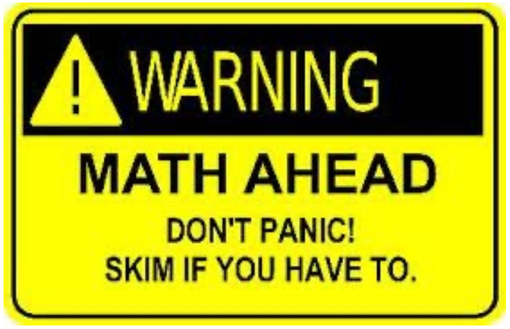

LMP 1210H: Basic Principles of Machine Learning in Biomedical Research

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UHN Peter Munk Cardiac Centre

Administrative Details

1. Homework
    a. Homework 1 is out! Due: **Feb 2, 9:59am**
    b. Homework 2 will be released on **Feb 2**

2. Final Project
    a. Team: 2-3 students
    b. Proposal due: **Feb 20.**
    c. Visit the office hour before submitting the proposal
    d. Proposal will **not** be graded
    e. Team without proposal submissions **cannot** participate in the final project.

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More on the final projects

1. How to form a good team?

   Keywords: Multidisciplinary, Open Communications, Piazza

2. How to write a good proposal?

   Keywords: Concise, Experimental Design, Office Hours

3. How to provide a good presentation?

   Keywords: Clear Structures, Memorable

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Recap: K - Nearest Neighbors (KNN)

- Nearest neighbors sensitive to noise or mis-labeled data ("class noise"). Solution?
- Smooth by having k nearest neighbors vote

Algorithm (kNN):

1. Find k examples $\{\mathbf{x}^{(i)}, t^{(i)}\}$ closest to the test instance $\mathbf{x}$
2. Classification output is majority class

$$y = \underset{t^{(z)}}{\operatorname{argmax}} \sum_{i=1}^{k} \mathbb{I}\{t^{(z)} = t^{(i)}\}$$

$\mathbb{I}\{\text{statement}\}$ is the identity function and is equal to one whenever the statement is true. We could also write this as $\delta(t^{(z)}, t^{(i)})$ with $\delta(a, b) = 1$ if $a = b$, 0 otherwise. $\mathbb{I}\{1\}$.

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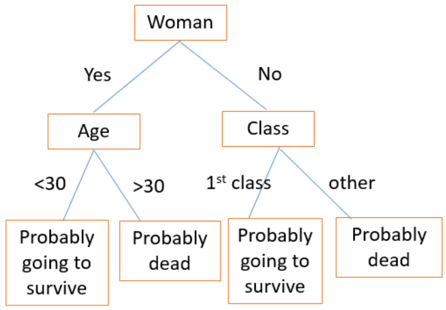
Recap: K - Nearest Neighbors (KNN)

- Simple algorithm that does all its work at test time — in a sense, no learning!
- Can be used for regression too, which we encounter later.
- Can control the complexity by varying k
- Suffers from the Curse of Dimensionality

Decision Trees

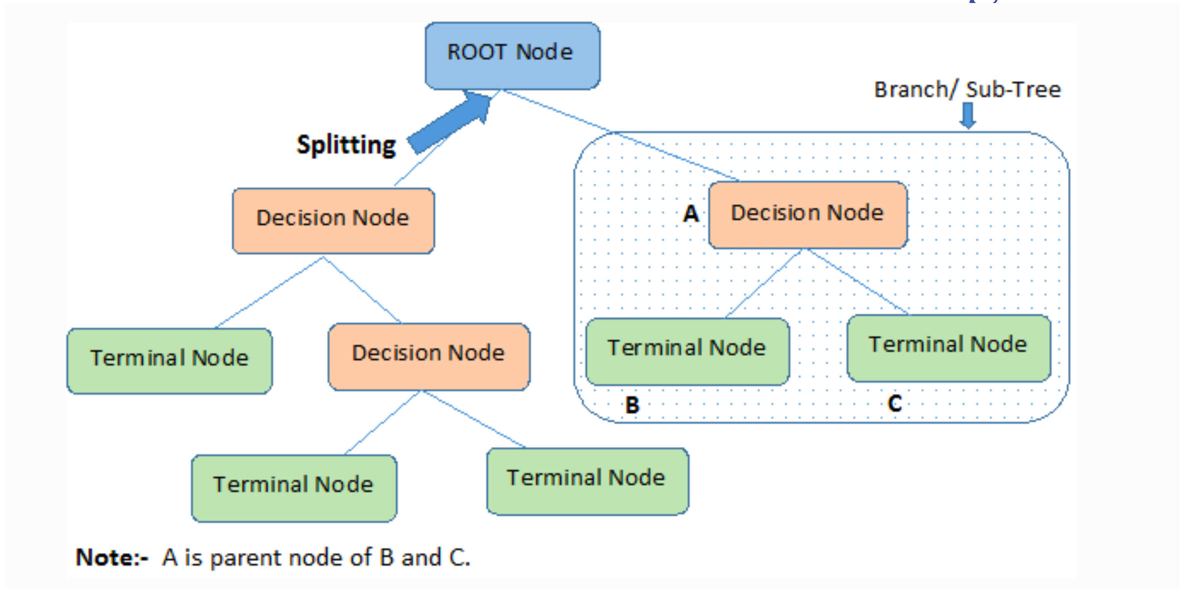
A normal tree

A decision tree



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

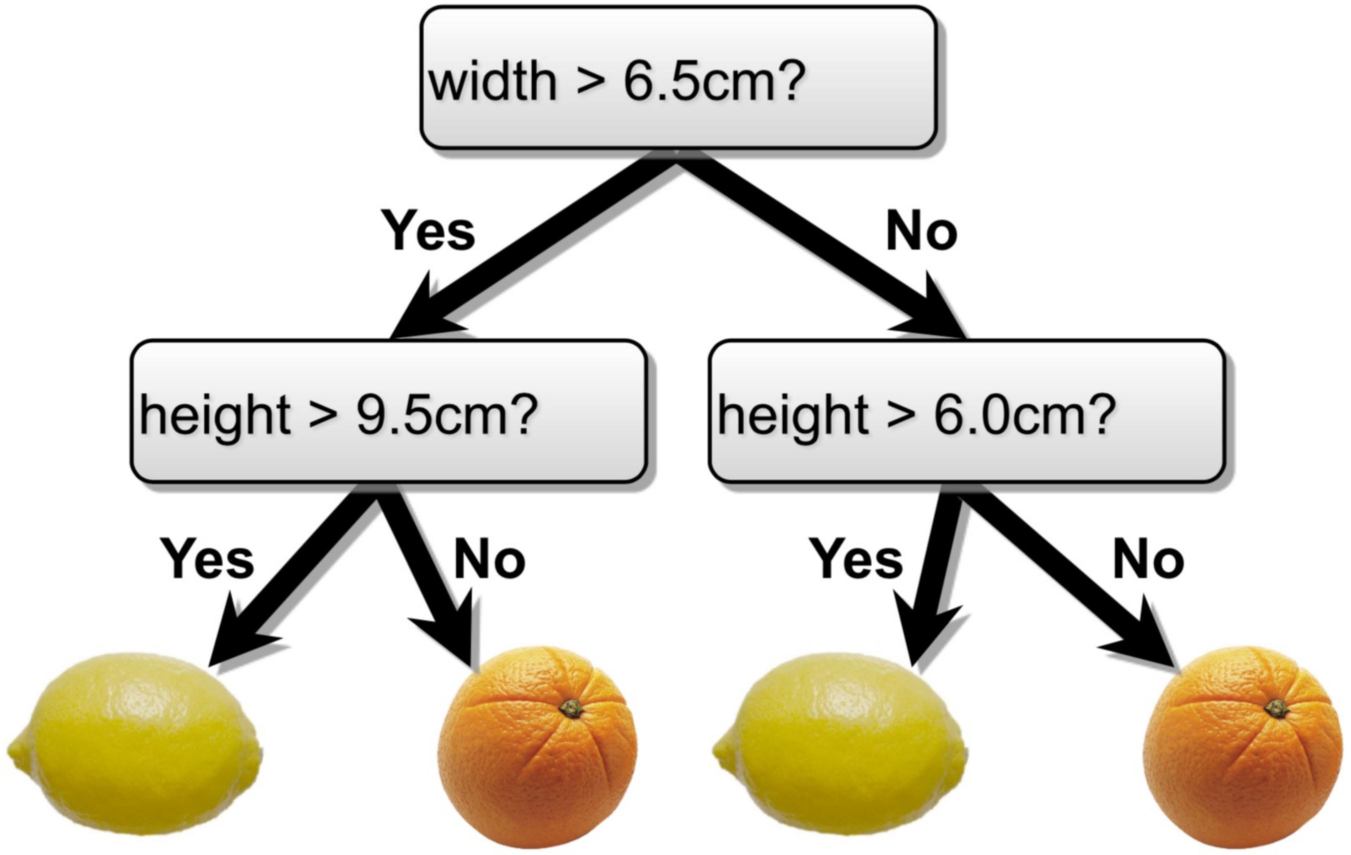
Decision Trees : Basic Terminologies



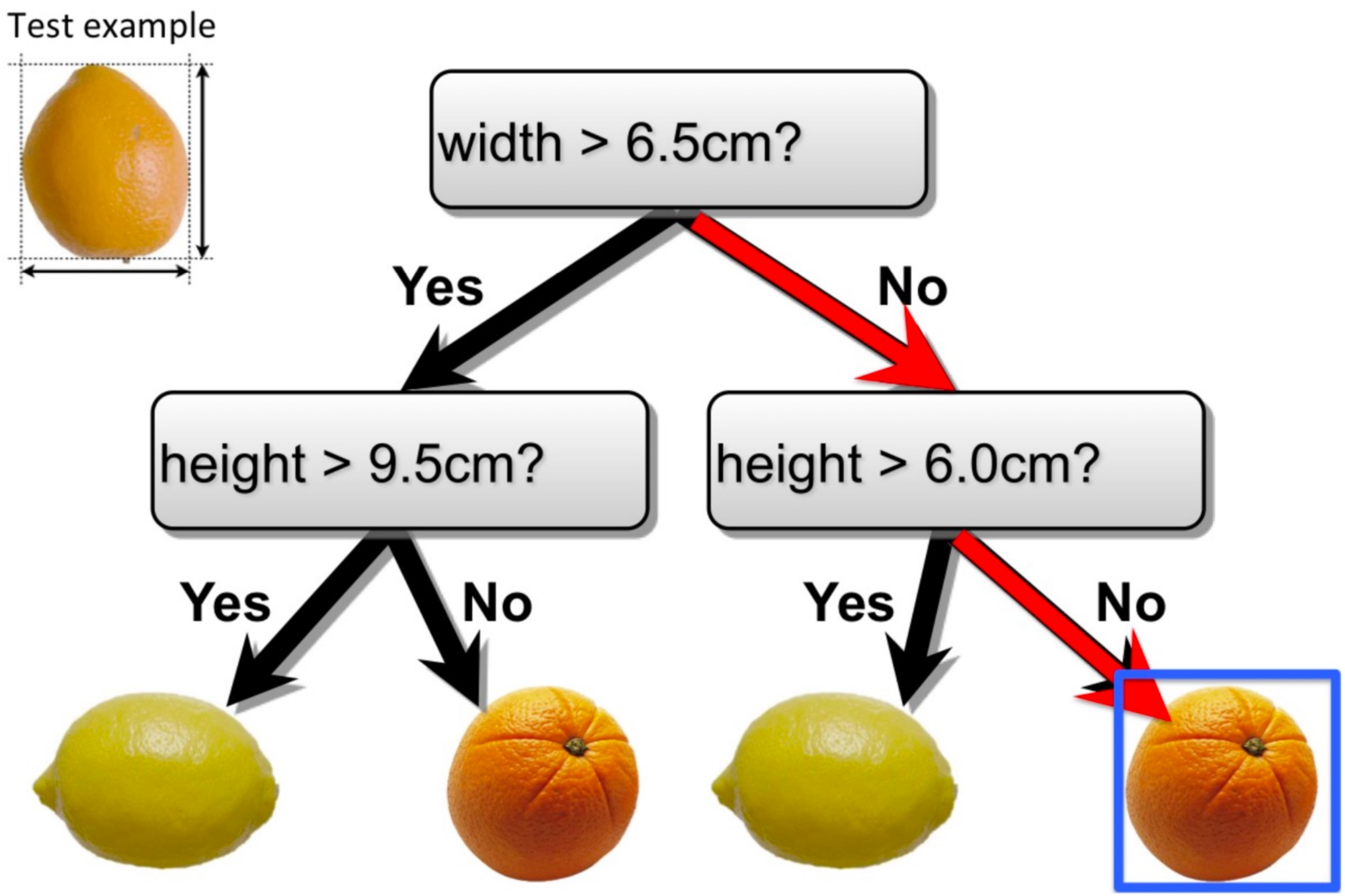
1. **Root Node:** This attribute is used for dividing the data into two or more sets. The feature attribute in this node is selected based on Attribute Selection Techniques.
2. **Branch or Sub-Tree:** A part of the entire decision tree is called a branch or sub-tree.
3. **Splitting:** Dividing a node into two or more sub-nodes based on if-else conditions.
4. **Decision Node:** After splitting the sub-nodes into further sub-nodes, then it is called the decision node.
5. **Leaf or Terminal Node:** This is the end of the decision tree where it cannot be split into further sub-nodes.

Decision Trees: A simple example

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



Decision Trees: A simple example



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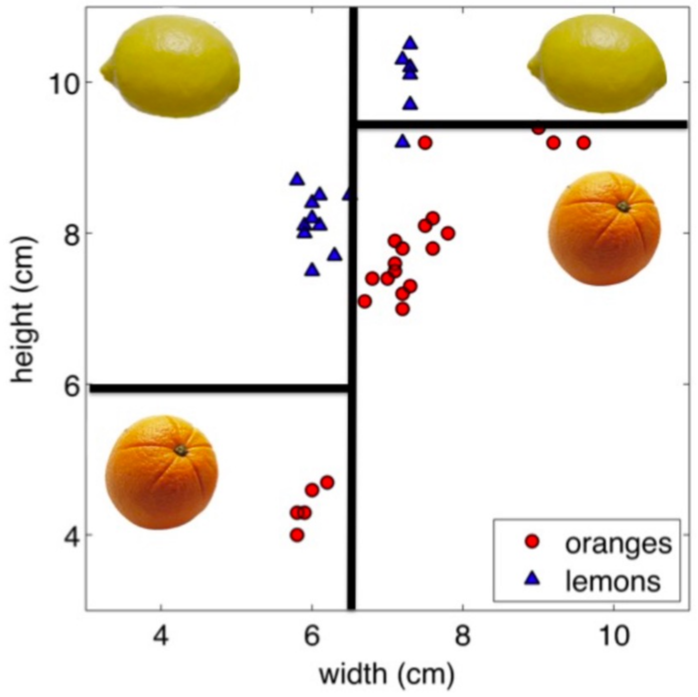
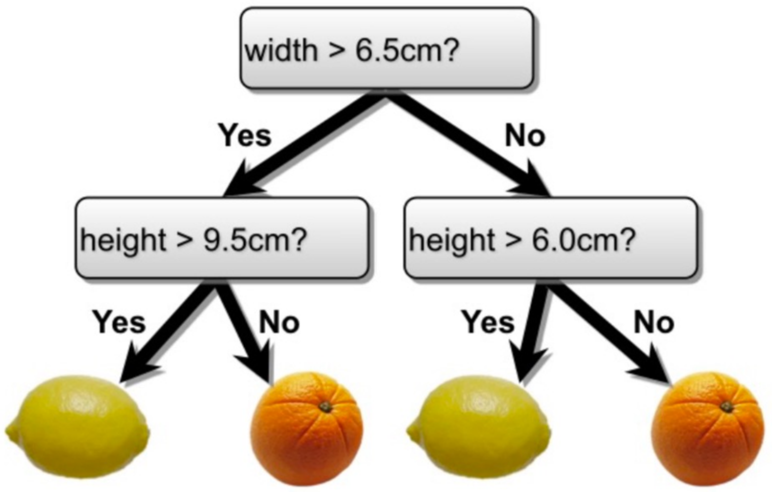
Decision Trees: A simple example

- For continuous attributes, split based on less than or greater than some threshold
- Thus, input space is divided into regions with boundaries parallel to axes





Decision Trees: Wait or Not

You can tell a lot about a fellow's character by his way of eating jellybeans.

----Ronald Reagan

You can tell a lot about a fellow's character by his way of eating at a restaurant.

----Bo Wang

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Decision Trees: Wait or Not

- What if the attributes are discrete?

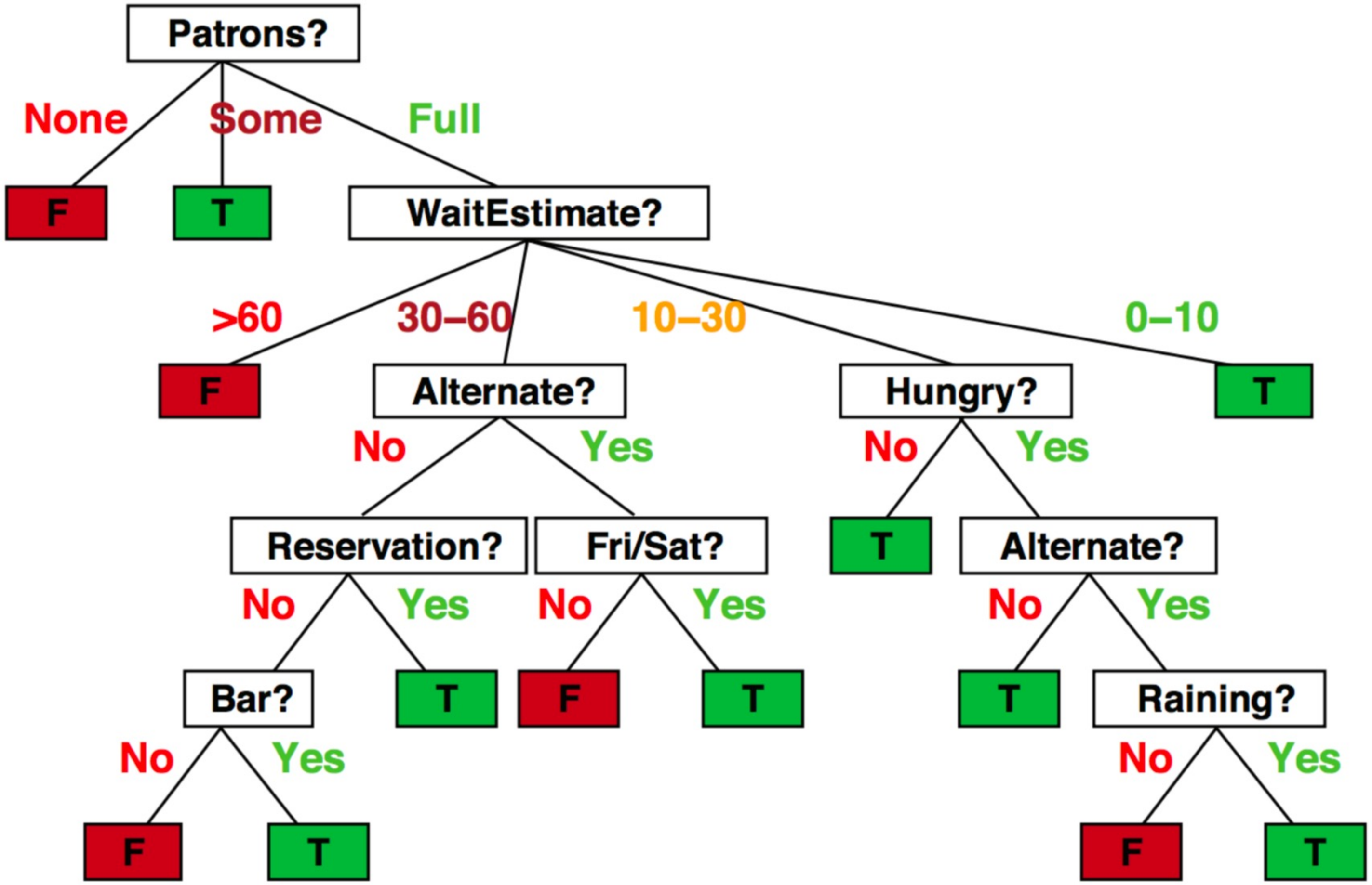
Example	Input Attributes										Goal
	Alt	*Bar*	*Fri*	*Hun*	*Pat*	*Price*	*Rain*	*Res*	*Type*	*Est*	*WillWait*
$\mathbf{x}_1$	Yes	No	No	Yes	Some	\$\$\$	No	Yes	French	0–10	$y_1 =$ Yes
$\mathbf{x}_2$	Yes	No	No	Yes	Full	\$	No	No	Thai	30–60	$y_2 =$ No
$\mathbf{x}_3$	No	Yes	No	No	Some	\$	No	No	Burger	0–10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

Attributes:

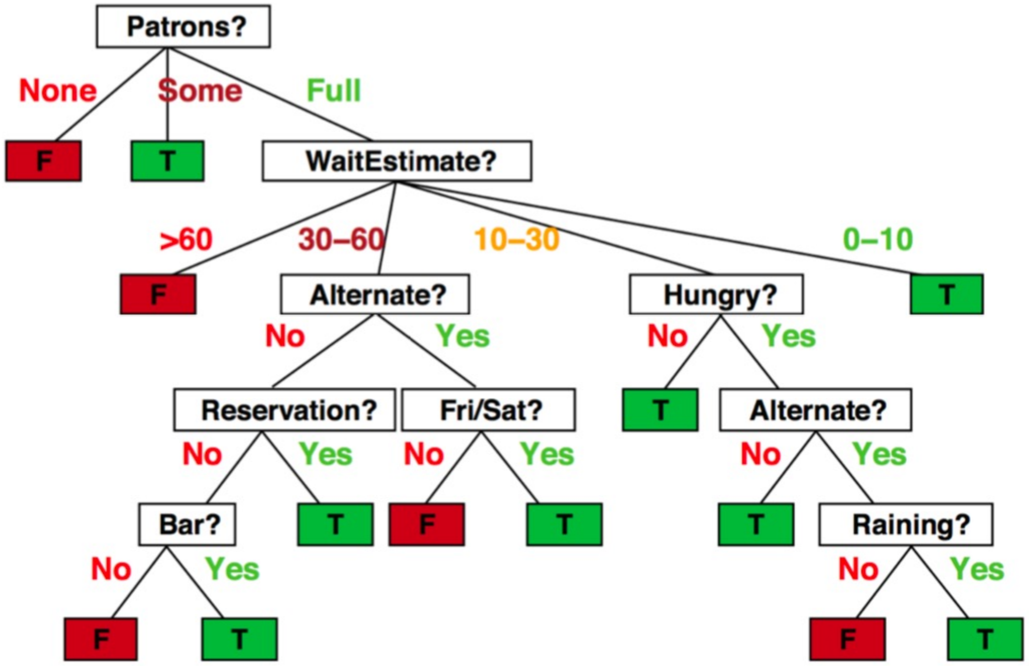
1.	Alternate: whether there is a suitable alternative restaurant nearby.
2.	Bar: whether the restaurant has a comfortable bar area to wait in.
3.	Fri/Sat: true on Fridays and Saturdays.
4.	Hungry: whether we are hungry.
5.	Patrons: how many people are in the restaurant (values are None, Some, and Full).
6.	Price: the restaurant's price range (\$, \$\$, \$\$\$).
7.	Raining: whether it is raining outside.
8.	Reservation: whether we made a reservation.
9.	Type: the kind of restaurant (French, Italian, Thai or Burger).
10.	WaitEstimate: the wait estimated by the host (0-10 minutes, 10-30, 30-60, >60).

Decision Trees: Wait or Not

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



Decision Trees: Wait or Not

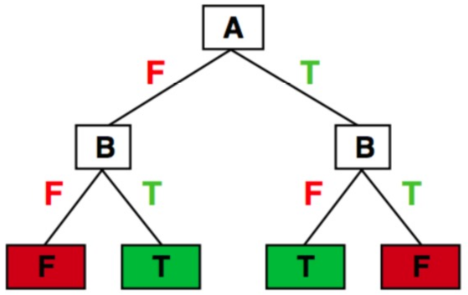


- **Internal nodes** test **attributes**
- **Branching** is determined by **attribute value**
- **Leaf nodes** are **outputs** (predictions)

Decision Trees

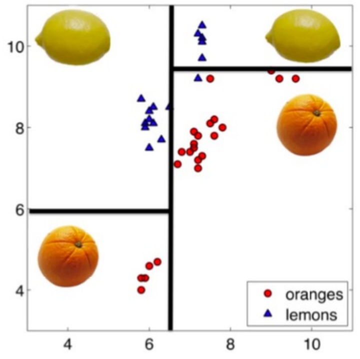
- **Discrete-input, discrete-output case:**
  - Decision trees can express any function of the input attributes
  - Example: For Boolean functions, the truth table row $\rightarrow$ path to leaf

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



- **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

Decision Trees



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

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

How to ***learn*** the trees

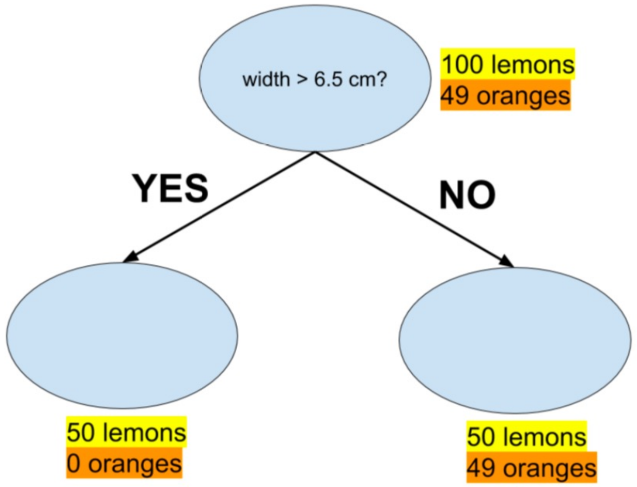
Learning the simplest (smallest) decision tree which correctly classifies training set is an NP complete problem (if you are interested, check: Hyafil & Rivest'76).

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

- When should we stop?
- Which attribute is the "best" (and where should we split, if continuous)?
  - Choose based on accuracy?
  - Loss: misclassification error
  - Say region R is split in R_1 and R_2 based on loss $L(R)$.
  - Accuracy gain is $L(R) - \frac{|R_1|L(R_1)+|R_2|L(R_2)}{|R_1|+|R_2|}$

How to ***learn*** the trees

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



- Is this split good? Zero accuracy gain

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

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

How to *learn* the trees

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

Entropy: a way to measure uncertainty

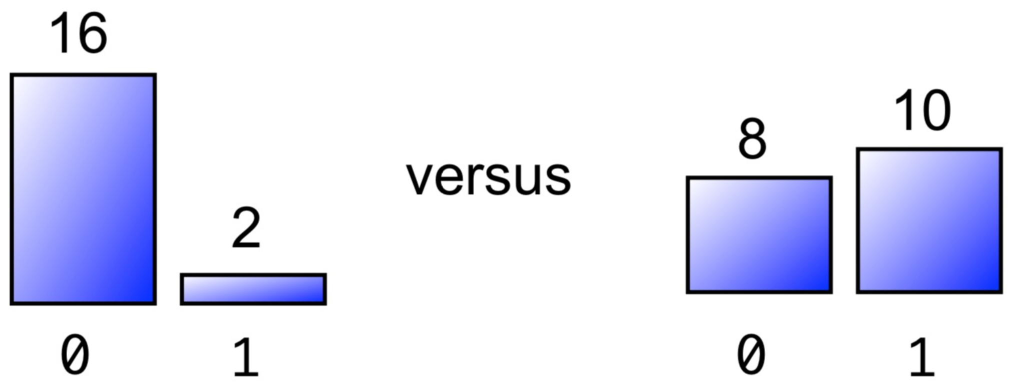
Q: Which coin is more uncertain?

Sequence 1:

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

Sequence 2:

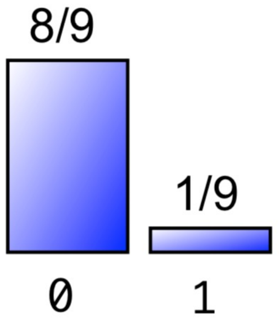
```
0 1 0 1 0 1 1 1 0 1 0 0 1 1 0 1 0 1 ... ?
```

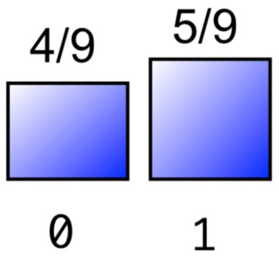


Entropy: a way to measure uncertainty

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

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





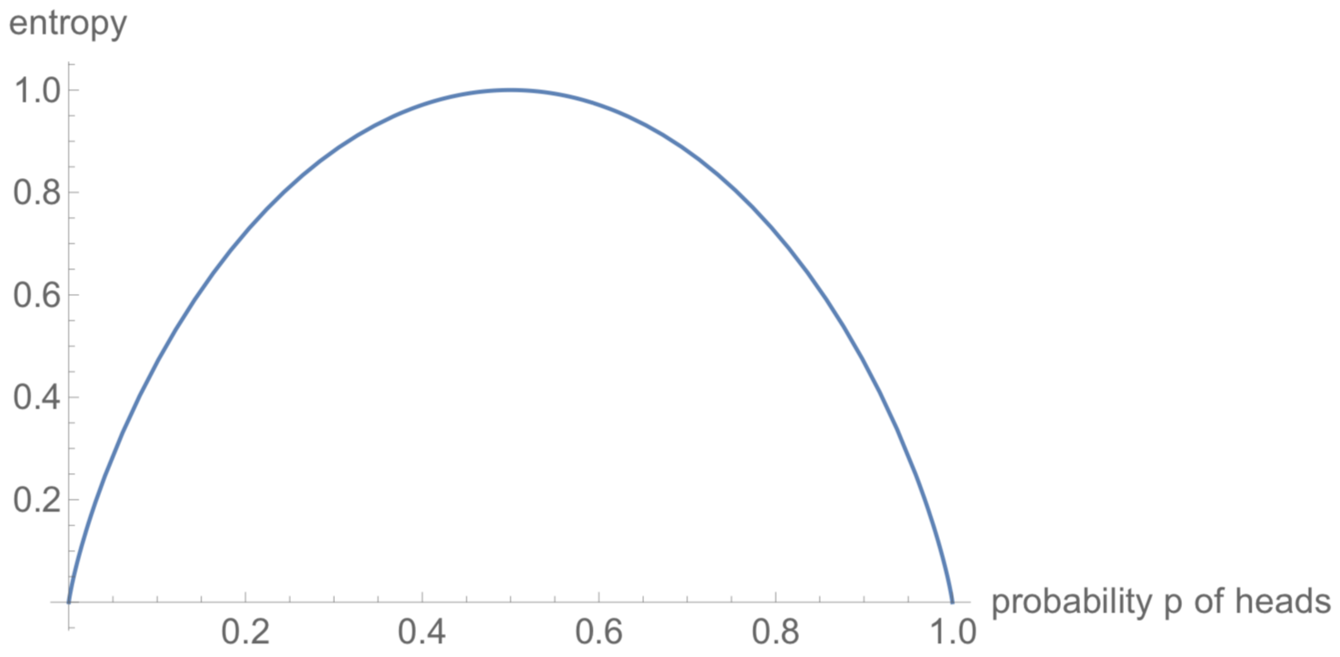
$$-\frac{8}{9}\log_2\frac{8}{9} - \frac{1}{9}\log_2\frac{1}{9} \approx \frac{1}{2}$$

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

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

Entropy: a way to measure uncertainty

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



Entropy: a way to measure uncertainty

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

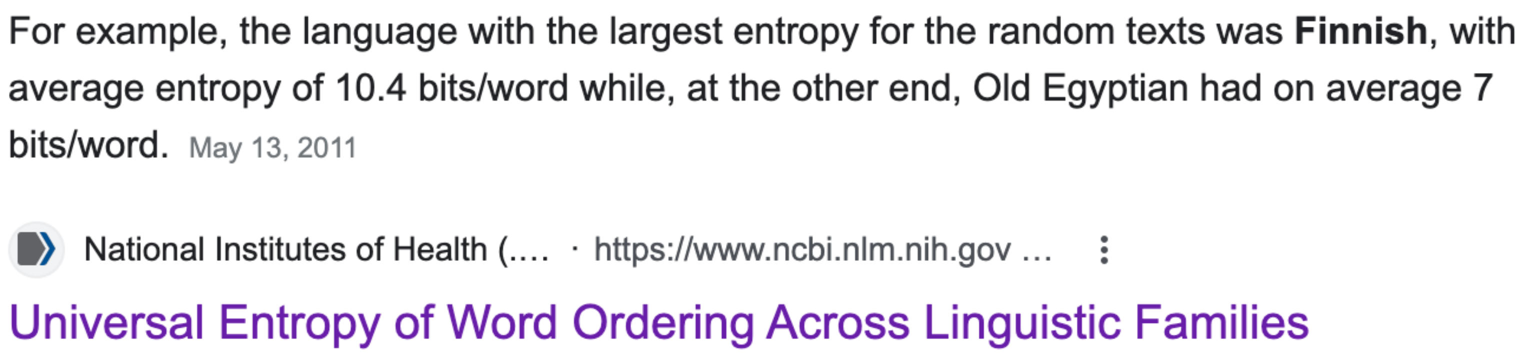
What is the entropy of *English*?

27 characters (A-Z, space).

100,000 words (avg 5.5 characters each)

- Assuming independence between successive characters:
  - uniform character distribution: $\log 27 = 4.75$ bits/character
  - true character distribution: 4.03 bits/character

Fun Fact: Which language has the largest entropy?



For example, the language with the largest entropy for the random texts was **Finnish**, with average entropy of 10.4 bits/word while, at the other end, Old Egyptian had on average 7 bits/word. May 13, 2011

National Institutes of Health (.... · https://www.ncbi.nlm.nih.gov ...

Universal Entropy of Word Ordering Across Linguistic Families

Entropy: a way to measure uncertainty

- 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

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

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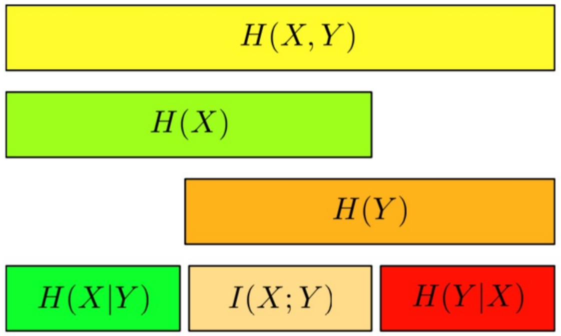
Entropy: a way to measure uncertainty

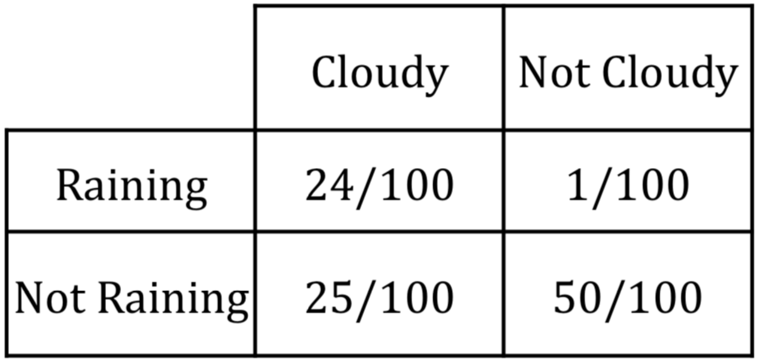


- Some useful properties for the discrete case:
  - H is always non-negative.
  - Chain rule: $H(X,Y) = H(X|Y) + H(Y) = H(Y|X) + H(X)$.
  - If X and Y independent, then X does not tell us anything about Y: $H(Y|X) = H(Y)$.
  - If X and Y independent, then $H(X,Y) = H(X) + H(Y)$.
  - But Y tells us everything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

Exercise: Verify these!

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

Entropy: a way to measure uncertainty



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

- The expected conditional entropy:

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

Entropy: a way to measure uncertainty

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

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

- What is the entropy of cloudiness, given the knowledge of whether or not it is raining?

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

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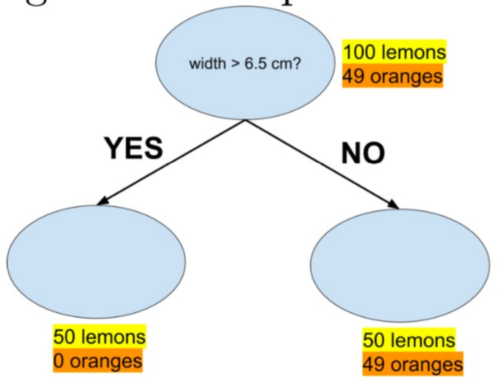
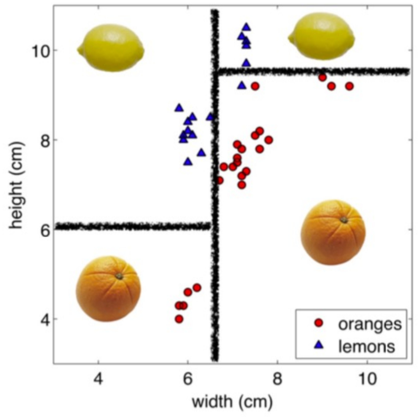
Learn the Decision Trees with Entropy

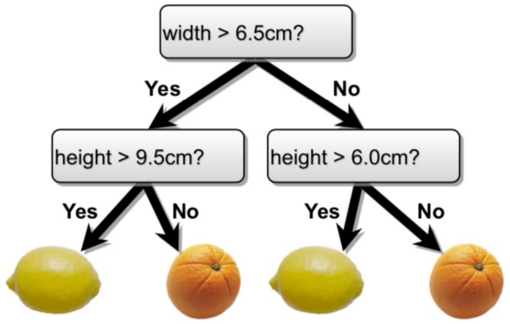
- Information gain measures the informativeness of a variable, which is exactly what we desire in a decision tree attribute!
- What is the information gain of this split?



- Let Y be r.v. denoting lemon or orange, B be r.v. denoting whether left or right split taken, and treat counts as probabilities.
- Root entropy: $H(Y) = -\frac{49}{149}\log_2(\frac{49}{149}) - \frac{100}{149}\log_2(\frac{100}{149}) \approx 0.91$
- Leafs entropy: $H(Y|B = \text{left}) = 0$, $H(Y|B = \text{right}) \approx 1$.
- $$\begin{aligned} IG(Y|B) &= H(Y) - H(Y|B) \\ &= H(Y) - \{H(Y|B{=}\text{left})\mathbb{P}(B{=}\text{left}) + H(Y|B{=}\text{right})\mathbb{P}(B{=}\text{right})\} \\ &\approx 0.91 - (0 \cdot \tfrac{1}{3} + 1 \cdot \tfrac{2}{3}) \approx 0.24 > 0 \end{aligned}$$

Learn the Decision Trees with Entropy



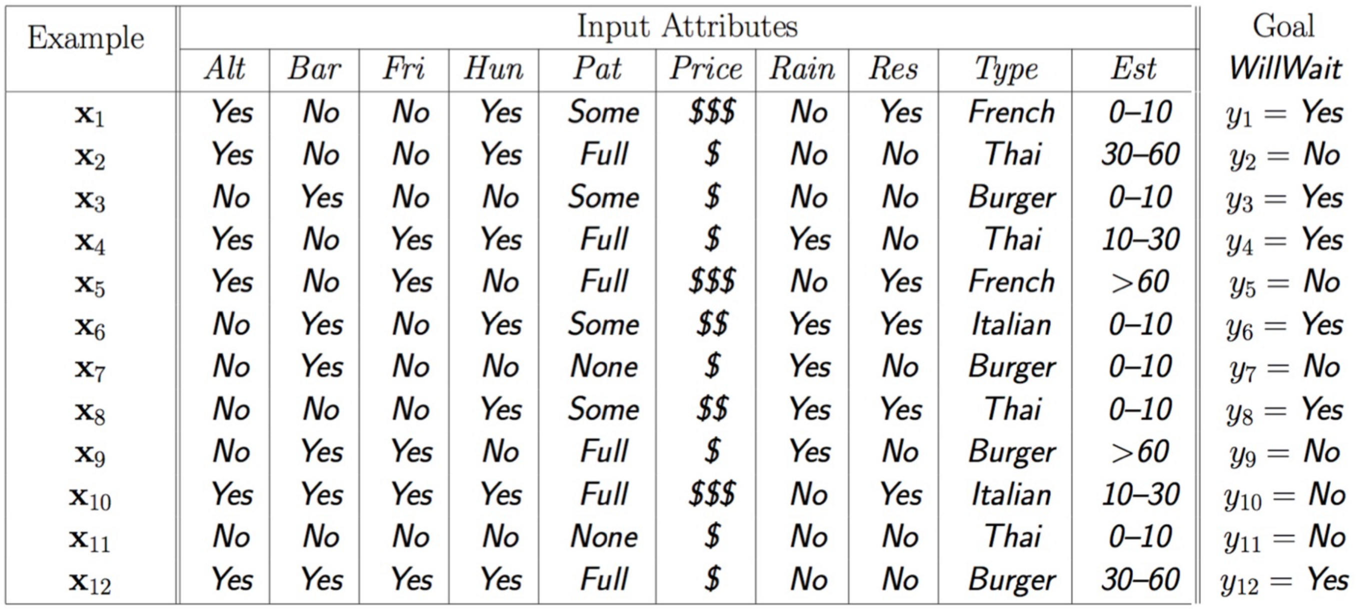


- At each level, one must choose:
  1. Which variable to split.
  2. Possibly where to split it.
- Choose them based on how much information we would gain from the decision! (choose attribute that gives the **best** gain)

Learn the Decision Trees with Entropy

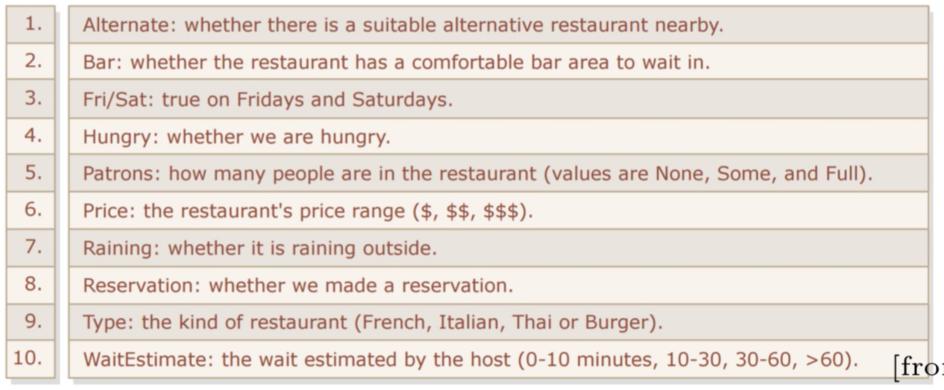
- Simple, greedy, recursive approach, builds up tree node-by-node
- Start with empty decision tree and complete training set
    - Split on the most informative attribute, partitioning dataset
    - Recurse on subpartitions
- Possible termination condition: end if all examples in current subpartition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

Get Back to the Restaurant: Wait or Not



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

Attributes:

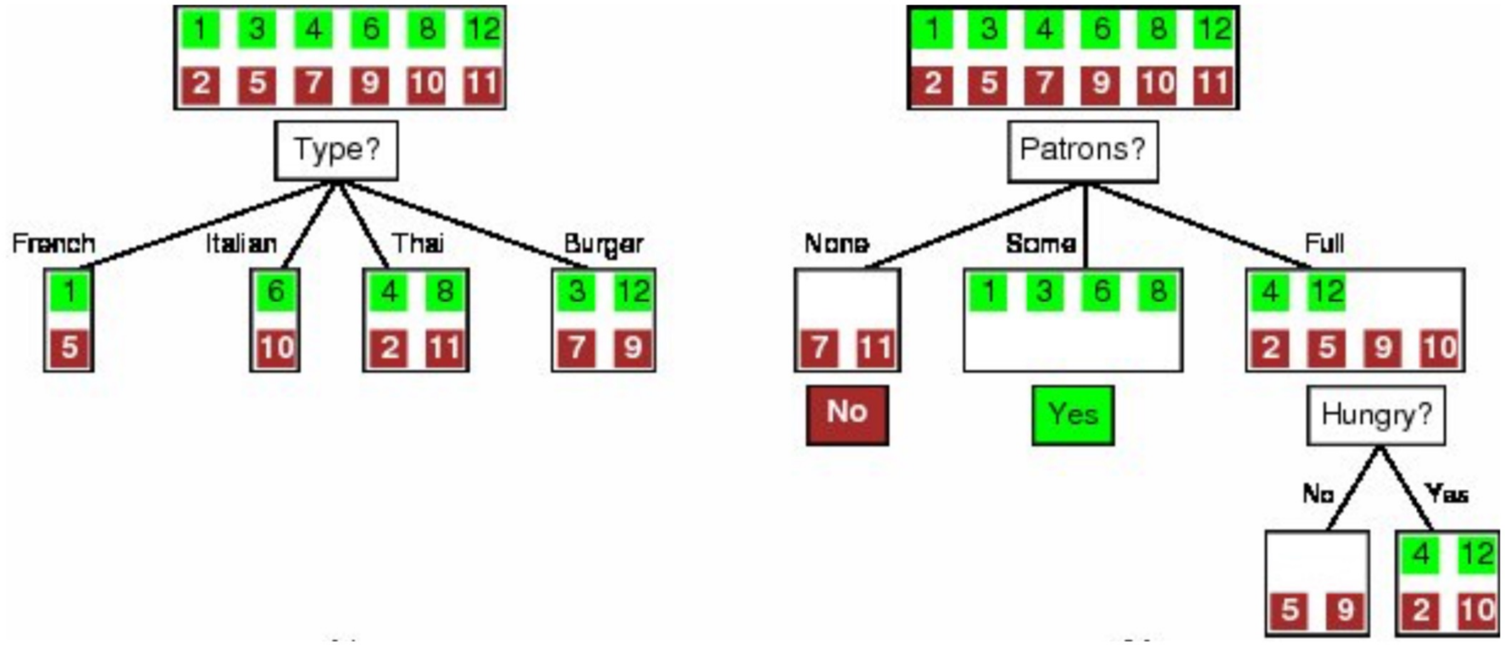


1.	Alternate: whether there is a suitable alternative restaurant nearby.
2.	Bar: whether the restaurant has a comfortable bar area to wait in.
3.	Fri/Sat: true on Fridays and Saturdays.
4.	Hungry: whether we are hungry.
5.	Patrons: how many people are in the restaurant (values are None, Some, and Full).
6.	Price: the restaurant's price range (\$, \$\$, \$\$\$).
7.	Raining: whether it is raining outside.
8.	Reservation: whether we made a reservation.
9.	Type: the kind of restaurant (French, Italian, Thai or Burger).
10.	WaitEstimate: the wait estimated by the host (0-10 minutes, 10-30, 30-60, >60).

[from: Russell & Norvig]

Get Back to the Restaurant: Wait or Not

Which attribute is better?



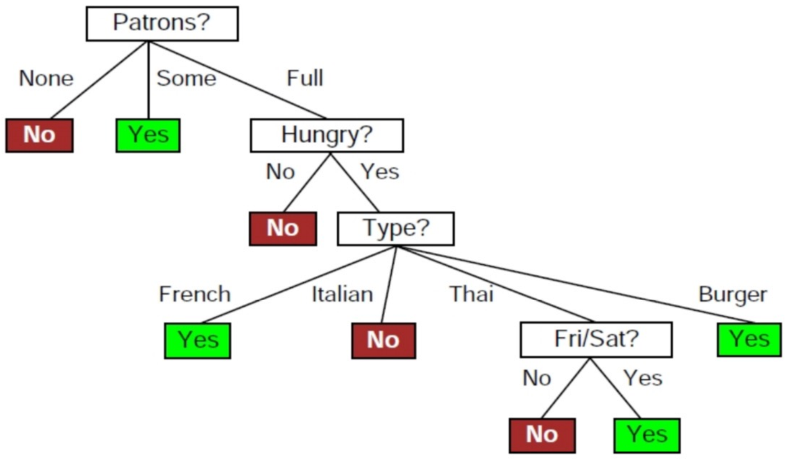
$$IG(Y) = H(Y) - H(Y|X)$$

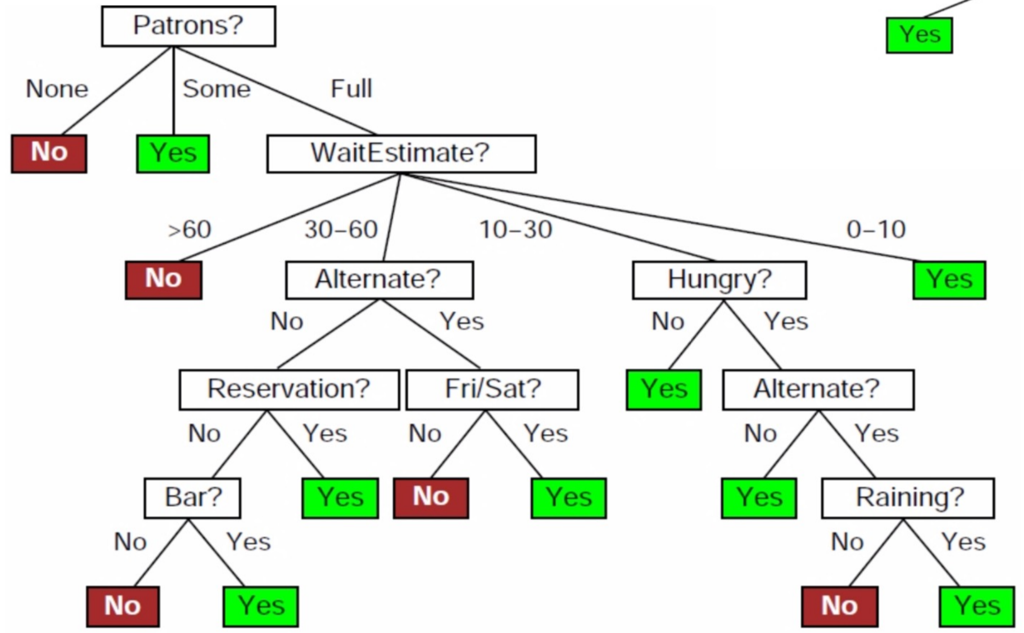
$$IG(type) = 1 - \left[\frac{2}{12}H(Y|\text{Fr.}) + \frac{2}{12}H(Y|\text{It.}) + \frac{4}{12}H(Y|\text{Thai}) + \frac{4}{12}H(Y|\text{Bur.})\right] = 0$$

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

Get Back to the Restaurant: Wait or Not

Which tree is better?

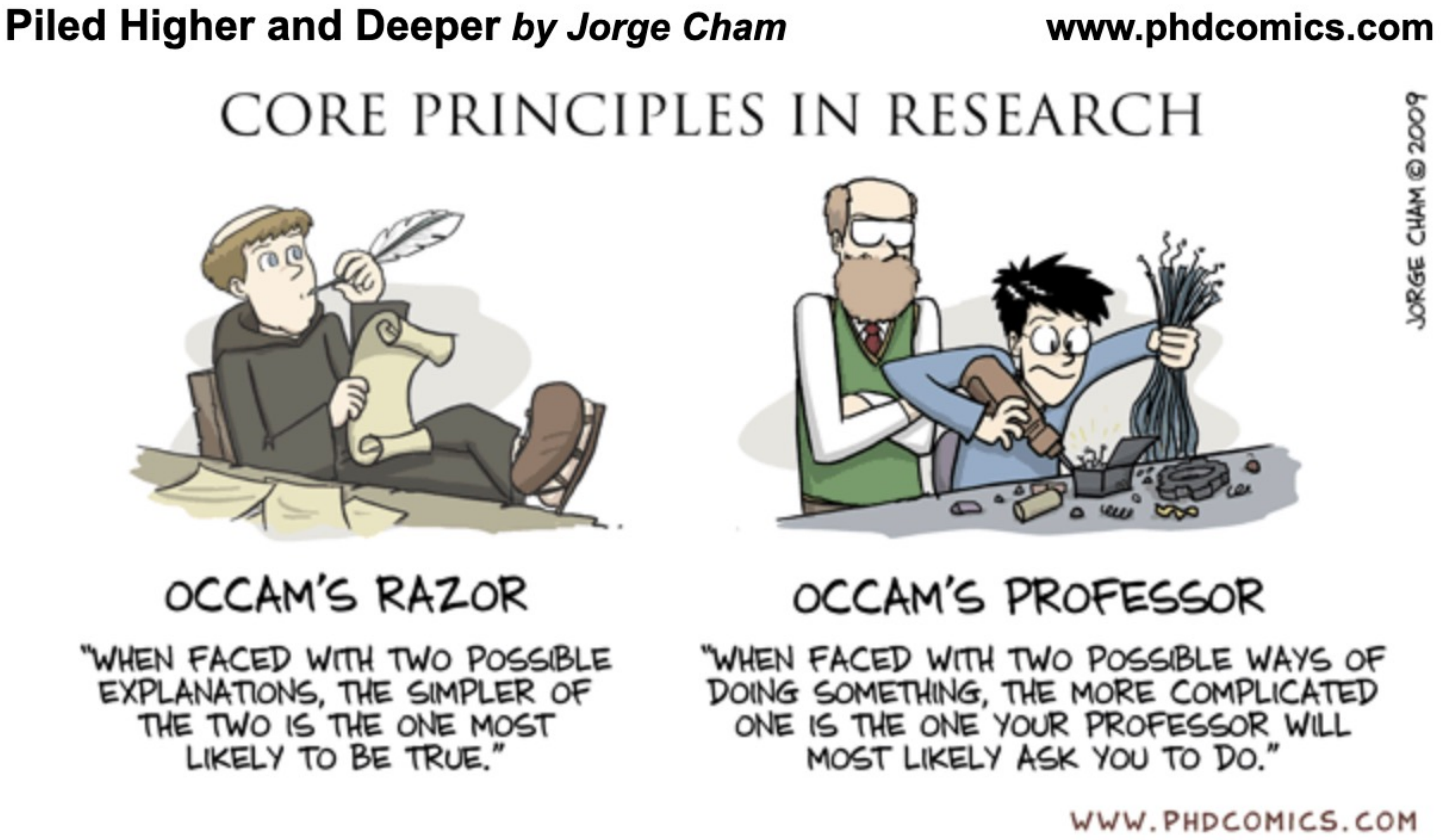




Model Selection: Which Tree is Better?

- 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

Model Selection: Occam's Razor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CORE PRINCIPLES IN RESEARCH
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OCCAM'S RAZOR
"WHEN FACED WITH TWO POSSIBLE EXPLANATIONS, THE SIMPLER OF THE TWO IS THE ONE MOST LIKELY TO BE TRUE."
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"WHEN FACED WITH TWO POSSIBLE WAYS OF DOING SOMETHING, THE MORE COMPLICATED ONE IS THE ONE YOUR PROFESSOR WILL MOST LIKELY ASK YOU TO DO."
WWW.PHDCOMICS.COM

title: "Core Principles" - originally published 10/12/2009

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Decision Trees: Pitfalls

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

Decision Trees v.s. KNN

Advantages of decision trees over k-NN

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

Decision Trees v.s. KNN

Advantages of k-NN over decision trees

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

Decision Trees in Healthcare

Fun Facts:

Decision trees is the most widely-adopted method in healthcare.

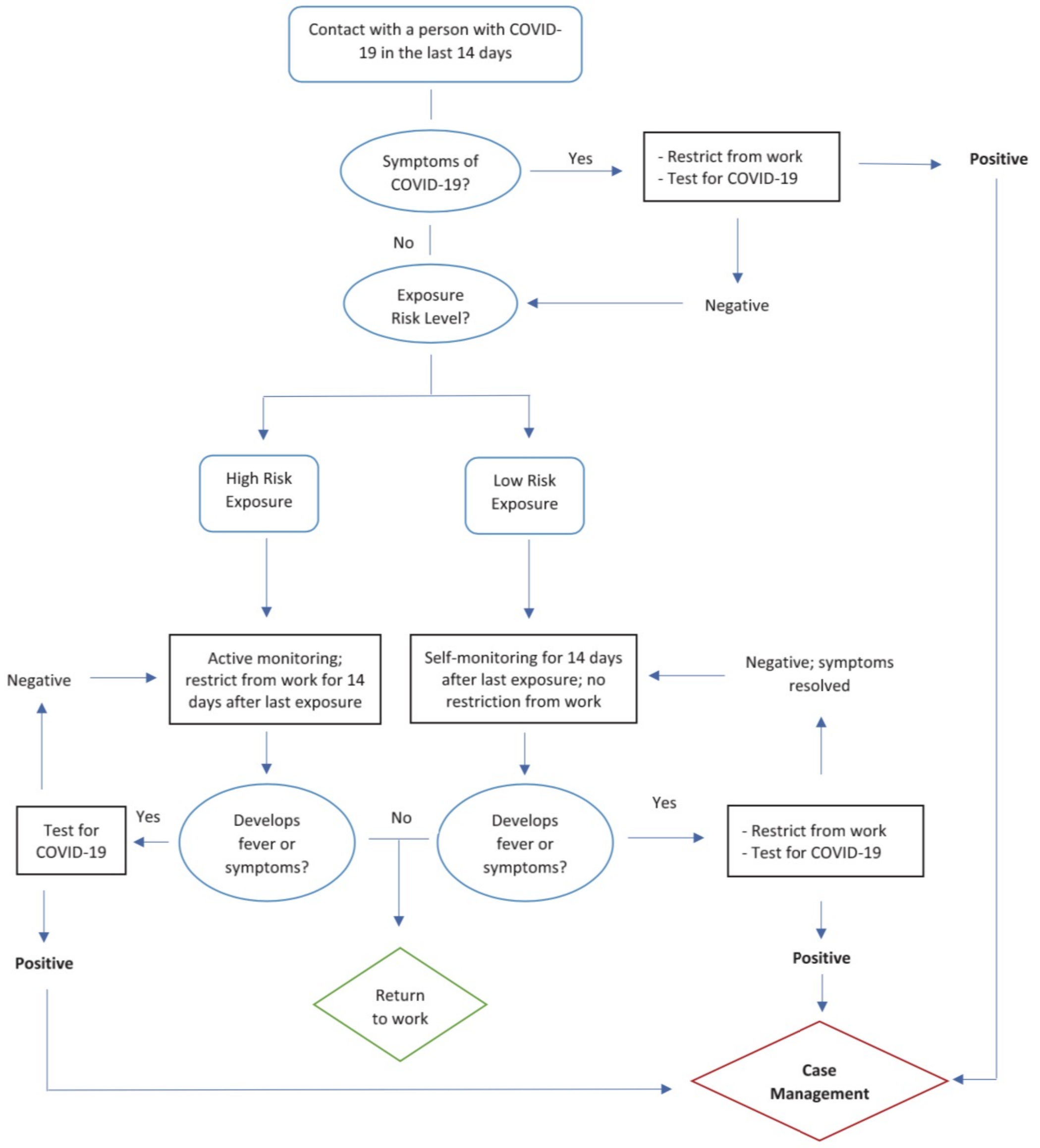
Class Discussion:

Name one application of decision trees in healthcare and discuss its pros and cons.

Decision Trees in COVID Management

Figure: Flowchart for management of HCWs with exposure to a person with COVID-19

Source: https://www.cdc.gov/



Contact with a person with COVID-19 in the last 14 days
Symptoms of COVID-19?
Yes
- Restrict from work
- Test for COVID-19
Positive
No
Negative
Exposure Risk Level?
High Risk Exposure
Low Risk Exposure
Active monitoring; restrict from work for 14 days after last exposure
Self-monitoring for 14 days after last exposure; no restriction from work
Negative
Negative; symptoms resolved
Test for COVID-19
Yes
Develops fever or symptoms?
No
Develops fever or symptoms?
Yes
- Restrict from work
- Test for COVID-19
Positive
Return to work
Positive
Case Management

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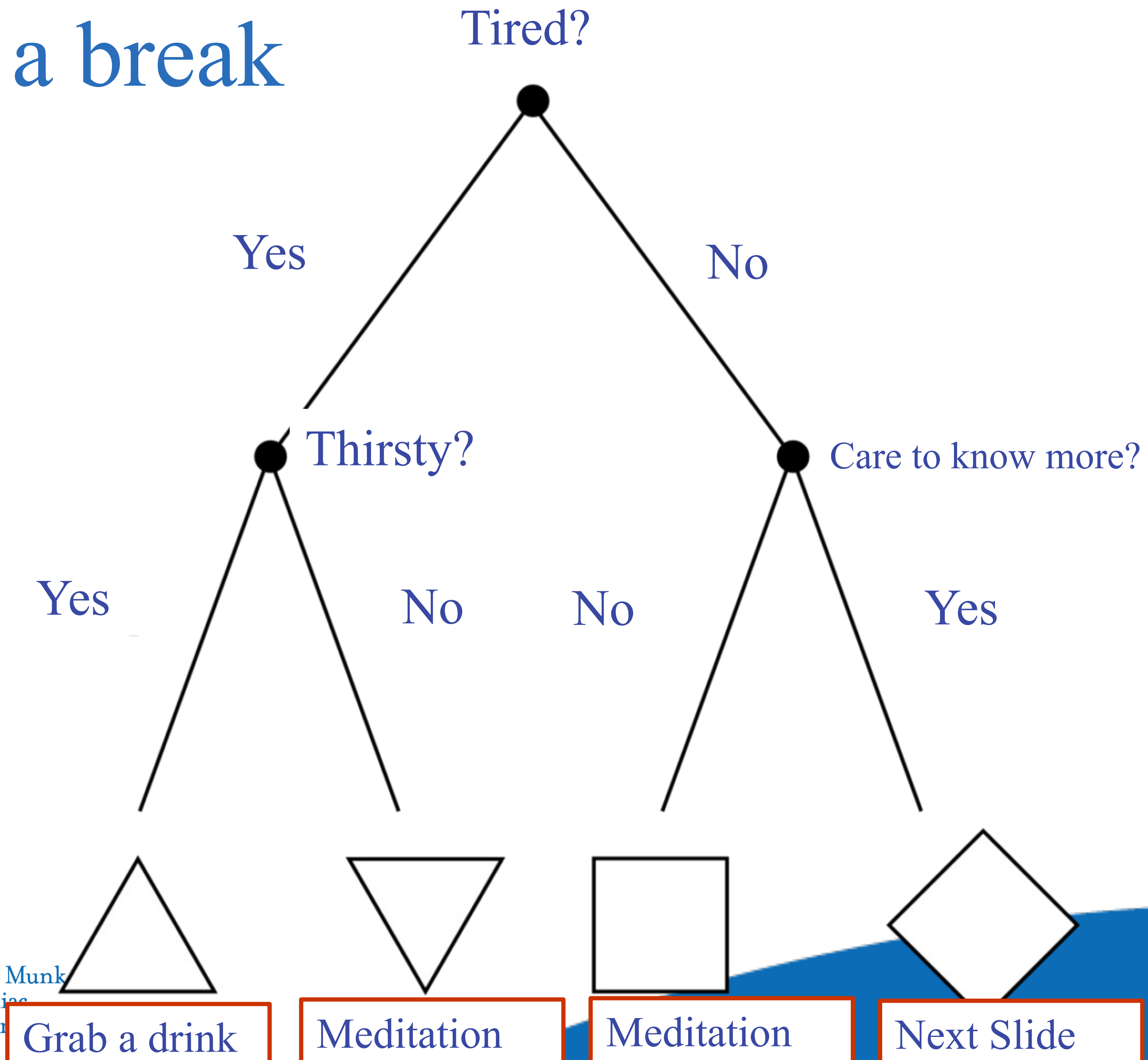
Decision Trees : Take-Home Messages

1. Decision Trees is simple and interpretable.

2. Decision Trees uses information gains to ***learn*** to split the trees.

3. Decision Trees tends to overfit

Take a break



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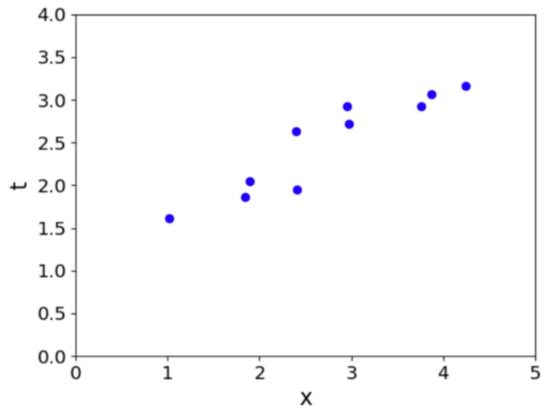
Linear Models

- So far, we have talked about *procedures* for learning.
  - KNN and decision trees.
- For the remainder of this course, we will take a more modular approach:
  - choose a model describing the relationships between variables of interest
  - define a loss function quantifying how bad the fit to the data is
  - choose a regularizer saying how much we prefer different candidate models (or explanations of data)
  - fit the model that minimizes the loss function and satisfy the constraint/penalty imposed by the regularizer, possibly using an optimization algorithm
- Mixing and matching these modular components gives us a lot of new ML methods.

Linear Models -- Problem Setup



Recall that in supervised learning:

- There is target $t \in \mathcal{T}$ (also called response, outcome, output, class)
- There are features $\mathbf{x} \in \mathcal{X}$ (also called inputs and covariates)
- Objective is to learn a function $f : \mathcal{X} \to \mathcal{T}$ such that

$$t \approx y = f(x)$$

based on some data $\mathcal{D} = \{(\mathbf{x}^{(i)}, t^{(i)}) \text{ for } i = 1, 2, ..., N\}$.

Linear Models -- Problem Setup

- Model: In linear regression, we use linear functions of the inputs $\mathbf{x} = (x_1, \ldots, x_D)$ to make predictions y of the target value t:

$$y = f(\mathbf{x}) = \sum_j w_j x_j + b$$

  - y is the prediction
  - $\mathbf{w}$ is the weights
  - b is the bias (or intercept) (do not confuse with the bias-variance tradeoff in the next lecture)
- $\mathbf{w}$ and b together are the parameters
- We hope that our prediction is close to the target: $y \approx t$.

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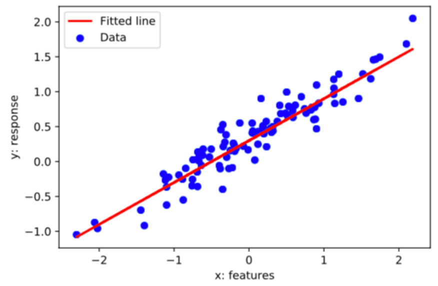
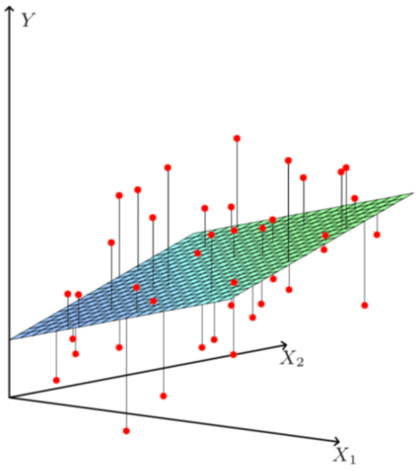
Linear Models -- Problem Setup



- If we have only 1 feature: $y = wx + b$ where $w, x, b \in \mathbb{R}$.
- y is linear in x.



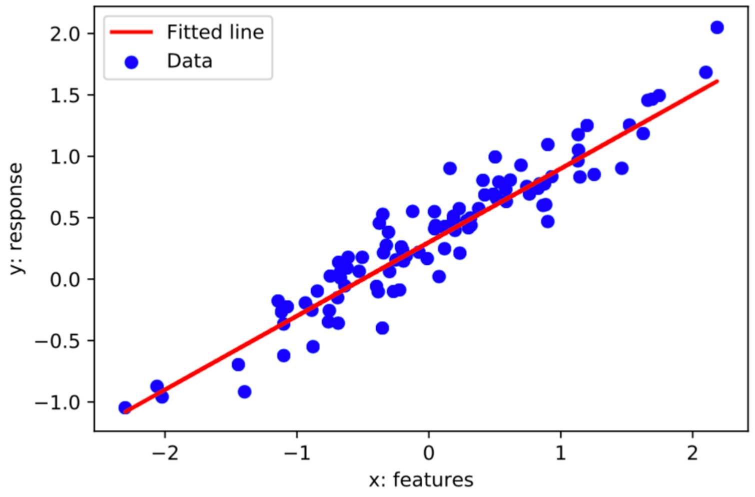
- If we have D features: $y = \mathbf{w}^\top \mathbf{x} + b$ where $\mathbf{w}, \mathbf{x} \in \mathbb{R}^D$, $b \in \mathbb{R}$
- y is linear in $\mathbf{x}$.

Relation between the prediction y and inputs $\mathbf{x}$ is linear in both cases.

Linear Models -- Problem Setup

We have a dataset $\mathcal{D} = \{(\mathbf{x}^{(i)}, t^{(i)}) \text{ for } i = 1, 2, ..., N\}$ where,

- $\mathbf{x}^{(i)} = (x_1^{(i)}, x_2^{(i)}, ..., x_D^{(i)})^\top \in \mathbb{R}^D$ are the inputs, e.g., age, height.
- $t^{(i)} \in \mathbb{R}$ is the target or response (e.g. income),
- predict $t^{(i)}$ with a linear function of $\mathbf{x}^{(i)}$:



- $t^{(i)} \approx y^{(i)} = \mathbf{w}^\top \mathbf{x}^{(i)} + b$
- Find the "best" line $(\mathbf{w}, b)$.
- $\underset{(\mathbf{w},b)}{\text{minimize}} \sum_{i=1}^{N} \mathcal{L}(y^{(i)}, t^{(i)})$

Linear Models -- Problem Setup

- How to quantify the quality of the fit to data?
- A loss function $\mathcal{L}(y, t)$ defines how bad it is if, for some example $\mathbf{x}$, the algorithm predicts y, but the target is actually t.
- Squared error loss function:

$$\mathcal{L}(y, t) = \tfrac{1}{2}(y - t)^2$$

- $y - t$ is the residual, and we want to make its magnitude small
- The $\frac{1}{2}$ factor is just to make the calculations convenient.
- Cost function: loss function averaged over all training examples

$$\begin{aligned}\mathcal{J}(\mathbf{w}, b) &= \frac{1}{2N}\sum_{i=1}^{N}\left(y^{(i)} - t^{(i)}\right)^2 \\ &= \frac{1}{2N}\sum_{i=1}^{N}\left(\mathbf{w}^\top \mathbf{x}^{(i)} + b - t^{(i)}\right)^2\end{aligned}$$

- The terminology is not universal. Some might call "loss" *pointwise loss* and the "cost function" the *empirical loss* or *average loss*.

Linear Models -- Vectorization

- We can organize all the training examples into a design matrix $\mathbf{X}$ with one row per training example, and all the targets into the target vector $\mathbf{t}$.

$$\mathbf{X} = \begin{pmatrix} \mathbf{x}^{(1)\top} \\ \mathbf{x}^{(2)\top} \\ \mathbf{x}^{(3)\top} \end{pmatrix} = \begin{array}{ccccc} & \text{one feature across all training examples} & & & \\ 8 & 0 & 3 & 0 & \\ 6 & -1 & 5 & 3 & \text{one training example (vector)} \\ 2 & 5 & -2 & 8 & \end{array}$$

- Computing the predictions for the whole dataset:

$$\mathbf{X}\mathbf{w} + b\mathbf{1} = \begin{pmatrix} \mathbf{w}^T\mathbf{x}^{(1)} + b \\ \vdots \\ \mathbf{w}^T\mathbf{x}^{(N)} + b \end{pmatrix} = \begin{pmatrix} y^{(1)} \\ \vdots \\ y^{(N)} \end{pmatrix} = \mathbf{y}$$

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Linear Models -- Vectorization

- Computing the squared error cost across the whole dataset:

$$\mathbf{y} = \mathbf{X}\mathbf{w} + b\mathbf{1}$$
$$\mathcal{J} = \frac{1}{2N}\|\mathbf{y} - \mathbf{t}\|^2$$

- Note that sometimes we may use $\mathcal{J} = \frac{1}{2}\|\mathbf{y} - \mathbf{t}\|^2$, without normalizer. That would correspond to the sum of losses, and not the average loss. The minimizer does not depend on N.
- We can also add a column of 1s to the design matrix, combine the bias and the weights, and conveniently write

$$\mathbf{X} = \begin{bmatrix} 1 & [\mathbf{x}^{(1)}]^\top \\ 1 & [\mathbf{x}^{(2)}]^\top \\ 1 & \vdots \end{bmatrix} \in \mathbb{R}^{N \times D+1} \quad \text{and} \quad \mathbf{w} = \begin{bmatrix} b \\ w_1 \\ w_2 \\ \vdots \end{bmatrix} \in \mathbb{R}^{D+1}$$

Then, our predictions reduce to $\mathbf{y} = \mathbf{X}\mathbf{w}$.

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Linear Models -- Vectorization

- Computing the prediction using a for loop:

```
y = b
for j in range(M):
    y += w[j] * x[j]
```

- For-loops in Python are slow, so we vectorize algorithms by expressing them in terms of vectors and matrices.

$$\mathbf{w} = (w_1, \ldots, w_D)^T \qquad \mathbf{x} = (x_1, \ldots, x_D)$$

$$y = \mathbf{w}^T \mathbf{x} + b$$

- This is simpler and much faster:

```
y = np.dot(w, x) + b
```

Linear Models -- Optimization

- We defined a cost function. This is what we would like to minimize.
- Recall from your calculus class: minimum of a smooth function (if it exists) occurs at a critical point, i.e., point where the derivative is zero.
- Multivariate generalization: set the partial derivatives to zero (or equivalently the gradient).
- We would like to find a point where the gradient is (close to) zero. How can we do it?
    - Sometimes it is possible to directly find the parameters that make the gradient zero in a closed-form. We call this the direct solution.
    - We may also use optimization techniques that iteratively get us closer to the solution. We will get back to this soon.

Optimization : What to do if we are first-year undergrad

- Partial derivatives: derivatives of a multivariate function with respect to one of its arguments.

$$\frac{\partial}{\partial x_1} f(x_1, x_2) = \lim_{h \to 0} \frac{f(x_1 + h, x_2) - f(x_1, x_2)}{h}$$

- To compute, take the single variable derivatives, pretending the other arguments are constant.
- Example: partial derivatives of the prediction y

$$\begin{aligned}\frac{\partial y}{\partial w_j} &= \frac{\partial}{\partial w_j}\left[\sum_{j'} w_{j'} x_{j'} + b\right] \\ &= x_j \\ \frac{\partial y}{\partial b} &= \frac{\partial}{\partial b}\left[\sum_{j'} w_{j'} x_{j'} + b\right] \\ &= 1\end{aligned}$$

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Optimization : What to do if we are first-year undergrad

- Chain rule for derivatives:

$$
\begin{aligned}
\frac{\partial \mathcal{L}}{\partial w_j} &= \frac{\mathrm{d}\mathcal{L}}{\mathrm{d}y}\frac{\partial y}{\partial w_j} \\
&= \frac{\mathrm{d}}{\mathrm{d}y}\left[\frac{1}{2}(y-t)^2\right]\cdot x_j \\
&= (y-t)x_j \\
\frac{\partial \mathcal{L}}{\partial b} &= y-t
\end{aligned}
$$

- Cost derivatives (average over data points):

$$
\begin{aligned}
\frac{\partial \mathcal{J}}{\partial w_j} &= \frac{1}{N}\sum_{i=1}^{N}(y^{(i)}-t^{(i)})\,x_j^{(i)} \\
\frac{\partial \mathcal{J}}{\partial b} &= \frac{1}{N}\sum_{i=1}^{N}y^{(i)}-t^{(i)}
\end{aligned}
$$

Optimization : What to do if we are first-year undergrad

- The minimum must occur at a point where the partial derivatives are zero, i.e.,

$$\frac{\partial \mathcal{J}}{\partial w_j} = 0 \quad (\forall j), \qquad \frac{\partial \mathcal{J}}{\partial b} = 0.$$

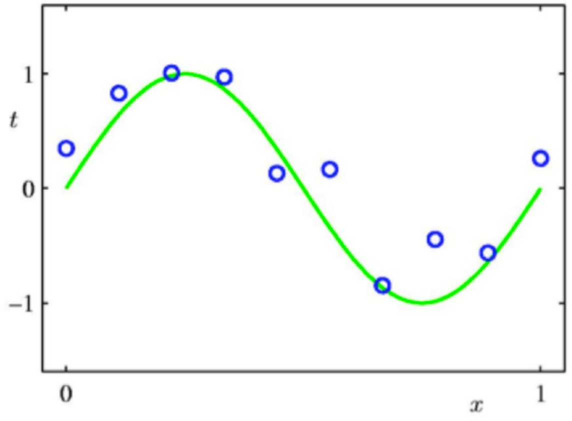
- If $\partial \mathcal{J} / \partial w_j \neq 0$, you could reduce the cost by changing w_j.
- This turns out to give a system of linear equations, which we can solve efficiently. **Full derivation in the preliminaries.pdf.**
- Optimal weights:

$$\mathbf{w}^{\mathrm{LS}} = (\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T \mathbf{t}$$

- Linear regression is one of only a handful of models in this course that permit direct solution.

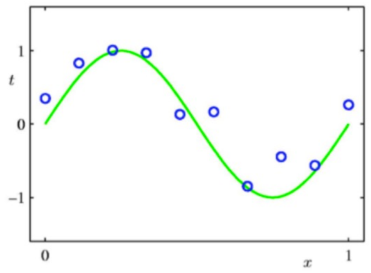
Linear Models – Feature Mapping

- The relation between the input and output may not be linear.



- We can still use linear regression by mapping the input feature to another space using feature mapping (or basis expansion) $\boldsymbol{\psi}(\mathbf{x}) : \mathbb{R}^D \to \mathbb{R}^d$ and treat the mapped feature (in $\mathbb{R}^d$) as the input of a linear regression procedure.
- Let us see how it works when $\mathbf{x} \in \mathbb{R}$ and we use polynomial feature mapping.

Linear Models – Feature Mapping



Fit the data using a degree-M polynomial function of the form:

$$y = w_0 + w_1 x + w_2 x^2 + \ldots + w_M x^M = \sum_{i=0}^{M} w_i x^i$$

- Here the feature mapping is $\boldsymbol{\psi}(x) = [1, x, x^2, \ldots]^\top$.
- We can still use least squares to find $\mathbf{w}$ since $y = \boldsymbol{\psi}(x)^\top \mathbf{w}$ is linear in $w_0, w_1, \ldots$.
- In general, $\boldsymbol{\psi}$ can be any function. Another example: $\boldsymbol{\psi} = [1, \sin(2\pi x), \cos(2\pi x), \sin(4\pi x), \cos(4\pi x), \sin(6\pi x), \cos(6\pi x), \cdots]^\top$.

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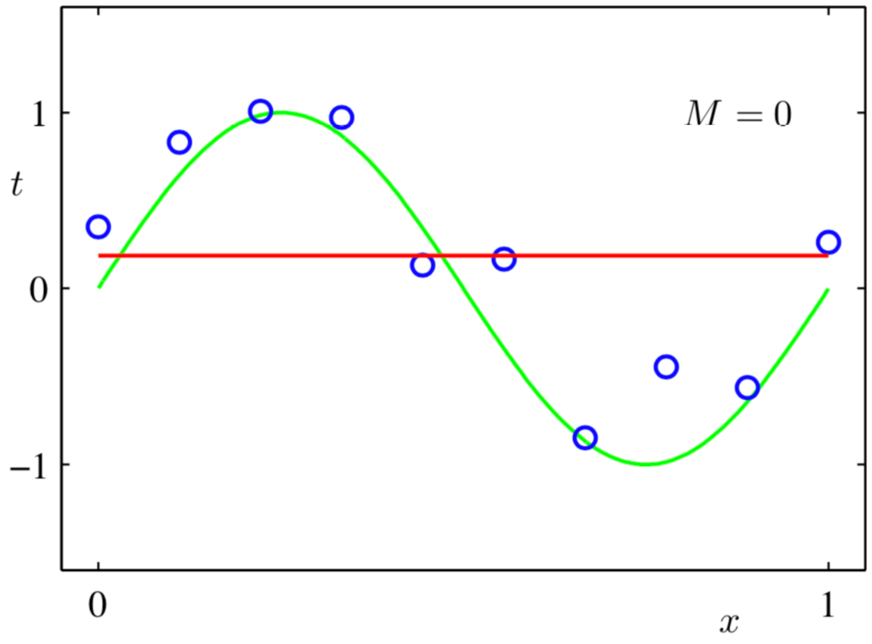
Linear Models – Feature Mapping

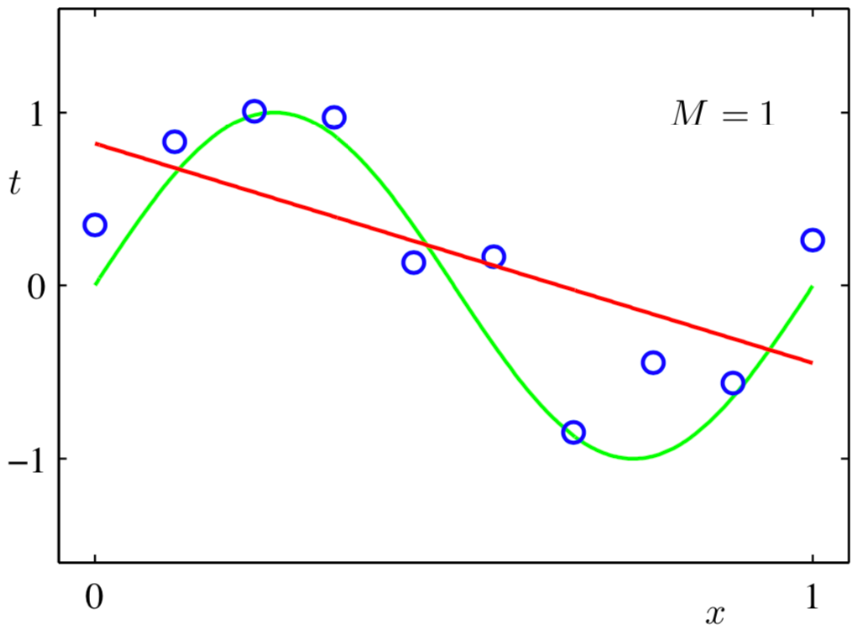
$$y = w_0$$



-Pattern Recognition and Machine Learning, Christopher Bishop.

Linear Models – Feature Mapping

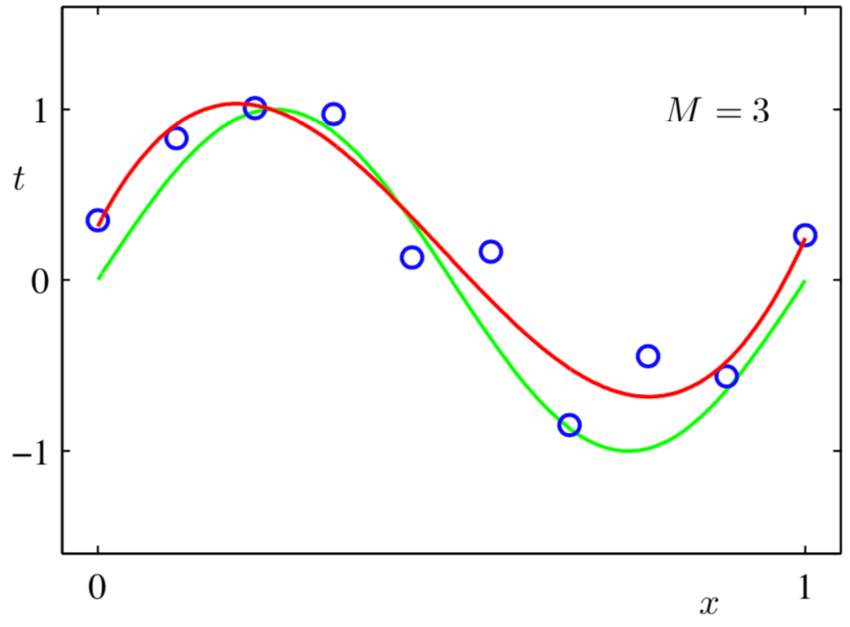
$$y = w_0 + w_1 x$$



-Pattern Recognition and Machine Learning, Christopher Bishop.

Linear Models – Feature Mapping

$$y = w_0 + w_1 x + w_2 x^2 + w_3 x^3$$



-Pattern Recognition and Machine Learning, Christopher Bishop.

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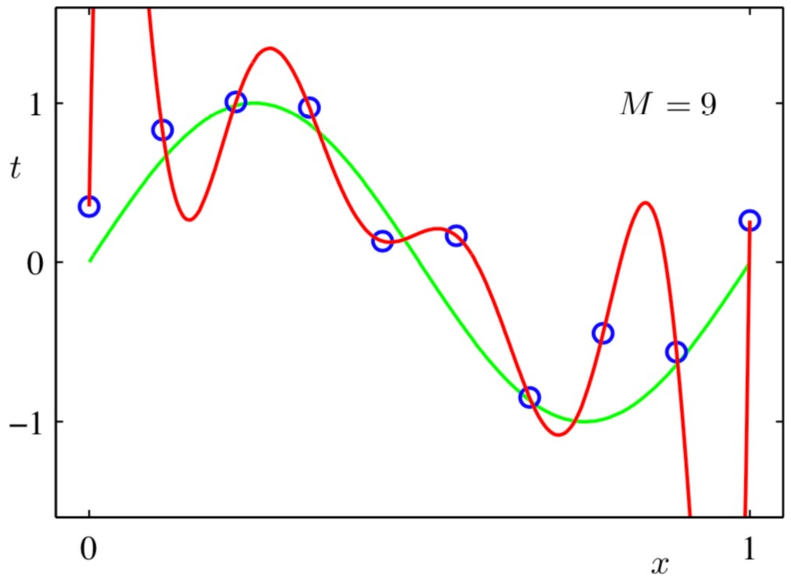
Linear Models – Feature Mapping

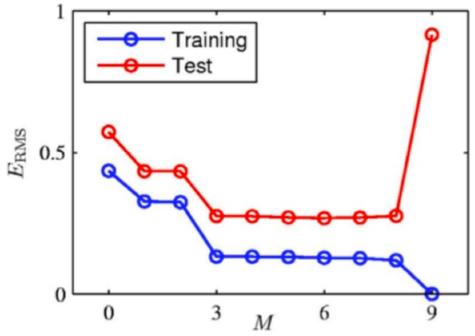
$$y = w_0 + w_1 x + w_2 x^2 + w_3 x^3 + \ldots + w_9 x^9$$

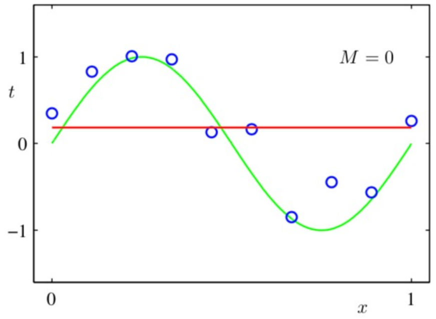


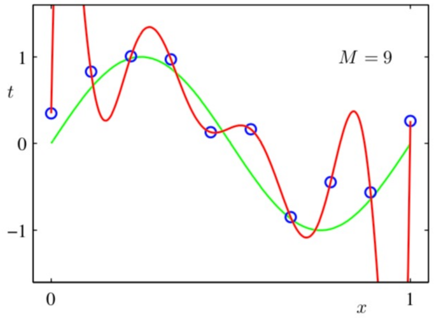
-Pattern Recognition and Machine Learning, Christopher Bishop.

Linear Models – Model Selection

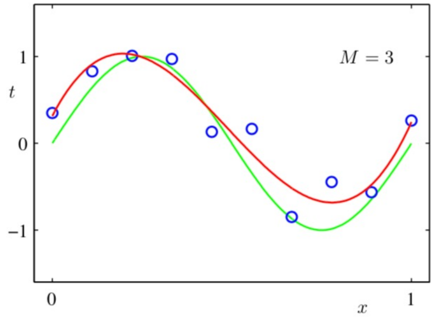
Underfitting (M=0): model is too simple — does not fit the data.
Overfitting (M=9): model is too complex — fits perfectly.





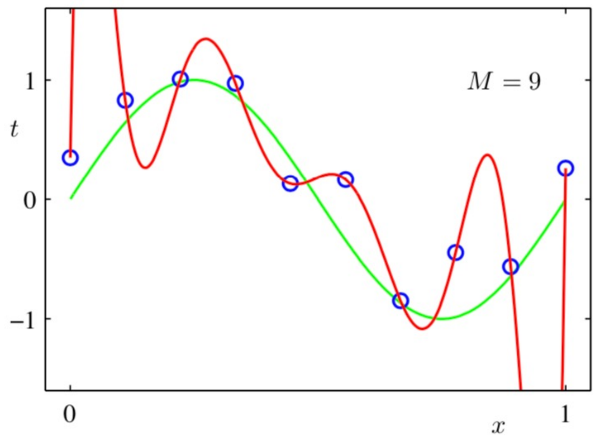


Good model (M=3): Achieves small test error (generalizes well).



Linear Models – Model Selection

	$M=0$	$M=1$	$M=3$	$M=9$
$w_0^\star$	0.19	0.82	0.31	0.35
$w_1^\star$		-1.27	7.99	232.37
$w_2^\star$			-25.43	-5321.83
$w_3^\star$			17.37	48568.31
$w_4^\star$				-231639.30
$w_5^\star$				640042.26
$w_6^\star$				-1061800.52
$w_7^\star$				1042400.18
$w_8^\star$				-557682.99
$w_9^\star$				125201.43



- As M increases, the magnitude of coefficients gets larger.
- For $M=9$, the coefficients have become finely tuned to the data.
- Between data points, the function exhibits large oscillations.

Linear Models – Model Selection

- The degree of the polynomial M controls the complexity of the model.
- The value of M is a hyperparameter for polynomial expansion, just like k in KNN. We can tune it using a validation set.
- Restricting the number of parameters of a model (M here) is a crude approach to control the complexity of the model.
- A better solution: keep the number of parameters of the model large, but enforce "simpler" solutions within the same space of parameters.
- This is done through regularization or penalization.
    - Regularizer (or penalty): a function that quantifies how much we prefer one hypothesis vs. another
- Q: How?!

Linear Models -- Regularization

- We can encourage the weights to be small by choosing as our regularizer the ℓ_2 (or L^2) penalty.

$$\mathcal{R}(\mathbf{w}) = \tfrac{1}{2}\|\mathbf{w}\|_2^2 = \frac{1}{2}\sum_j w_j^2.$$

  - Note: To be precise, we are regularizing the *squared* ℓ_2 norm.

- The regularized cost function makes a tradeoff between fit to the data and the norm of the weights:

$$\mathcal{J}_{\text{reg}}(\mathbf{w}) = \mathcal{J}(\mathbf{w}) + \lambda\mathcal{R}(\mathbf{w}) = \mathcal{J}(\mathbf{w}) + \frac{\lambda}{2}\sum_j w_j^2.$$

- The basic idea is that "simpler" functions have smaller ℓ_2-norm of their weights $\mathbf{w}$, and we prefer them to functions with larger ℓ_2-norms.
- If you fit training data poorly, $\mathcal{J}$ is large. If your optimal weights have high values, $\mathcal{R}$ is large.
- Large λ penalizes weight values more.
- Here, λ is a hyperparameter that we can tune with a validation set.

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Linear Models -- Regularization

For the least squares problem, we have $\mathcal{J}(\mathbf{w}) = \frac{1}{2N}\|\mathbf{X}\mathbf{w} - \mathbf{t}\|^2$.

- When $\lambda > 0$ (with regularization), regularized cost gives

$$\begin{aligned} \mathbf{w}_{\lambda}^{\text{Ridge}} = \underset{\mathbf{w}}{\operatorname{argmin}}\, \mathcal{J}_{\text{reg}}(\mathbf{w}) &= \underset{\mathbf{w}}{\operatorname{argmin}}\, \frac{1}{2N}\|\mathbf{X}\mathbf{w} - \mathbf{t}\|_2^2 + \frac{\lambda}{2}\|\mathbf{w}\|_2^2 \\ &= (\mathbf{X}^T\mathbf{X} + \lambda N\mathbf{I})^{-1}\mathbf{X}^T\mathbf{t} \end{aligned}$$

- The case $\lambda = 0$ (no regularization) reduces to least squares solution!
- Q: What happens when $\lambda \to \infty$?
- Note that it is also common to formulate this problem as $\operatorname{argmin}_{\mathbf{w}} \|\mathbf{X}\mathbf{w} - \mathbf{t}\|_2^2 + \frac{\lambda}{2}\|\mathbf{w}\|_2^2$ in which case the solution is $\mathbf{w}_{\lambda}^{\text{Ridge}} = (\mathbf{X}^T\mathbf{X} + \lambda\mathbf{I})^{-1}\mathbf{X}^T\mathbf{t}$.

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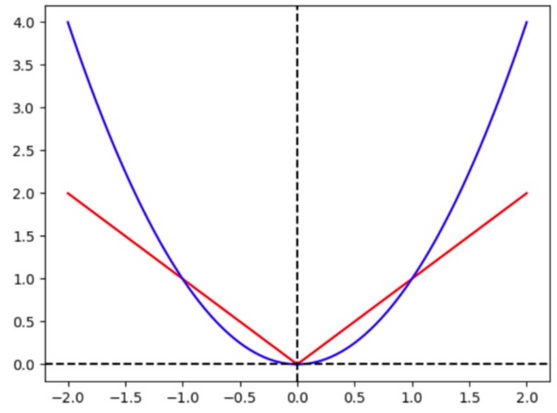
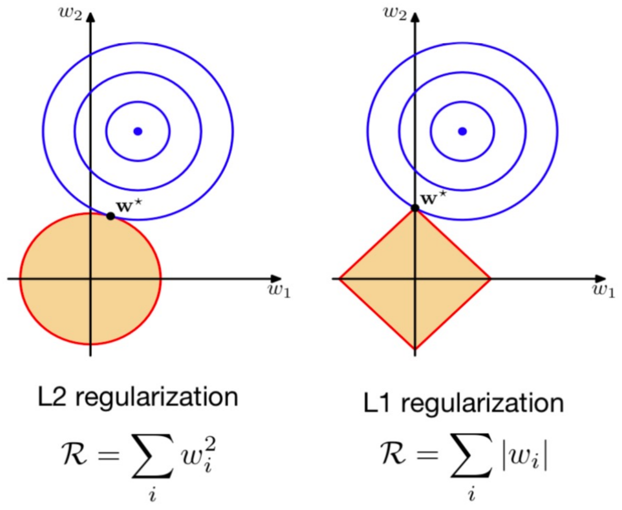
Linear Models -- Regularization

- The ℓ_1 norm, or sum of absolute values, is another regularizer that encourages weights to be exactly zero. (How can you tell?)
- We can design regularizers based on whatever property we'd like to encourage.





— Bishop, *Pattern Recognition and Machine Learning*

Optimization :
A more generalized approach

- Now let's see a second way to minimize the cost function which is more broadly applicable: gradient descent.
- Gradient descent is an iterative algorithm, which means we apply an update repeatedly until some criterion is met.
- We initialize the weights to something reasonable (e.g. all zeros) and repeatedly adjust them in the direction of steepest descent.

Gradient Descent

- Observe:
  - if $\partial \mathcal{J}/\partial w_j > 0$, then increasing w_j increases $\mathcal{J}$.
  - if $\partial \mathcal{J}/\partial w_j < 0$, then increasing w_j decreases $\mathcal{J}$.
- The following update decreases the cost function:

$$\begin{aligned} w_j &\leftarrow w_j - \alpha \frac{\partial \mathcal{J}}{\partial w_j} \\ &= w_j - \frac{\alpha}{N} \sum_{i=1}^{N} (y^{(i)} - t^{(i)})\, x_j^{(i)} \end{aligned}$$

- α is a learning rate. The larger it is, the faster $\mathbf{w}$ changes.
  - We'll see later how to tune the learning rate, but values are typically small, e.g. 0.01 or 0.0001

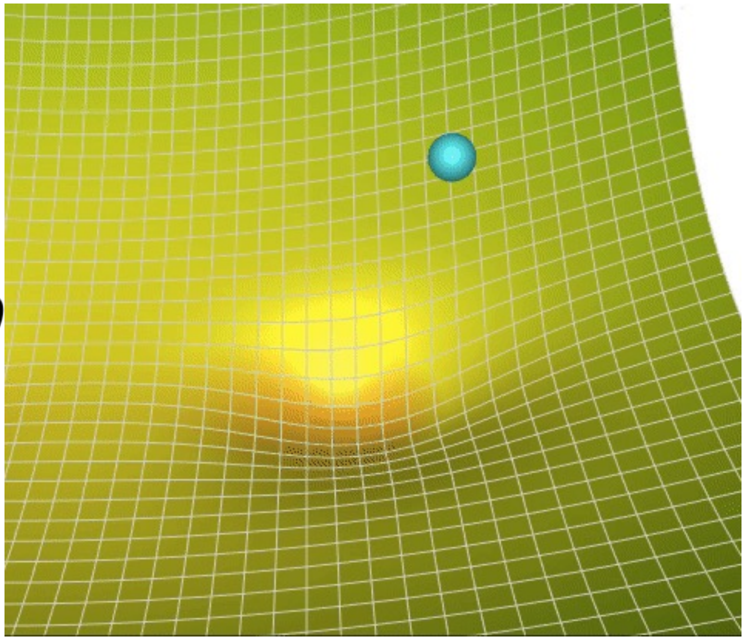
Gradient Descent

- Goal: we want to minimize a specific objective function (cost or loss):

$$\mathcal{J}(\boldsymbol{\theta}) = \frac{1}{N}\sum_{i=1}^{N} \mathcal{J}^{(i)}(\boldsymbol{\theta}) = \frac{1}{N}\sum_{i=1}^{N} \mathcal{L}(y(\mathbf{x}^{(i)}, \boldsymbol{\theta}), t^{(i)}).$$

- Step 1: Calculate Gradient (by linearity)

$$\nabla \mathcal{J}(\boldsymbol{\theta}) = \frac{1}{N}\sum_{i=1}^{N} \nabla \mathcal{J}^{(i)}(\boldsymbol{\theta}$$



- Step 2: Update the parameters:

$$\boldsymbol{\theta} = \boldsymbol{\theta} - \alpha \nabla \mathcal{J}(\boldsymbol{\theta})$$

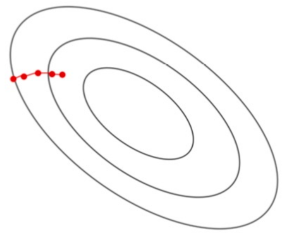
Source: https://towardsdatascience.com/a-visual-explanation-of-gradient-descent-methods-momentum-adagrad-rmsprop-adam-f898b102325c

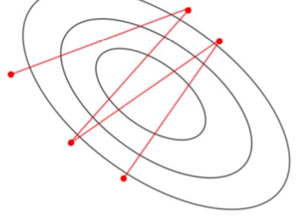
Gradient Descent

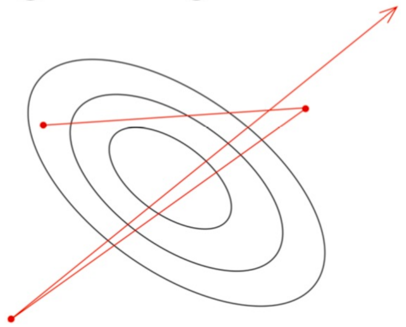
- Even for linear regression, where there is a direct solution, we sometimes need to use GD.
- Why gradient descent, if we can find the optimum directly?
  - GD can be applied to a much broader set of models
  - GD can be easier to implement than direct solutions
  - For regression in high-dimensional spaces, GD is more efficient than direct solution
    - Linear regression solution: $(\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{t}$
    - matrix inversion is an $\mathcal{O}(D^3)$ algorithm
    - each GD update costs $O(ND)$
    - Huge difference if $D \gg 1$

Gradient Descent

- In gradient descent, the learning rate α is a hyperparameter we need to tune. Here are some things that can go wrong:


α too small: slow progress

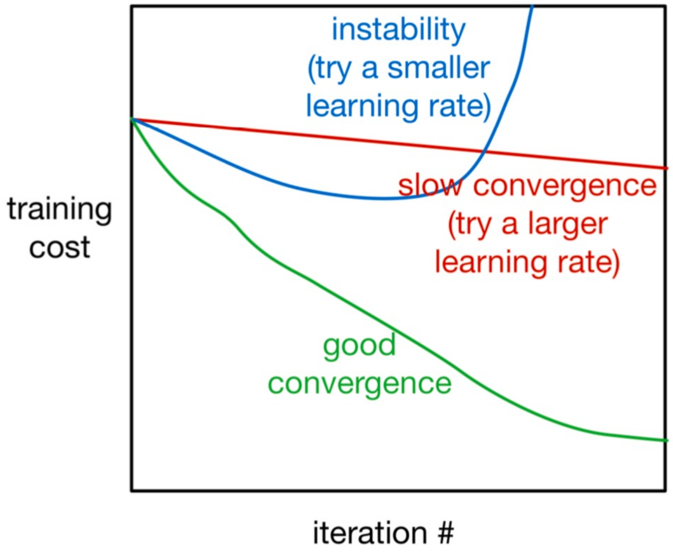

α too large: oscillations


α much too large: instability

- Good values are typically between 0.001 and 0.1. You should do a grid search if you want good performance (i.e. try $0.1, 0.03, 0.01, \ldots$).

Gradient Descent

- To diagnose optimization problems, it's useful to look at training curves: plot the training cost as a function of iteration.



- Warning: it's very hard to tell from the training curves whether an optimizer has converged. They can reveal major problems, but they can't guarantee convergence.

Linear Models

Why vectorize?

- The equations, and the code, will be simpler and more readable. Gets rid of dummy variables/indices!
- Vectorized code is much faster
  - Cut down on Python interpreter overhead
  - Use highly optimized linear algebra libraries
  - Matrix multiplication is very fast on a Graphics Processing Unit (GPU)

A general theme

Linear regression exemplifies recurring themes of this course:

- choose a model and a loss function
- formulate an optimization problem
- solve the minimization problem using one of two strategies
  - direct solution (set derivatives to zero)
  - gradient descent (see appendix)
- vectorize the algorithm, i.e. represent in terms of linear algebra
- make a linear model more powerful using features
- improve the generalization by adding a regularizer

Linear Model: Take-Home Messages

1. Linear Model is simple and interpretable.

2. Regularization on weights can help with overfitting.

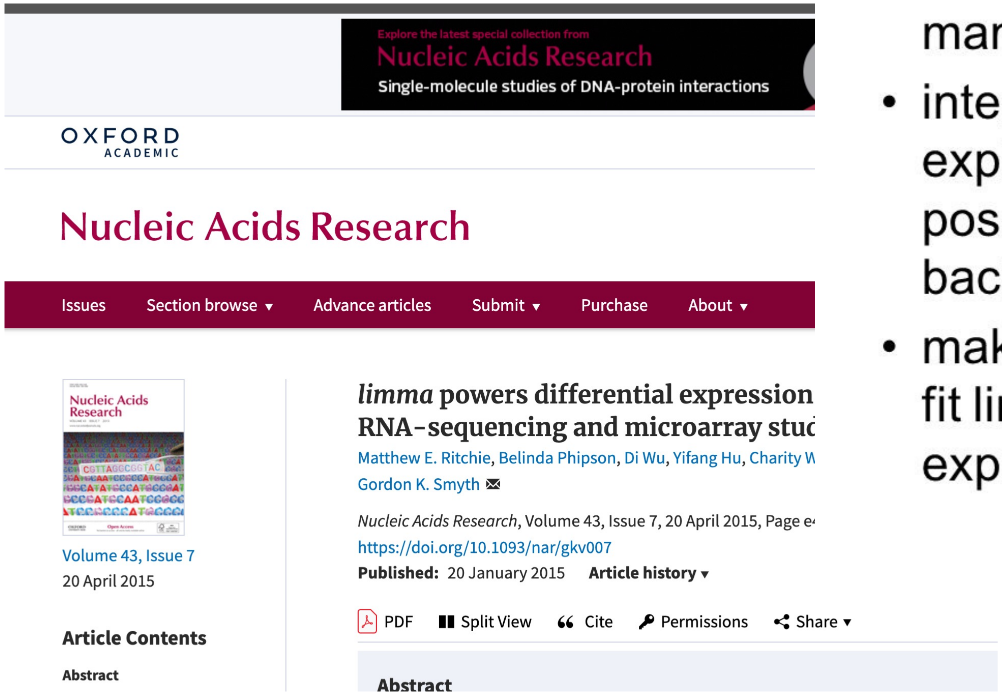
3. Gradient descent is a general way to solve optimization problems in machine learning.

4. Linear model may fail when linearity assumption does not hold.

Linear Models in Medicine

LIMMA: Linear models for microarray data

Nearly 20K citations!



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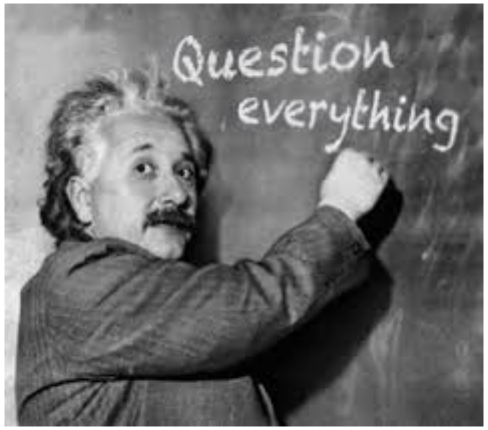
Article Contents

Abstract

Abstract

My experience

- limma has excellent documentation and many examples
- integration with preprocessing and exploratory data analysis makes it possible to test different options for background subtraction and normalization
- makes it possible for a non-statistician to fit linear models and find differentially expressed genes



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