomposition

Lemons or Oranges

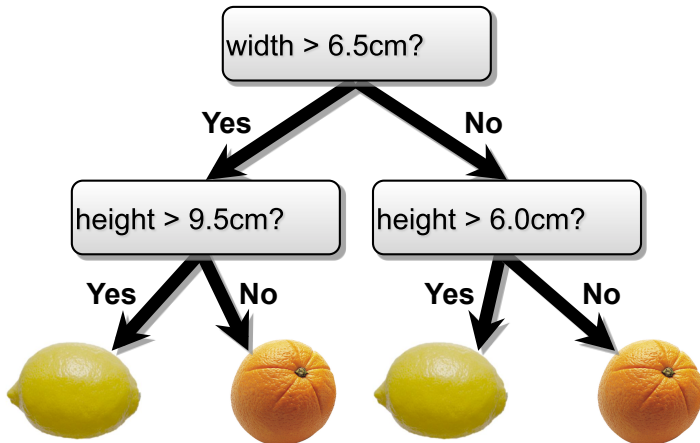


Scenario: You run a sorting facility for citrus fruits

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

Decision Trees

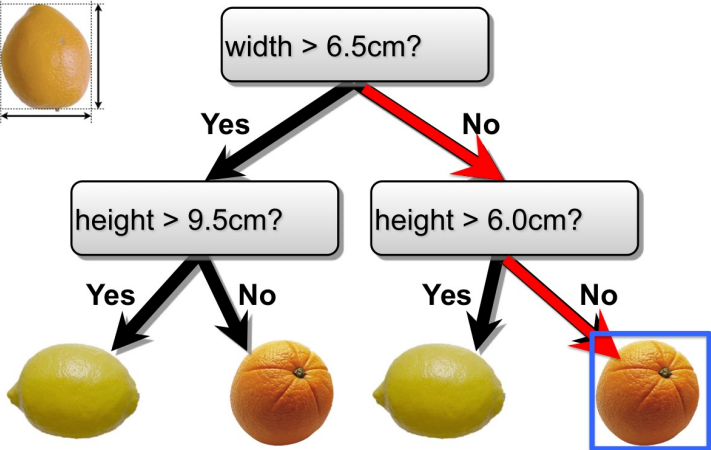
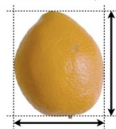
- Make predictions by splitting on features according to a tree structure.



Decision Trees

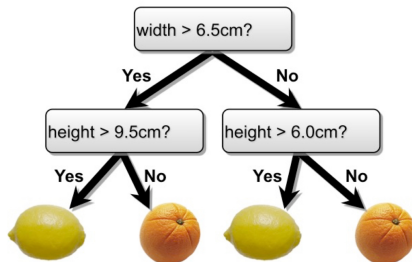
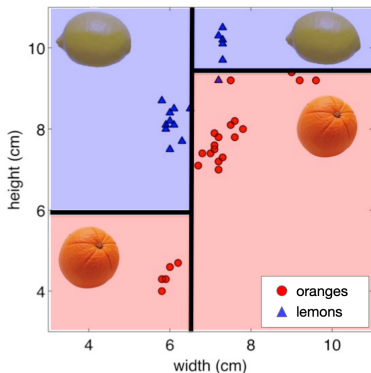
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Test example

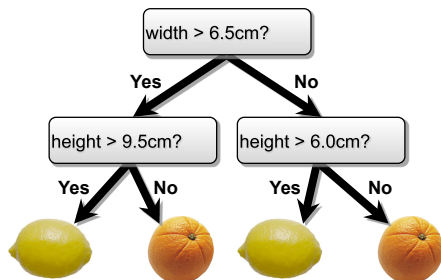


Decision Trees—Continuous Features

- 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

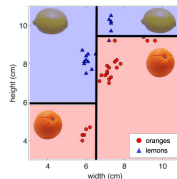


- Internal nodes test a feature
- Branching is determined by the feature value
- Leaf nodes are outputs (predictions)

Question: What are the hyperparameters of this model?

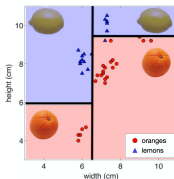
Decision Trees—Classification and Regression

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



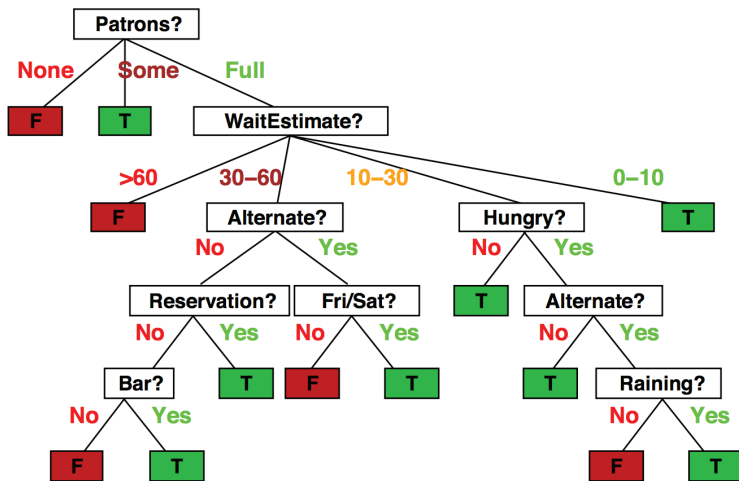
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- Regression tree:
 - ▶ continuous output
 - ▶ leaf value y^m typically set to the mean value in $\{t^{(m_1)}, \dots, t^{(m_k)}\}$
- Classification tree (we will focus on this):
 - ▶ discrete output
 - ▶ leaf value y^m typically set to the most common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



Decision Trees—Discrete Features

- Will I eat at this restaurant?



Decision Trees—Discrete Features

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

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	$y_2 = \text{No}$
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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).

Features:

Learning Decision Trees

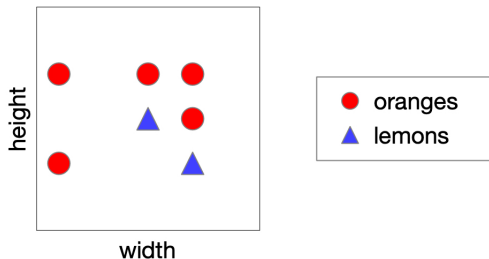
- Decision trees are universal function approximators.
 - ▶ For any training set we can construct a decision tree that has exactly the one leaf for every training point, but it probably won't generalize.
 - ▶ Example - If all D features were binary, and we had $N = 2^D$ unique training examples, a **Full Binary Tree** would have one leaf per example.
- Finding the smallest decision tree that correctly classifies a training set is NP complete.
 - ▶ 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?
 - ▶ 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?

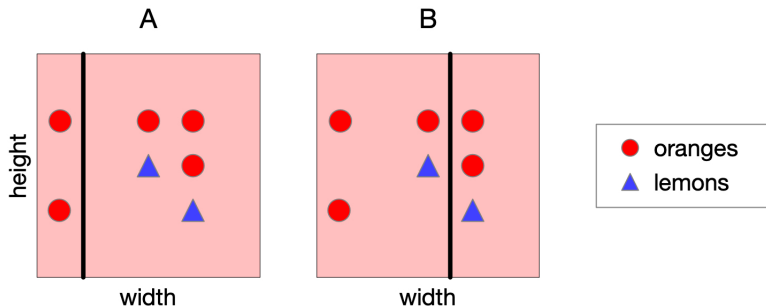
Choosing a Good Split

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



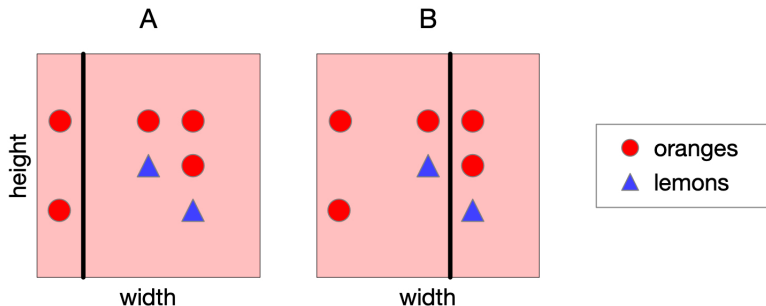
Choosing a Good Split

- 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.
- 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

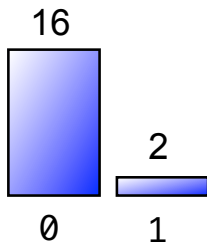
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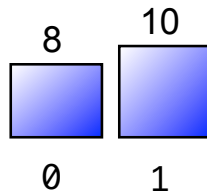
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Sequence 2:

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



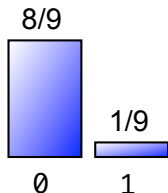
versus



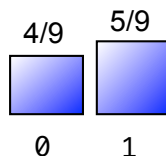
Quantifying Uncertainty

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

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



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

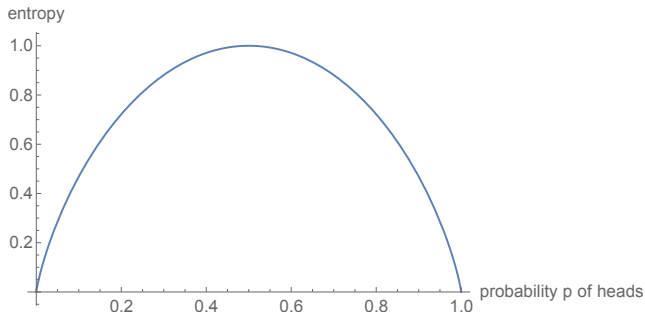


$$-\frac{4}{9} \log_2 \frac{4}{9} - \frac{5}{9} \log_2 \frac{5}{9} \approx 0.99$$

- 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.

Quantifying Uncertainty

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



- 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

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- **“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]

- 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 .

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

- 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:

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

Conditional Entropy

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

	Cloudy	Not Cloudy
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- 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

$$IG(Y|X) = H(Y) - H(Y|X) \quad (1)$$

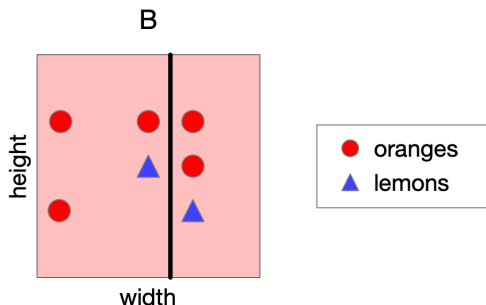
- If X is completely uninformative about Y : $IG(Y|X) = 0$
- If X is completely informative about Y : $IG(Y|X) = H(Y)$

Revisiting Our Original Example

- Information gain measures the informativeness of a variable, which is exactly what we desire in a decision tree 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

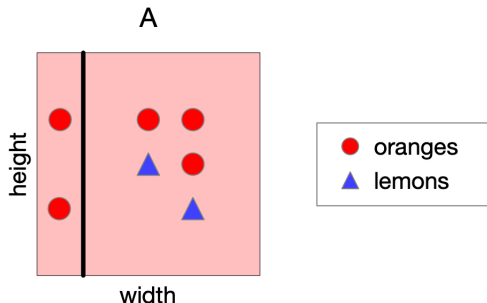
- What is the information gain of split B? Not terribly informative...



- 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:
 $H(Y|left) \approx 0.81, H(Y|right) \approx 0.92$
- $IG(split) \approx 0.86 - (\frac{4}{7} \cdot 0.81 + \frac{3}{7} \cdot 0.92) \approx 0.006$

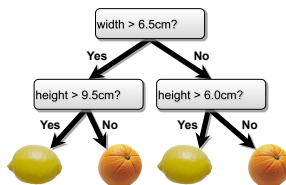
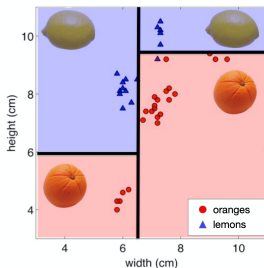
Information Gain of Split A

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



- 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:
 $H(Y|left) = 0, H(Y|right) \approx 0.97$
- $IG(split) \approx 0.86 - (\frac{2}{7} \cdot 0 + \frac{5}{7} \cdot 0.97) \approx 0.17!!$

Constructing Decision Trees



- At each level, one must choose:
 - Which feature to split.
 - 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

- 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

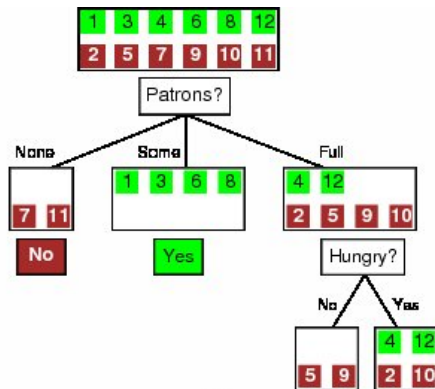
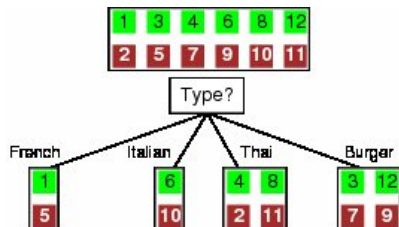
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[from: Russell & Norvig]

Features:

Feature Selection

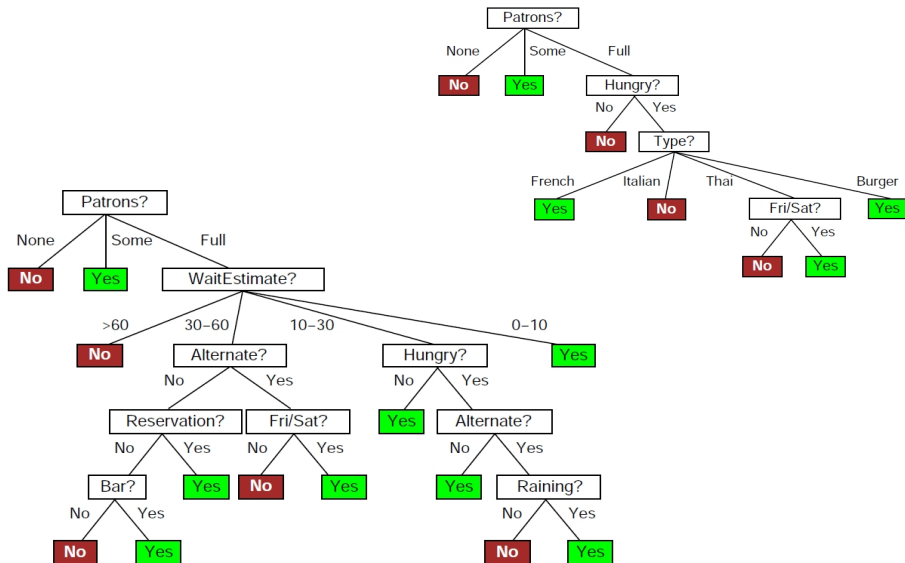


$$IG(Y) = H(Y) - H(Y|X)$$

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

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

Which Tree is Better? Vote!



What Makes a Good Tree?

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 - ▶ Useful principle, but hard to formalize (how to define simplicity?)
 - ▶ See Domingos, 1999, “The role of Occam’s razor in knowledge discovery”

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- We desire small trees with informative nodes near the root

Decision Tree Miscellany

- Problems:

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- ▶ Too big of a tree can overfit the data
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- Handling continuous attributes

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 - ▶ Too big of a tree can overfit the data
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- 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

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Advantages of KNNs over decision trees

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

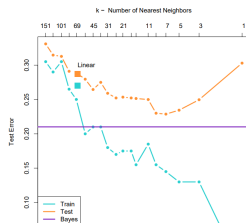
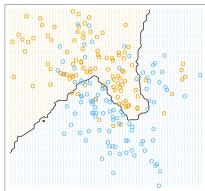
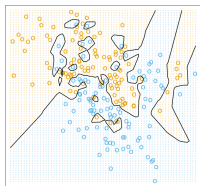
- We've seen many classification algorithms.
- We can combine multiple classifiers into an **ensemble**, which is a set of predictors whose individual decisions are combined in some way to classify new examples
 - ▶ E.g., (possibly weighted) majority vote
- For this to be nontrivial, the classifiers 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.

- 1 Introduction
- 2 Decision Trees
- 3 Bias-Variance Decomposition

- 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.

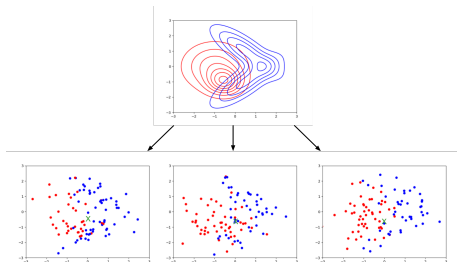
Bias-Variance Decomposition

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



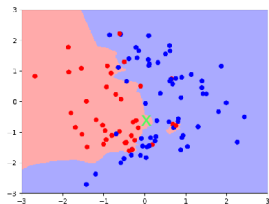
Basic Setup for Classification

- 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} .

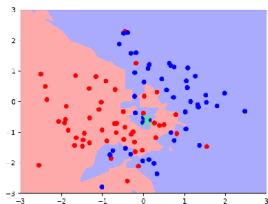


Basic Setup for Classification

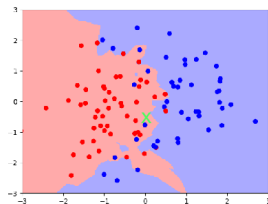
- Run our learning algorithm on each training set, and compute its prediction y at the query point \mathbf{x} .
- We can view y as a random variable, where the randomness comes from the choice of training set.
- The classification accuracy is determined by the distribution of y .
- Since y is a random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



$y = \bullet$

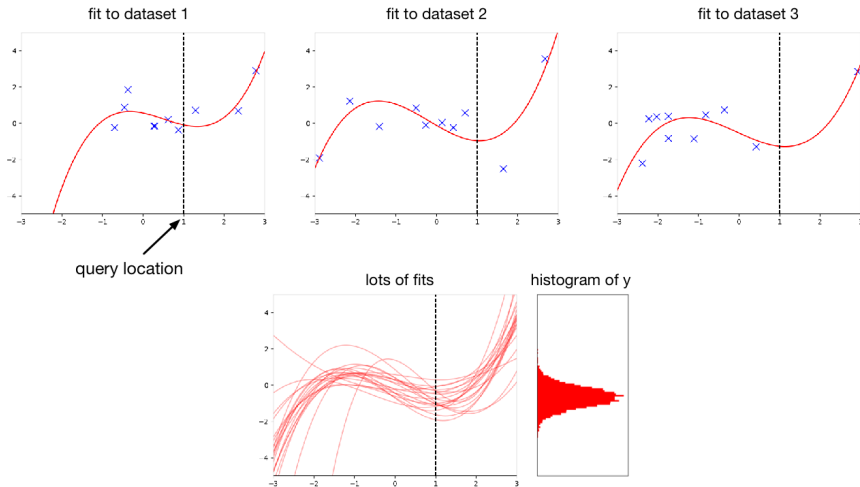


$y = \bullet$



$y = \bullet$

Basic Setup for Regression



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?)

Basic Setup

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Comments:

- Notice: y is independent of t . (Why?)
- This gives a distribution over the loss at \mathbf{x} , with expectation $\mathbb{E}[L(y, t) | \mathbf{x}]$.
- 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 .

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:**

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

Bayes Optimality

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

- The first term is nonnegative, and can be made 0 by setting $y = y_*$.
- The second term 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 $p(t | \mathbf{x})$ 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):

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

Bayes Optimality

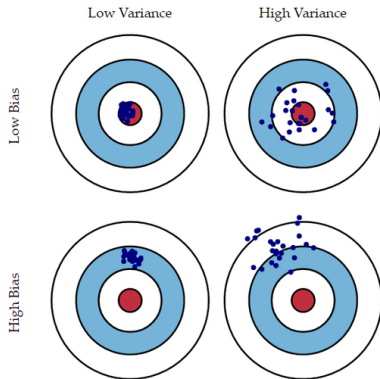
$$\mathbb{E}[(y - t)^2] = \underbrace{(y_\star - \mathbb{E}[y])^2}_{\text{bias}} + \underbrace{\text{Var}(y)}_{\text{variance}} + \underbrace{\text{Var}(t)}_{\text{Bayes error}}$$

We 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

Bias and Variance

- Throwing darts = predictions for each draw of a dataset



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