Decision Trees

Dan Roth
danroth@seas.upenn.edu | http://www.cis.upenn.edu/~danroth/ | 461C, 3401 Walnut

Slides were created by Dan Roth (for CIS519/419 at Penn or CS446 at UIUC),
Some slides were taken with approval from other authors who have made their ML slides available.

Penn Engineering

Administration (9/21/20)

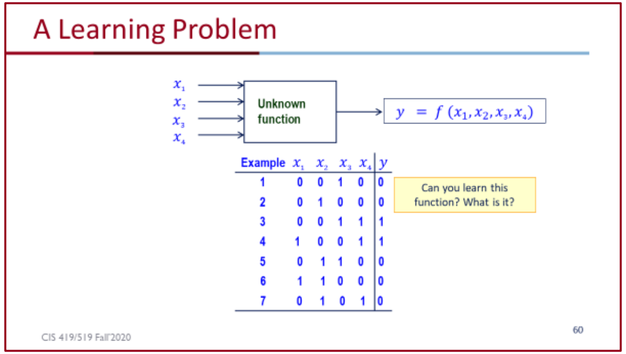
Are we recording? YES!

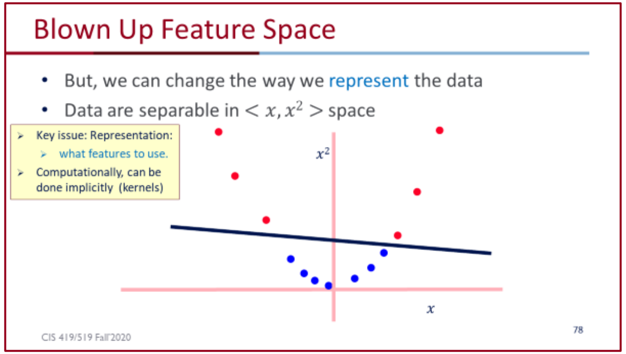
Available on the web site

- Quiz1
  - Statistics
  - We already got some positive feedback – the more feedback, the better.
- Remember that all the lectures are available on the website before the class
  - Go over it and be prepared
- HW 1 will be released today
  - I will discuss it on Wednesday, once you had a chance to read and think about it
  - You will see some new material there; for example, regarding procedures for evaluating classifiers and statistical significance. This is intentional. The material should be self explanatory.
  - Start working on it now. Don't wait until the last day (or two) since it could take a lot of your time
- Go to the recitations and office hours
- Questions?
  - Please ask/comment during class.
  - Give us feedback

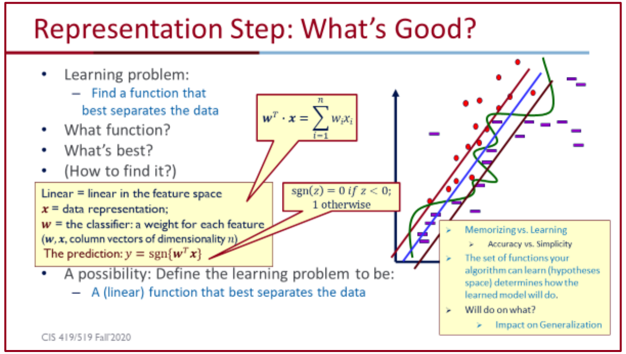
Introduction – Summary

- The importance of a hypothesis space
  - The need to make some assumptions of the function we are trying to learn





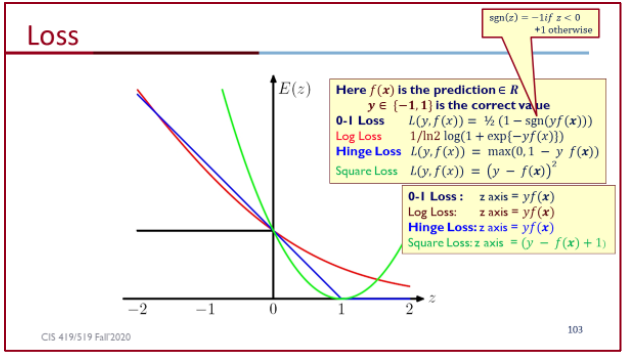
- Expressivity of functions and feature spaces

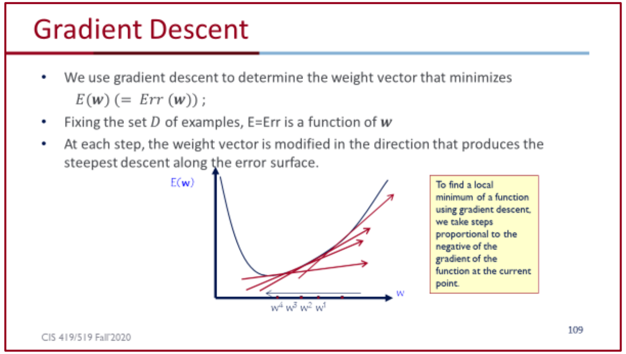


- And Linear functions

Introduction – Summary (2)

- Loss functions
  - They drive the search for a good hypothesis





- How to search?
  - Via gradient Descent

GD: averaging the gradient of the loss over the complete training set.

$$\Delta w_i = R \sum_{d \in D} (t_d - O_d) x_{id}$$

- Algorithms: GD and SGD
  - A sequence of weight vectors (hypotheses) from an initial guess to the final learned function.

SGD: update the weight vector based on a single example (or a small batch)

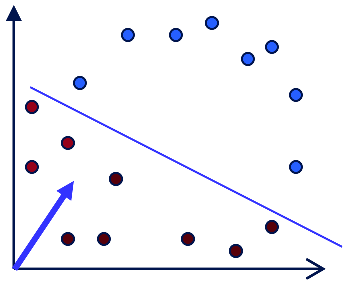
$$\Delta w_i = R (t_d - O_d) x_{id}$$

Questions? (No need to say "no"; just ask if you have any)

Start the presentation to see live content. For screen share software, share the entire screen. Get help at **pollev.com/app**

Introduction - Summary

- We introduced the technical part of the class by giving two (very important) examples for learning approaches to linear discrimination.
- There are many other solutions.
- Question 1: Our solution learns a linear function; in principle, the target function may not be linear, and this will have implications on the performance of our learned hypothesis.
  - **Can we learn a function that is more flexible in terms of what it does with the feature space?**



- Question 2: Do we understand what we learn (the interpretability of the model)?
- Question 3: Can we say something about the quality of what we learn (sample complexity, time complexity; quality)

Decision Trees

- Earlier, we decoupled the generation of the feature space from the learning.
- Argued that we can map the given examples into another space, in which the target functions are linearly separable.

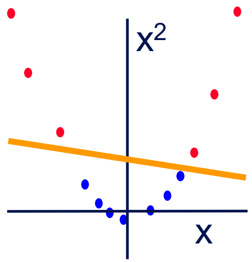
- Do we always want to do it?
- How do we determine what are good mappings?

Think about the Badges problem (vowel)

- The study of decision trees may shed some light on this.
- Learning is done directly from the given data representation.
- The algorithm ``transforms" the data itself.

What's the best learning algorithm?

- Some would argue: Boosted Decision Trees
  - Interpretation of the final model might also play a role



This Lecture

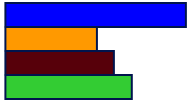
- Decision trees for (binary) classification
  - Non-linear classifiers
- Learning decision trees (ID3 algorithm)
  - Greedy heuristic (based on information gain)
    Originally developed for discrete features
  - Some extensions to the basic algorithm
- Overfitting
  - Some experimental issues

Introduction of Decision trees

Representing Data

- Think about a large table, N attributes, and assume you want to know something about the people represented as entries in this table.
- E.g. reads a lot of books or not;
- Simplest way: **Histogram** on the first attribute – reads

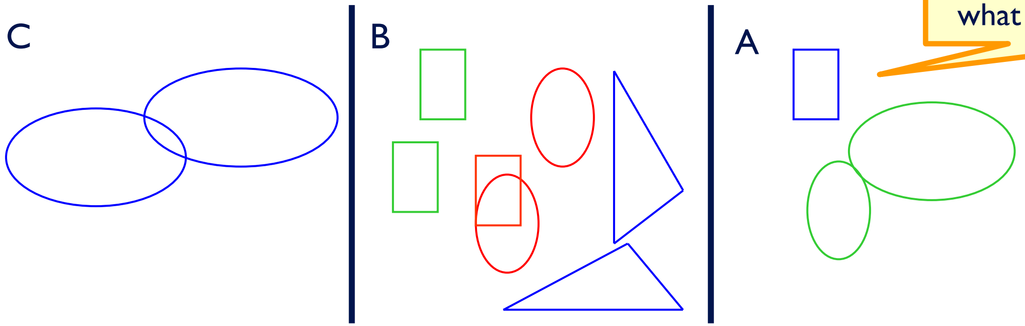
- Then, **histogram** on 1st and 2nd: (reads (0/1) & gender (0/1): 00, 01, 10, 11)



- But, what if the # of attributes is larger: N=16
- How large are the 1-d histograms (contingency tables) ? 16 numbers
- How large are the 2-d histograms? 16-choose-2 (all pairs) = 120 numbers
- How many 3-d tables? 560 numbers
- With 100 attributes, the 3-d tables need 161,700 numbers
- We need to figure out a way to represent data in a better way;
  - In part, this depends on identifying the important attributes, since we want to look at these first.
  - Information theory has something to say about it – we will use it to better represent the data.

Decision Trees

- A hierarchical data structure that represents data by implementing a divide and conquer strategy
  - Can be used as a non-parametric classification and regression method (real numbers associated with each example, rather than a categorical label)
- Process:
  - Given a collection of examples, learn a decision tree that represents it.
  - Use this representation to classify new examples



Given this collection of shapes, what shapes are type A, B, and C?

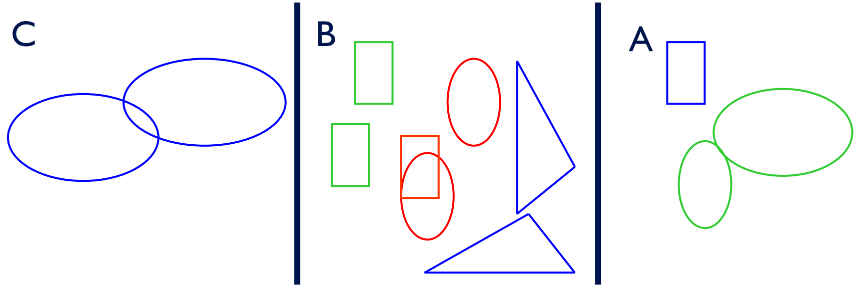
The Representation

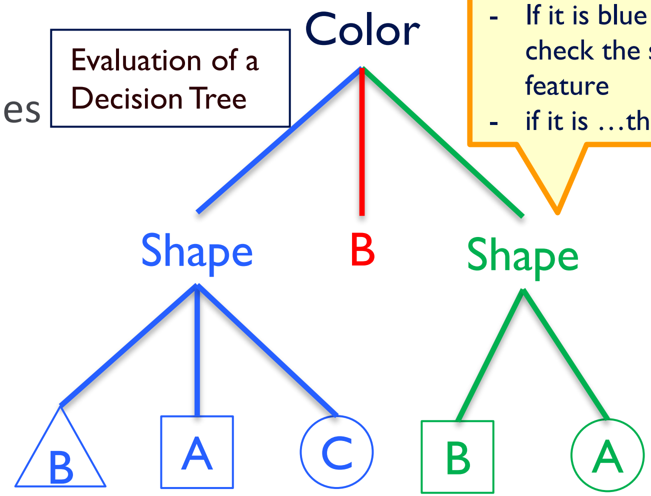
- Decision Trees are classifiers for instances represented as feature vectors
  - color={red, blue, green} ; shape={circle, triangle, rectangle} ; label= {A, B, C}
  - An example: <(color = green; shape = rectangle), label = B>
- Nodes are tests for feature values
- There is one branch for each value of the feature
- Leaves specify the category (labels)
- Can categorize instances into multiple disjoint categories

Learning a Decision Tree?

Evaluation of a Decision Tree

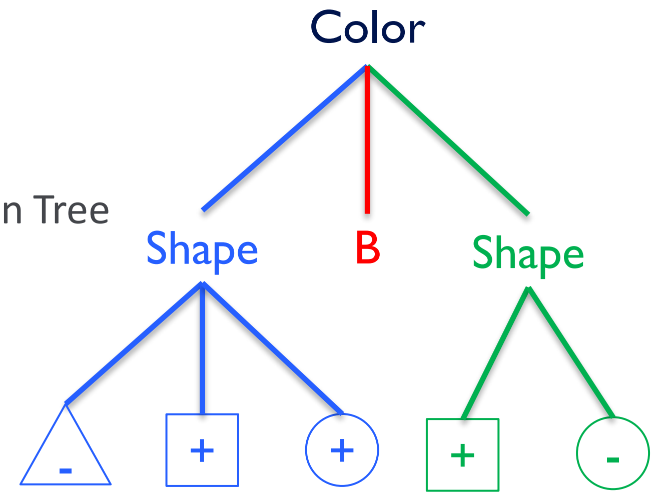
- Check the color feature.
- If it is blue than check the shape feature
- if it is …then…





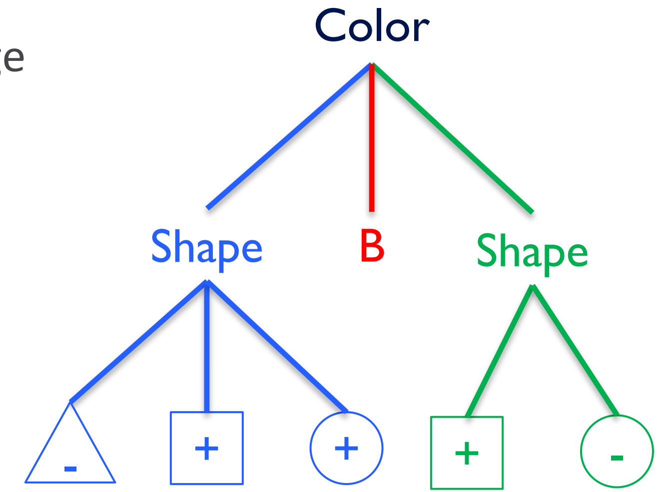
Expressivity of Decision Trees

- As Boolean functions they can represent any Boolean function.
- Can be rewritten as rules in Disjunctive Normal Form (DNF)
  - Green ∧ Square → positive
  - Blue ∧ Circle → positive
  - Blue ∧ Square → positive
- The disjunction of these rules is equivalent to the Decision Tree
- What did we show? What is the hypothesis space here?
  - 2 dimensions: color and shape
  - 3 values each: color(red, blue, green), shape(triangle, square, circle)
  - |X| = 9: (red, triangle), (red, circle), (blue, square) …
  - |Y| = 2: + and -
  - |H| = 2^9
- And, all these functions can be represented as decision trees.



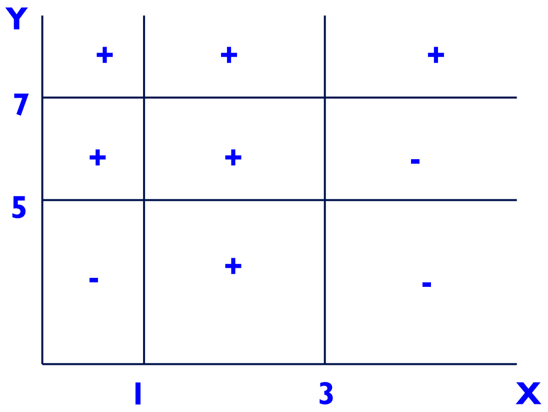
Decision Trees

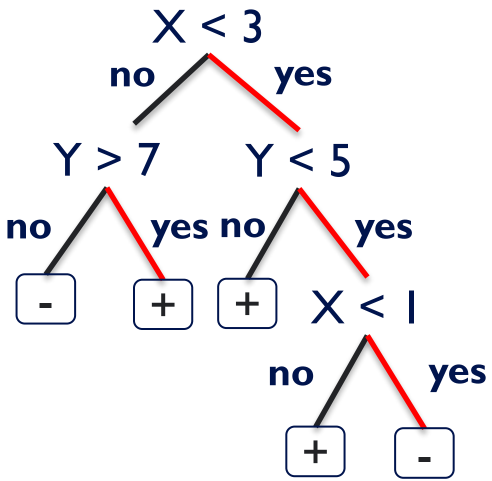
- Output is a discrete category. Real valued outputs are possible (regression trees)
- There are efficient algorithms for processing large amounts of data (but not too many features)
- There are methods for handling **noisy data** (classification noise and attribute noise) and for handling missing attribute values



Decision Boundaries

- Usually, instances are represented as attribute-value pairs (color=blue, shape = square, +)
- Numerical values can be used either by discretizing or by using thresholds for splitting nodes
- In this case, the tree divides the features space into axis-parallel rectangles, each labeled with one of the labels



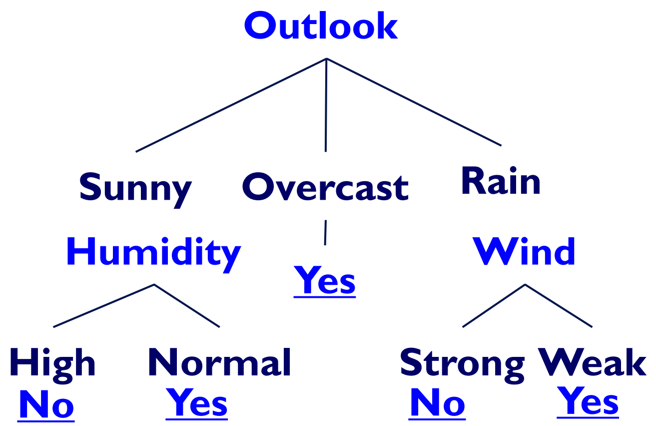


Learning decision trees (ID3 algorithm

Decision Trees

- Can represent any Boolean Function
- Can be viewed as a way to compactly represent a lot of data.
- Natural representation: (20 questions)
- The evaluation of the Decision Tree Classifier is easy

- Clearly, given data, there are many ways to represent it as a decision tree.
- Learning a good representation from data is the challenge.



Given data you can always represent it using a decision tree (agree? convince yourself); if so, what is a "good" decision tree?

Start the presentation to see live content. For screen share software, share the entire screen. Get help at **pollev.com/app**

Will I play tennis today?

- **Features**
  - Outlook: {Sun, Overcast, Rain}
  - Temperature: {Hot, Mild, Cool}
  - Humidity: {High, Normal, Low}
  - Wind: {Strong, Weak}

- **Labels**
  - Binary classification task: Y = {+, -}

Will I play tennis today?

	O	T	H	W	Play?
1	S	H	H	W	-
2	S	H	H	S	-
3	O	H	H	W	+
4	R	M	H	W	+
5	R	C	N	W	+
6	R	C	N	S	-
7	O	C	N	S	+
8	S	M	H	W	-
9	S	C	N	W	+
10	R	M	N	W	+
11	S	M	N	S	+
12	O	M	H	S	+
13	O	H	N	W	+
14	R	M	H	S	-

Outlook: S(unny), O(vercast), R(ainy)

Temperature: H(ot), M(edium), C(ool)

Humidity: H(igh), N(ormal), L(ow)

Wind: S(trong), W(eak)

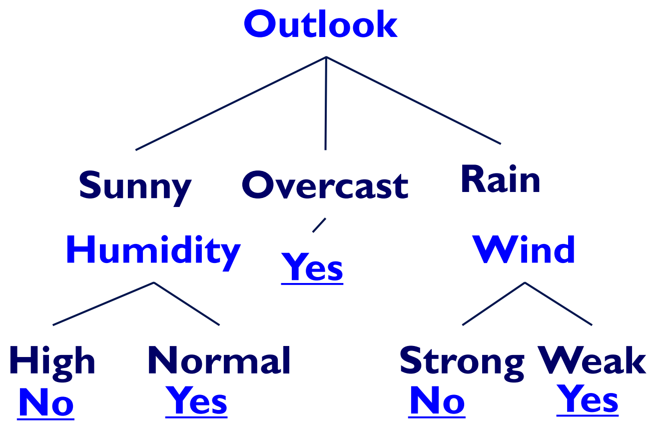
Suggest an algorithm to learn a decision tree from this data; what would be the goal of the first step of the algorithm?

Start the presentation to see live content. For screen share software, share the entire screen. Get help at **pollev.com/app**

Basic Decision Trees Learning Algorithm

	O	T	H	W	Play?
1	S	H	H	W	-
2	S	H	H	S	-
3	O	H	H	W	+
4	R	M	H	W	+
5	R	C	N	W	+
6	R	C	N	S	-
7	O	C	N	S	+
8	S	M	H	W	-
9	S	C	N	W	+
10	R	M	N	W	+
11	S	M	N	S	+
12	O	M	H	S	+
13	O	H	N	W	+
14	R	M	H	S	-

- Data is processed in Batch (i.e. all the data available) Algorithm?
- Recursively build a decision tree top down.



Basic Decision Tree Algorithm

- Let S be the set of Examples
  - Label is the target attribute (the prediction)
  - Attributes is the set of measured attributes
- ID3(*S*, Attributes, Label)

If all examples are labeled the same return a single node tree with Label

Otherwise Begin

A = attribute in Attributes that ***best*** classifies S (Create a Root node for tree)

for each possible value v of A

Add a new tree branch corresponding to A=v

Let *Sv* be the subset of examples in S with A=v

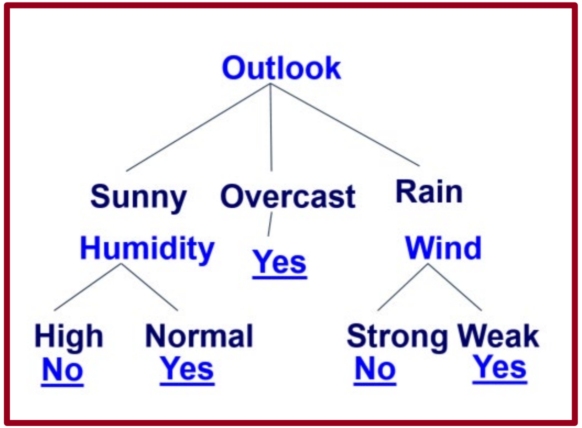
if *Sv* is empty: add leaf node with the common value of Label in S

Else: below this branch add the subtree

ID3(*Sv*, Attributes - {a}, Label)

End

Return Root



why?

For evaluation time

Picking the Root Attribute

- The goal is to have the resulting decision tree as small as possible (Occam's Razor)
  - But, finding the minimal decision tree consistent with the data is NP-hard
- The recursive algorithm is a greedy heuristic search for a simple tree, but cannot guarantee optimality.
- The main decision in the algorithm is the selection of the next attribute to condition on.

Picking the Root Attribute

- Consider data with two Boolean attributes (A,B).

  < (A=0,B=0), - >: 50 examples

  < (A=0,B=1), - >: 50 examples

  < (A=1,B=0), - >: 0 examples

  < (A=1,B=1), + >: 100 examples

- What should be the first attribute we select?

What should be the first attribute we select?

A

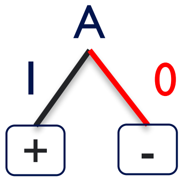
B

Ill defined; there is no advantage to one over the other.

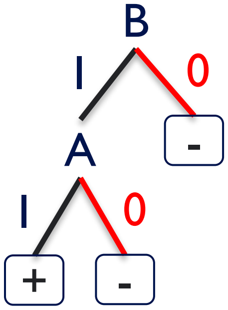
Start the presentation to see live content. For screen share software, share the entire screen. Get help at **pollev.com/app**

Picking the Root Attribute

- Consider data with two Boolean attributes (A,B).
  - < (A=0,B=0), - >: 50 examples
  - < (A=0,B=1), - >: 50 examples
  - < (A=1,B=0), - >: 0 examples
  - < (A=1,B=1), + >: 100 examples
- What should be the first attribute we select?
  - Splitting on A: we get purely labeled nodes.
  - Splitting on B: we don't get purely labeled nodes.
  - What if we have: <(A=1,B=0), - >: 3 examples?
- (one way to think about it: # of queries required to label a random data point)



splitting on A



splitting on B

Picking the Root Attribute

- Consider data with two Boolean attributes (A,B).

  < (A=0,B=0), - >: 50 examples

  < (A=0,B=1), - >: 50 examples

  < (A=1,B=0), - >: ~~0 examples~~ 3 examples

  < (A=1,B=1), + >: 100 examples

- What should be the first attribute we select?

What should be the first attribute we select?

A

B

Ill defined; there is no advantage to one over the other.

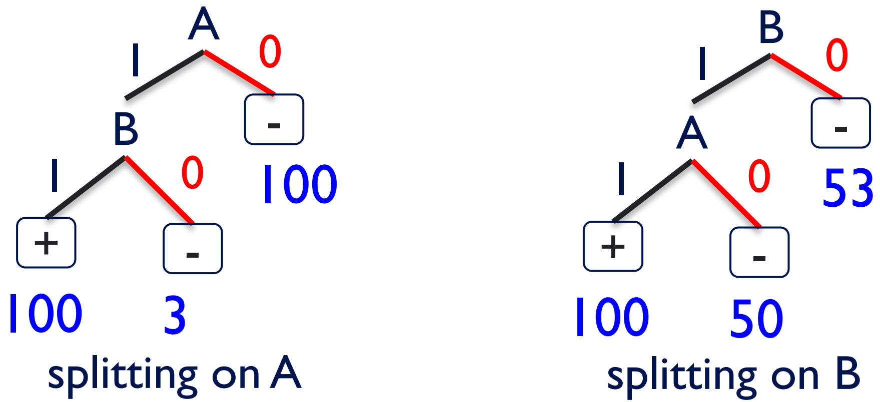
Start the presentation to see live content. For screen share software, share the entire screen. Get help at **pollev.com/app**

Picking the Root Attribute

- Consider data with two Boolean attributes (A,B).
  - < (A=0,B=0), - >: 50 examples
  - < (A=0,B=1), - >: 50 examples
  - < (A=1,B=0), - >: ~~0 examples~~ 3 examples
  - < (A=1,B=1), + >: 100 examples
- What should be the first attribute we select?
- Trees looks structurally similar; which attribute should we choose?

Advantage A. But…
Need a way to quantify things

- One way to think about it: # of queries required to label a random data point.
- If we choose A we have less uncertainty about the labels.



Picking the Root Attribute

- The goal is to have the resulting decision tree as small as possible (Occam's Razor)
  – The main decision in the algorithm is the selection of the next attribute to condition on.
- We want attributes that split the examples to sets that are relatively pure in one label; this way we are closer to a leaf node.
  – The most popular heuristics is based on information gain, originated with the ID3 system of Quinlan.

Entropy

- Entropy (impurity, disorder) of a set of examples, S, relative to a binary classification is:

$$Entropy(S) = -p_+ \log(p_+) - p_- \log(p_-)$$

- p_+ is the proportion of positive examples in S and
- p_- is the proportion of negatives examples in S
  - If all the examples belong to the same category [(1,0) or (0,1)]: Entropy = 0
  - If all the examples are equally mixed (0.5, 0.5): Entropy = 1
  - Entropy = Level of uncertainty.
- In general, when p_i is the fraction of examples labeled i:

$$Entropy(S[p_1, p_2, \ldots, p_k]) = -\sum_1^k p_i \log(p_i)$$

- Entropy can be viewed as the number of bits required, on average, to encode the class of labels. If the probability for + is 0.5, a single bit is required for each example; if it is 0.8 – can use less then 1 bit.

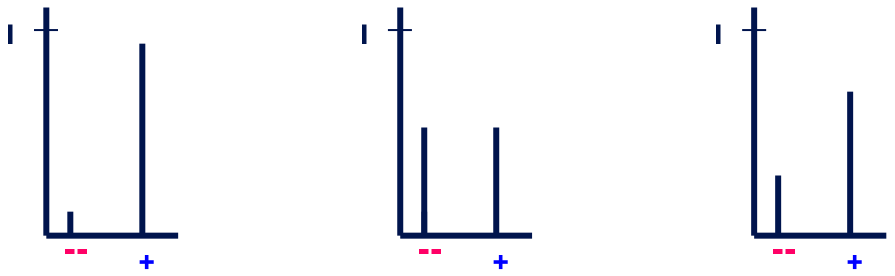
Entropy

- Entropy (impurity, disorder) of a set of examples, S, relative to a binary classification is:

$$Entropy(S) = -p_{+} \log(p_{+}) - p_{-} \log(p_{-})$$

- p_{+} is the proportion of positive examples in S and
- p_{-} is the proportion of negatives examples in S
  - If all the examples belong to the same category: Entropy = 0
  - If all the examples are equally mixed (0.5, 0.5): Entropy = 1
  - **Entropy = Level of uncertainty.**

Test yourself: assign high, medium, low to each of these distributions



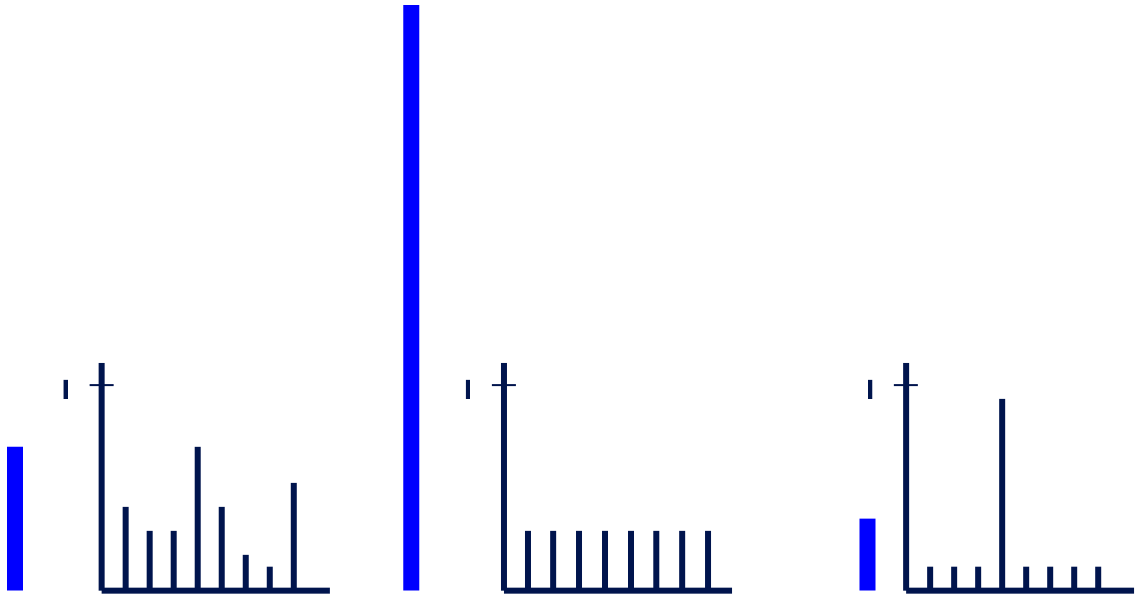
Entropy

(Convince yourself that the max value would be $\log(k)$)

(Also note that the base of the log only introduces a constant factor; therefore, we'll think about base 2)

$$Entropy(S[p_1, p_2, \ldots, p_k]) = -\sum_{1}^{k} p_i \log(p_i)$$

Test yourself again: assign high, medium, low to each of these distributions. For the middle distribution, try to guess the value of the entropy.

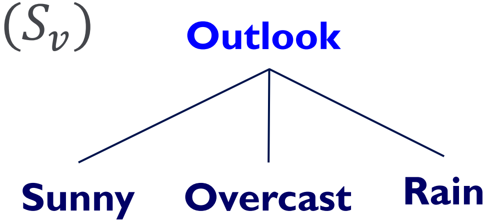


Information Gain

High Entropy – High level of Uncertainty
Low Entropy – No Uncertainty.

- The information gain of an attribute a is the expected reduction in entropy caused by partitioning on this attribute

$$Gain(S,a) = Entropy(S) - \sum_{v \in values(S)} \frac{|S_v|}{|S|} Entropy(S_v)$$



- Where:
  - S_v is the subset of S for which attribute a has value v, and
  - the entropy of partitioning the data is calculated by **weighing the entropy of each partition** by its size relative to the original set

- Partitions of low entropy (imbalanced splits) lead to high gain
- Go back to check which of the A, B splits is better

Administration (9/21/20)

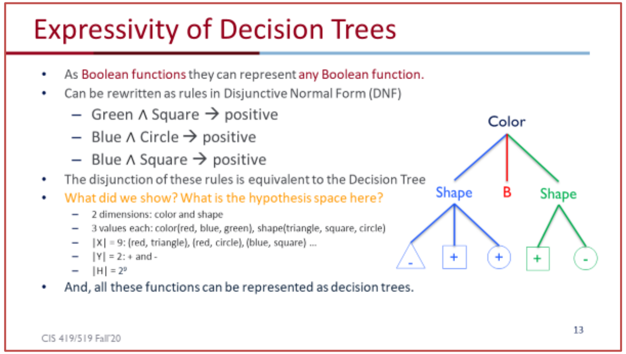
Are we recording? YES!

Available on the web site

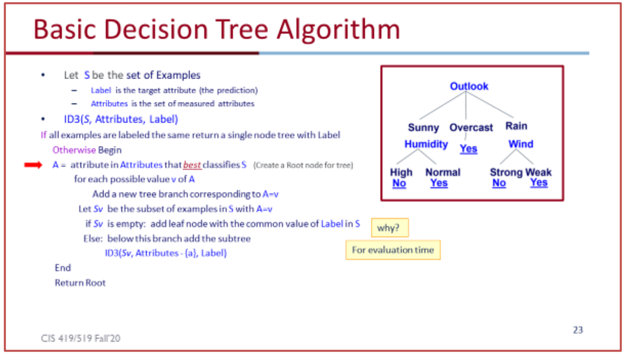
- Remember that all the lectures are available on the website before the class
  - Go over it and be prepared
- HW 1 was released on Monday
  - Covers: SGD, DT, Feature Extraction, Ensemble Models, & Experimental Machine Learning
  - Start working on it now. Don't wait until the last day (or two) since it could take a lot of your time
- Go to the recitations and office hours
- No Class on Monday 9/28 for Yom Kippur
- Questions?
  - Please ask/comment during class.
  - Give us feedback

What Have We Done?

1. Decision Trees
   - Expressivity

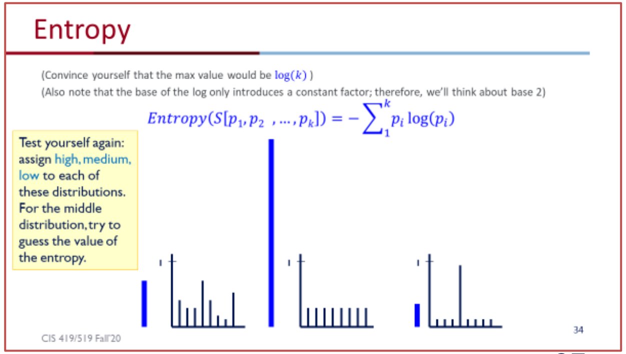


2. A Recursive Decision Tree Algorithm



3. Entropy and Information Gain

$$Gain(S,a) = Entropy(S) - \sum_{v \in values(S)} \frac{|S_v|}{|S|} Entropy(S_v)$$



Will I play tennis today?

	O	T	H	W	Play?
1	S	H	H	W	-
2	S	H	H	S	-
3	O	H	H	W	+
4	R	M	H	W	+
5	R	C	N	W	+
6	R	C	N	S	-
7	O	C	N	S	+
8	S	M	H	W	-
9	S	C	N	W	+
10	R	M	N	W	+
11	S	M	N	S	+
12	O	M	H	S	+
13	O	H	N	W	+
14	R	M	H	S	-

Outlook: S(unny), O(vercast), R(ainy)

Temperature: H(ot), M(edium), C(ool)

Humidity: H(igh), N(ormal), L(ow)

Wind: S(trong), W(eak)

Will I play tennis today?

	O	T	H	W	Play?
1	S	H	H	W	-
2	S	H	H	S	-
3	O	H	H	W	+
4	R	M	H	W	+
5	R	C	N	W	+
6	R	C	N	S	-
7	O	C	N	S	+
8	S	M	H	W	-
9	S	C	N	W	+
10	R	M	N	W	+
11	S	M	N	S	+
12	O	M	H	S	+
13	O	H	N	W	+
14	R	M	H	S	-

calculate current entropy

- $p_+ = \frac{9}{14} \quad p_- = \frac{5}{14}$
- $Entropy(Play) = -p_+ \log_2(p_+) - p_- \log_2(p_-)$

$$= -\frac{9}{14}\log_2\frac{9}{14} - \frac{5}{14}\log_2\frac{5}{14}$$

$$\approx 0.94$$

Information Gain: Outlook

	O	T	H	W	Play?
1	S	H	H	W	-
2	S	H	H	S	-
3	O	H	H	W	+
4	R	M	H	W	+
5	R	C	N	W	+
6	R	C	N	S	-
7	O	C	N	S	+
8	S	M	H	W	-
9	S	C	N	W	+
10	R	M	N	W	+
11	S	M	N	S	+
12	O	M	H	S	+
13	O	H	N	W	+
14	R	M	H	S	-

$$Gain(S,a) = Entropy(S) - \sum_{v \in values(S)} \frac{|S_v|}{|S|} Entropy(S_v)$$

Outlook = sunny:

$p_+ = 2/5 \quad p_- = 3/5$ **Entropy(O = S) = 0.971**

Outlook = overcast:

$p_+ = 4/4 \quad p_- = 0$ **Entropy(O = O) = 0**

Outlook = rainy:

$p_+ = 3/5 \quad p_- = 2/5$ **Entropy(O = R) = 0.971**

Expected entropy

= $\sum_{v \in values(S)} \frac{|S_v|}{|S|} Entropy(S_v)$

= (5/14)×0.971 + (4/14)×0 + (5/14)×0.971 = **0.694**

Information gain = 0.940 – 0.694 = **0.246**

Information Gain: Humidity

	O	T	H	W	Play?
1	S	H	H	W	-
2	S	H	H	S	-
3	O	H	H	W	+
4	R	M	H	W	+
5	R	C	N	W	+
6	R	C	N	S	-
7	O	C	N	S	+
8	S	M	H	W	-
9	S	C	N	W	+
10	R	M	N	W	+
11	S	M	N	S	+
12	O	M	H	S	+
13	O	H	N	W	+
14	R	M	H	S	-

$$Gain(S,a) = Entropy(S) - \sum_{v \in values(S)} \frac{|S_v|}{|S|} Entropy(S_v)$$

Humidity = high:

$p_+ = 3/7 \quad p_- = 4/7$ **Entropy(H = H) = 0.985**

Humidity = Normal:

$p_+ = 6/7 \quad p_- = 1/7$ **Entropy(H = N) = 0.592**

Expected entropy

= $\sum_{v \in values(S)} \frac{|S_v|}{|S|} Entropy(S_v)$

= (7/14)×0.985 + (7/14)×0.592 = **0.7785**

Information gain = 0.940 – 0.694 **= 0.246**

Which feature to split on?

	O	T	H	W	Play?
1	S	H	H	W	-
2	S	H	H	S	-
3	O	H	H	W	+
4	R	M	H	W	+
5	R	C	N	W	+
6	R	C	N	S	-
7	O	C	N	S	+
8	S	M	H	W	-
9	S	C	N	W	+
10	R	M	N	W	+
11	S	M	N	S	+
12	O	M	H	S	+
13	O	H	N	W	+
14	R	M	H	S	-

Information gain:

Outlook: 0.246
Humidity: 0.151
Wind: 0.048
Temperature: 0.029

→ Split on Outlook

How difficult was the lecture today?

Very difficult

Somewhat difficult

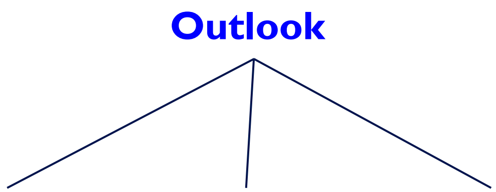
Just right

Easy

Too easy

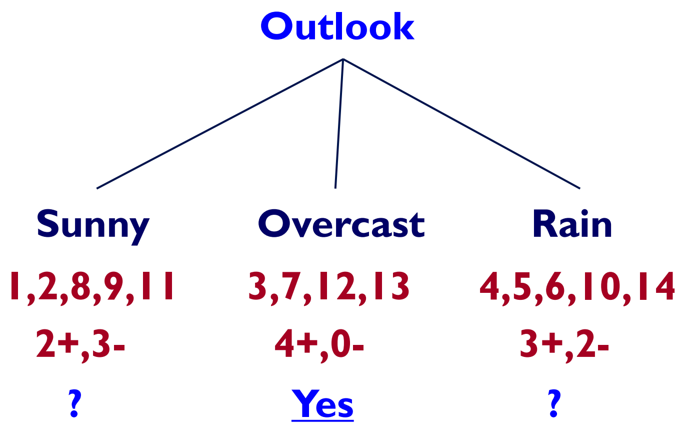
Start the presentation to see live content. For screen share software, share the entire screen. Get help at **pollev.com/app**

An Illustrative Example (III)



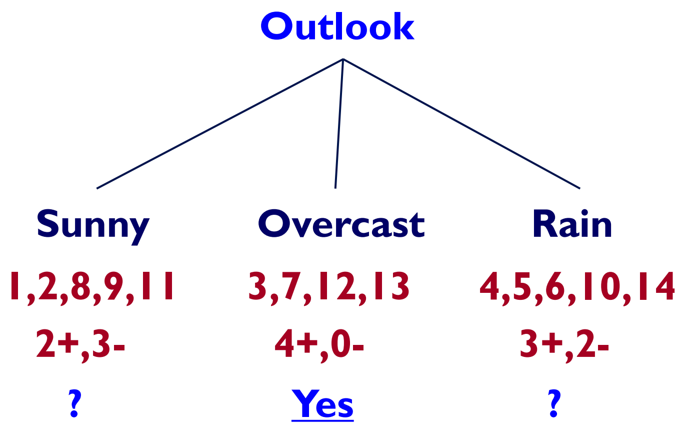
Gain(S,Humidity)=0.151
Gain(S,Wind) = 0.048
Gain(S,Temperature) = 0.029
Gain(S,Outlook) = 0.246

An Illustrative Example (III)



	O	T	H	W	Play?
1	S	H	H	W	-
2	S	H	H	S	-
3	O	H	H	W	+
4	R	M	H	W	+
5	R	C	N	W	+
6	R	C	N	S	-
7	O	C	N	S	+
8	S	M	H	W	-
9	S	C	N	W	+
10	R	M	N	W	+
11	S	M	N	S	+
12	O	M	H	S	+
13	O	H	N	W	+
14	R	M	H	S	-

An Illustrative Example (III)

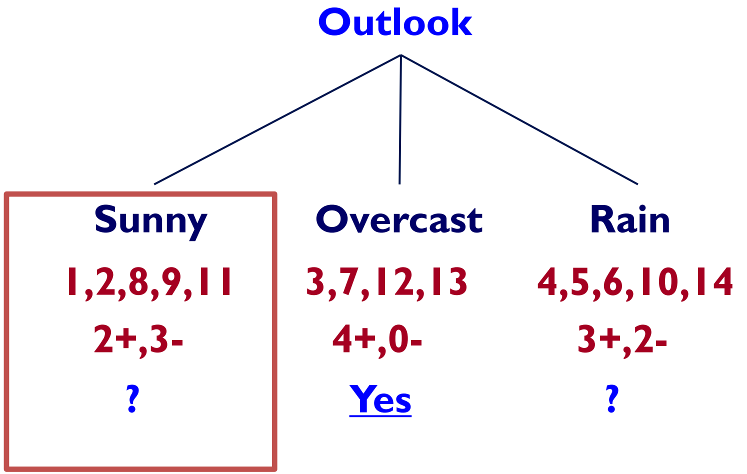


Continue until:

- Every attribute is included in path, or,
- All examples in the leaf have same label

	O	T	H	W	Play?
1	S	H	H	W	-
2	S	H	H	S	-
3	O	H	H	W	+
4	R	M	H	W	+
5	R	C	N	W	+
6	R	C	N	S	-
7	O	C	N	S	+
8	S	M	H	W	-
9	S	C	N	W	+
10	R	M	N	W	+
11	S	M	N	S	+
12	O	M	H	S	+
13	O	H	N	W	+
14	R	M	H	S	-

An Illustrative Example (IV)



$Gain(S_{sunny}, Humidity) = .97-(3/5)\ 0-(2/5)\ 0 = .97$

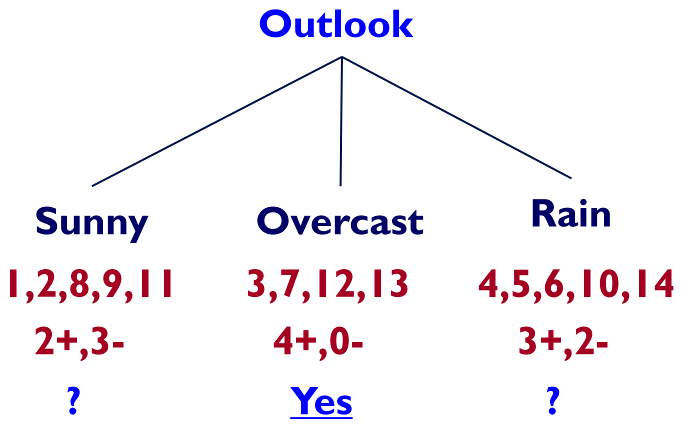
$Gain(S_{sunny}, Temp) = .97-\ 0-(2/5)\ 1 = .57$

$Gain(S_{sunny}, Wind) = .97-(2/5)\ 1 - (3/5)\ .92 = .02$

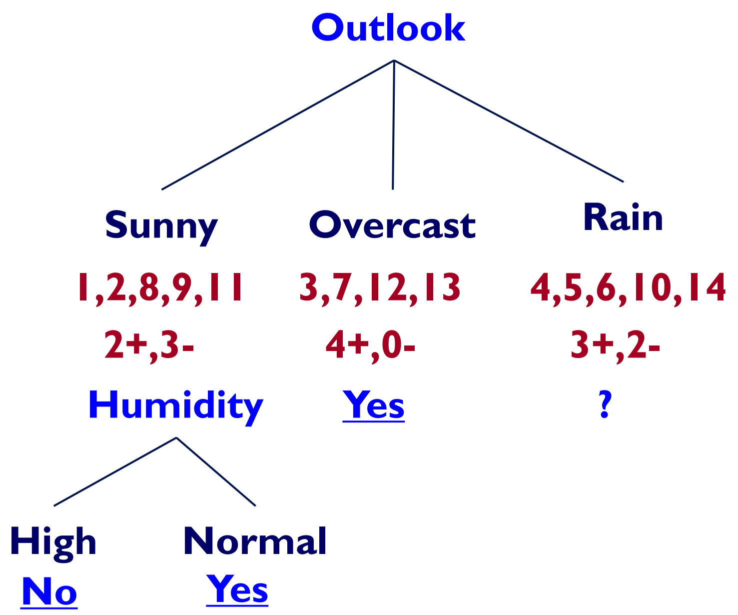
Split on Humidity

	O	T	H	W	Play?
1	S	H	H	W	-
2	S	H	H	S	-
4	R	M	H	W	+
5	R	C	N	W	+
6	R	C	N	S	-
7	O	C	N	S	+
8	S	M	H	W	-
9	S	C	N	W	+
10	R	M	N	W	+
11	S	M	N	S	+
12	O	M	H	S	+
13	O	H	N	W	+
14	R	M	H	S	-

An Illustrative Example (V)



An Illustrative Example (V)



induceDecisionTree(S)

- 1. Does S uniquely define a class?

  if all $s \in S$ have the same label y: **return** S;

- 2. Find the feature with the most information gain:

  $i = \text{argmax}_i\ \mathit{Gain}(S, X_i)$

- 3. Add children to S:

  for *k* **in** Values(X_i):

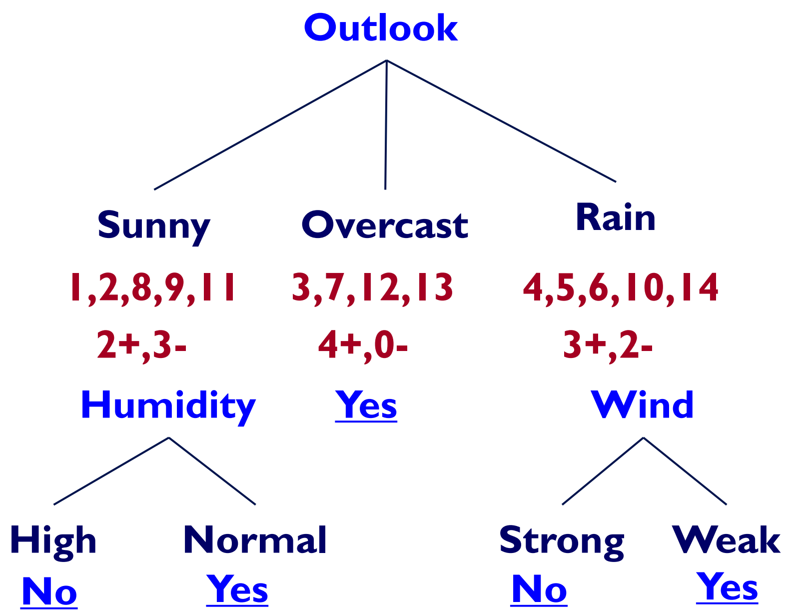
  $S_k = \{s \in S \mid x_i = k\}$

  addChild(S, S_k)

  induceDecisionTree(S_k)

  return S;

An Illustrative Example (VI)



Hypothesis Space in Decision Tree Induction

- Conduct a search of the space of decision trees which can represent all possible discrete functions. (pros and cons)
- Goal: to find the best decision tree
  - Best could be "smallest depth"
  - Best could be "minimizing the expected number of tests"
- Finding a minimal decision tree consistent with a set of data is NP-hard.
- Performs a greedy heuristic search: hill climbing without backtracking
- Makes statistically based decisions using all data

History of Decision Tree Research

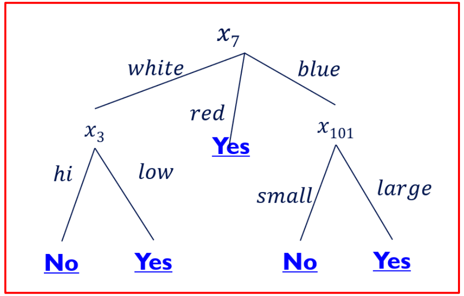
- Hunt and colleagues in Psychology used full search decision tree methods to model human concept learning in the 60s
  - Quinlan developed ID3, with the information gain heuristics in the late 70s to learn expert systems from examples
  - Breiman, Freidman and colleagues in statistics developed CART (classification and regression trees simultaneously)
- A variety of improvements in the 80s: coping with noise, continuous attributes, missing data, non-axis parallel etc.
  - Quinlan's updated algorithm, C4.5 (1993) is commonly used (New: C5)
- Boosting (or Bagging) over DTs is a very good general-purpose algorithm

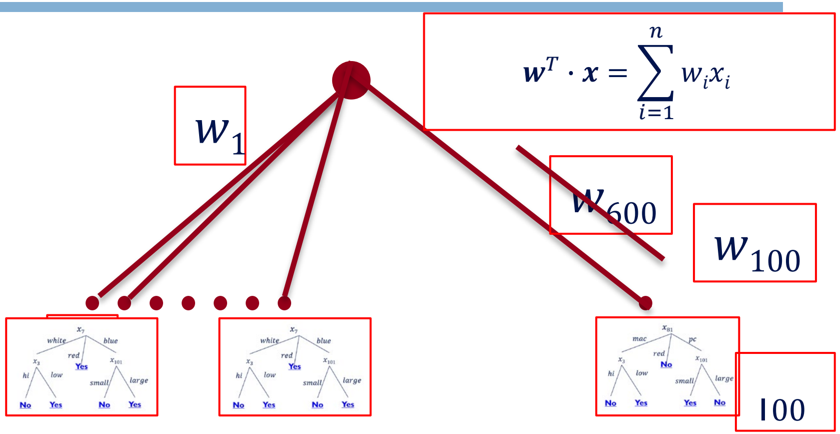
Untitled open-ended question

Start the presentation to see live content. For screen share software, share the entire screen. Get help at **pollev.com/app**

HW1 – Learning Algorithms

- SGD: You will learn the weights w_i
- DT/DT-stumps: learn a small DTs





Final Process:

For each example: $x_{1,600}$ → $(DT_1(x),\dots, DT_{100}(x))$

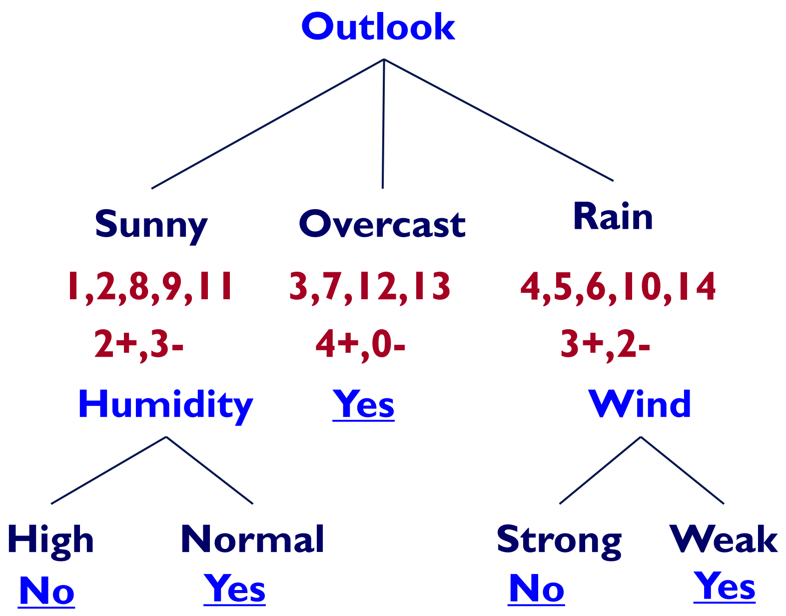
Run SGD on 100 dimensional examples

- SGD+Stumps
  - But, the DT algorithm is deterministic, and will give me the same DT every time
  - Run it on different data – in this case, use random 50% of the features; **100 times**
    - Not the only option; you could use random 50% of the data

Overfitting

Example

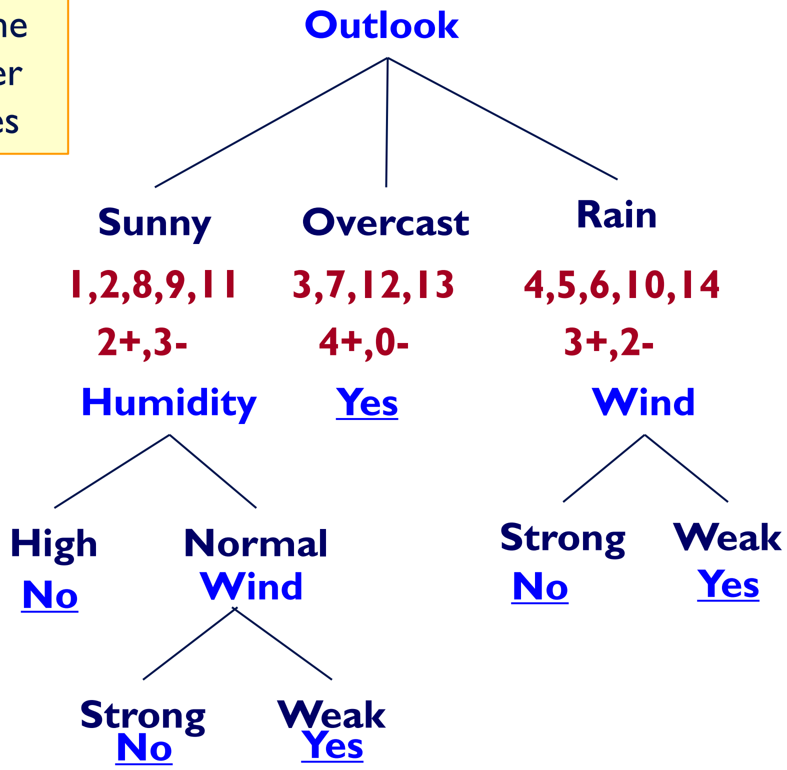
- Outlook = Sunny,
- Temp = Hot
- Humidity = Normal
- Wind = Strong
- label: NO
- this example doesn't exist in the tree



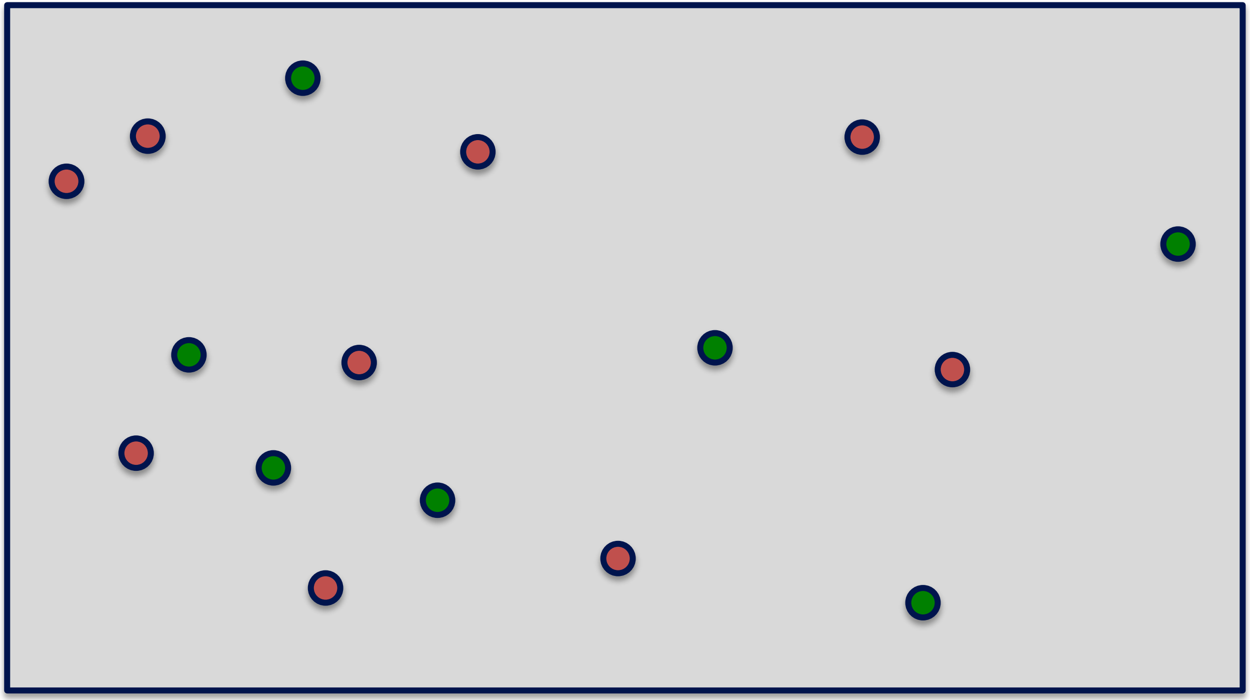
Overfitting - Example

This can always be done – may fit noise or other coincidental regularities

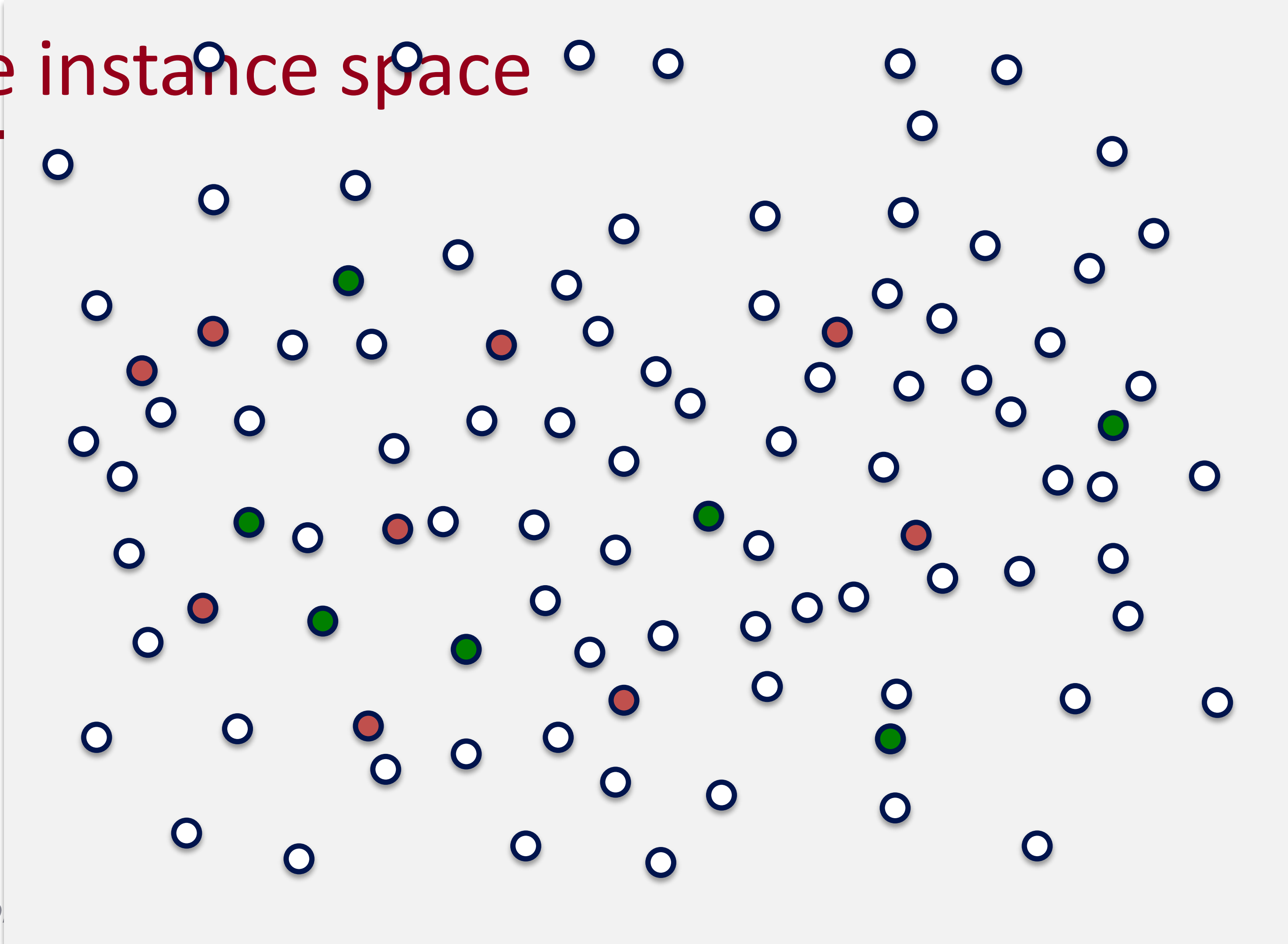
- Outlook = Sunny,
- Temp = Hot
- Humidity = Normal
- Wind = Strong
- label: NO
- this example doesn't exist in the tree



Our training data

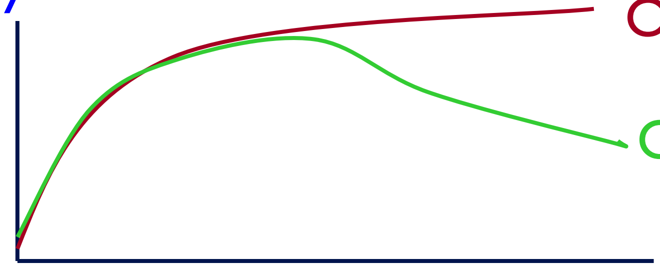


The instance space



Overfitting the Data

- Learning a tree that classifies the training data perfectly may not lead to the tree with the best generalization performance.
  - There may be noise in the training data the tree is fitting
  - The algorithm might be making decisions based on very little data
- A hypothesis h is said to overfit the training data if there is another hypothesis h', such that h has a smaller error than h' on the **training data** but h has larger error on the **test data** than h'.



Reasons for overfitting

- Too much variance in the training data
  - Training data is not a representative sample of the instance space
  - We split on features that are actually irrelevant

- Too much noise in the training data
  - Noise = some feature values or class labels are incorrect
  - We learn to predict the noise

- In both cases, it is a result of our will to minimize the empirical error when we learn, and the ability to do it (with DTs)

Pruning a decision tree

- Prune = remove leaves and assign majority label of the parent to all items
- Prune the children of node s if:
  - all children are leaves, and
  - the accuracy on the validation set does not decrease if we assign the most frequent class label to all items at s.

Avoiding Overfitting

How can this be avoided with linear classifiers?

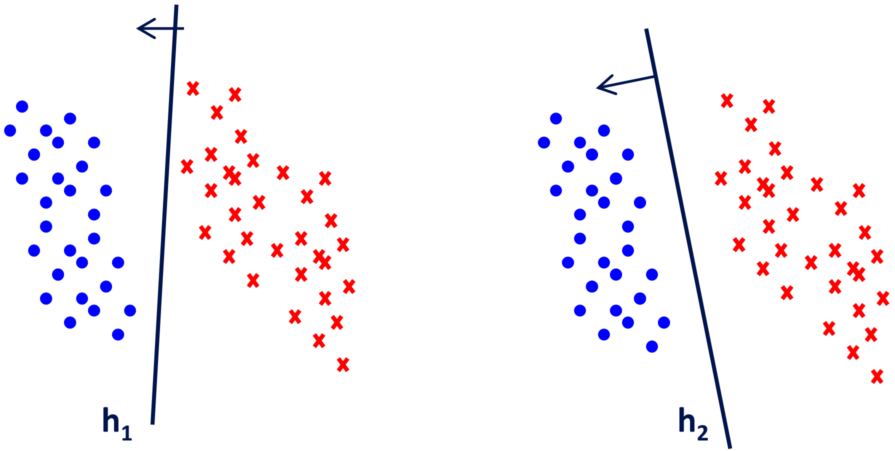
- Two basic approaches
  - Pre-pruning: Stop growing the tree at some point during construction when it is determined that there is not enough data to make reliable choices.
  - Post-pruning: Grow the full tree and then remove nodes that seem not to have sufficient evidence.
- Methods for evaluating subtrees to prune
  - Cross-validation: Reserve hold-out set to evaluate utility
  - Statistical testing: Test if the observed regularity can be dismissed as likely to occur by chance
  - Other

- The goal is to guarantee/improve generalization
- This is related to the notion of regularization that we will see in other contexts – keep the hypothesis simple.

Hand waving, for now.

Next: a brief detour into explaining generalization and overfitting

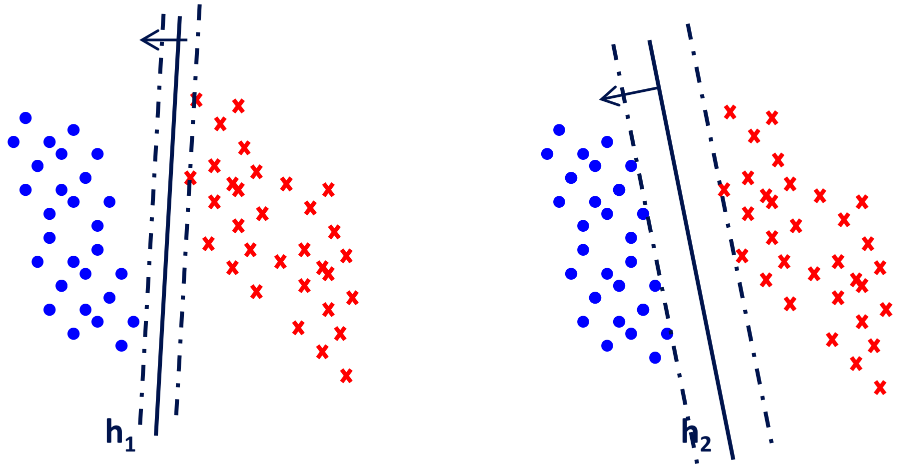
Preventing Overfitting



Untitled open-ended question

Start the presentation to see live content. For screen share software, share the entire screen. Get help at **pollev.com/app**

Preventing Overfitting



DT Extensions: continuous attributes and missing values

Penn Engineering

Continuous Attributes

- Real-valued attributes can, in advance, be discretized into ranges, such as big, medium, small
- Alternatively, one can develop splitting nodes based on thresholds of the form A<c that partition the data into examples that satisfy A<c and A>=c.
  - The information gain for these splits is calculated in the same way and compared to the information gain of discrete splits.

- How to find the split with the highest gain?
- For each continuous feature A:
  - Sort examples according to the value of A
  - For each ordered pair (x,y) with different labels
    - Check the mid-point as a possible threshold, i.e.
    - $S_{a < x}$ $S_{a >= y}$

Continuous Attributes

- Example:
  - Length (L): 10 15 21 28 32 40 50
  - labels: - + + - + + -
  - Check thresholds: L < 12.5; L < 24.5; L < 45
  - Subset of Examples= {…}, Split= k+,j-

- How to find the split with the highest gain ?
  - For each continuous feature A:
    - Sort examples according to the value of A
    - For each ordered pair (x,y) with different labels
      - Check the mid-point as a possible threshold. I.e,
      - $S_{a < x}, S_{a >= y}$

Missing Values

- Diagnosis = < fever, blood_pressure,..., blood_test=?,...>

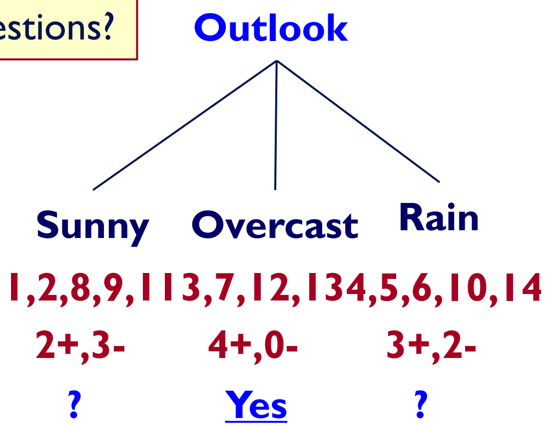
- Many times values are not available for all attributes during training or testing (e.g., medical diagnosis)

- Training: evaluate Gain(S,a) where in some of the examples a value for a is not given

Missing Values

$$Gain(S,a) = Entropy(S) - \sum \frac{|S_v|}{|S|} Entropy(S_v)$$

Other suggestions?



$Gain(S_{sunny}, Temp) =$ **.97- 0-(2/5) 1 = .57**

$Gain(S_{sunny}, Humidity) =$

- Fill in: assign the most likely value of X_i to **s**:
  argmax $_k$ $P(X_i = k)$: Normal
  - **97-(3/5) Ent[+0,-3] -(2/5) Ent[+2,-0] = .97**
- Assign fractional counts $P(X_i = k)$ for each value of X_i to **s**
  - **.97-(2.5/5) Ent[+0,-2.5] - (2.5/5) Ent[+2,-.5] < .97**

Day	Outlook	Temperature	Humidity	Wind	PlayTennis
1	Sunny	Hot	High	Weak	No
2	Sunny	Hot	High	Strong	No
8	Sunny	Mild	???	Weak	No
9	Sunny	Cool	Normal	Weak	Yes
11	Sunny	Mild	Normal	Strong	Yes

Missing Values

- Diagnosis = < fever, blood_pressure,..., blood_test=?,...>

- Many times values are not available for all attributes during training or testing (e.g., medical diagnosis)

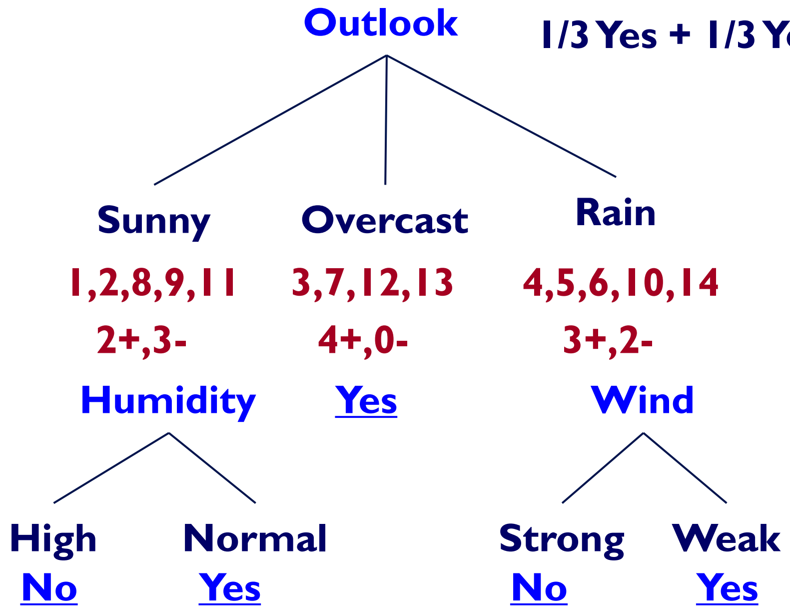
- Training: evaluate Gain(S,a) where in some of the examples a value for a is not given
- Testing: classify an example without knowing the value of a

Missing Values

Outlook = Sunny, Temp = Hot, Humidity = ???, Wind = Strong, label = ?? **Normal/High**

Outlook = ???, Temp = Hot, Humidity = Normal, Wind = Strong, label = ??

1/3 Yes + 1/3 Yes + 1/3 No = Yes



Other Issues

- Attributes with different costs
  - Change information gain so that low cost attribute are preferred
    - Dealing with features with different # of values
- Alternative measures for selecting attributes
  - When different attributes have different number of values information gain tends to prefer those with many values
- Oblique Decision Trees
  - Decisions are not axis-parallel
- Incremental Decision Trees induction
  - Update an existing decision tree to account for new examples incrementally (Maintain consistency?)

Summary: Decision Trees

- Presented the hypothesis class of Decision Trees
  - Very expressive, flexible, class of functions
- Presented a learning algorithm for Decision Tress
  - Recursive algorithm.
  - Key step is based on the notion of Entropy
- Discussed the notion of overfitting and ways to address it within DTs
  - In your problem set – look at the performance on the training vs. test
- Briefly discussed some extensions
  - Real valued attributes
  - Missing attributes
- Evaluation in machine learning
  - Cross validation
  - Statistical significance

Decision Trees as Features

- Rather than using decision trees to represent the target function it is becoming common to use small decision trees as features
- When learning over a large number of features, learning decision trees is difficult and the resulting tree may be very large

  → (over fitting)
- Instead, learn small decision trees, with limited depth.
- Treat them as "experts"; they are correct, but only on a small region in the domain. (what DTs to learn? same every time?)
- Then, learn another function, typically a linear function, over these as features.
- Boosting (but also other linear learners) are used on top of the small decision trees. (Either Boolean, or real valued features)
- In HW1 you learn a linear classifier over DTs.
  - Not learning the DTs sequentially; all are learned at once.
    - How can you learn multiple DTs?
  - Combining them using an SGD algorithm.

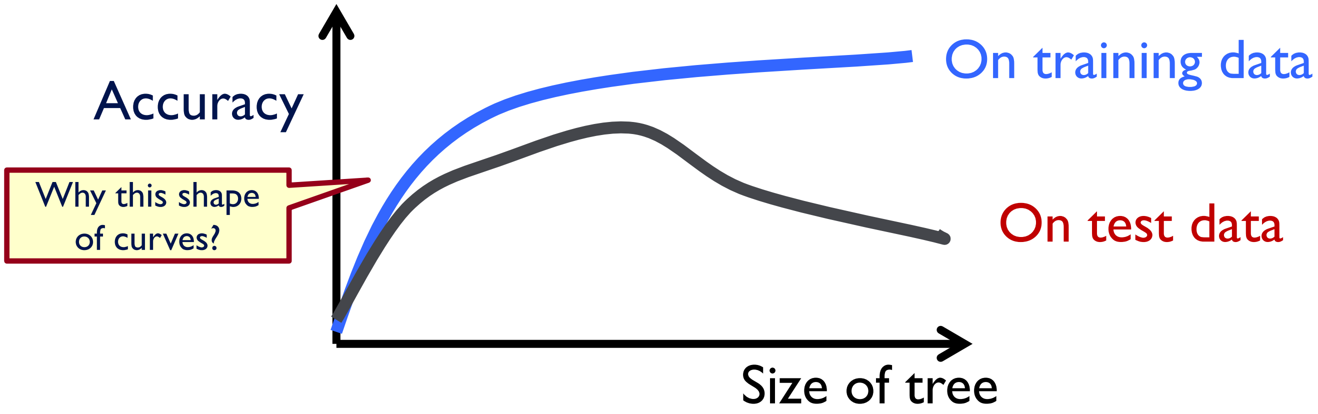
Comments/feedback on Today's Lecture?

Start the presentation to see live content. For screen share software, share the entire screen. Get help at **pollev.com/app**

The i.i.d. assumption

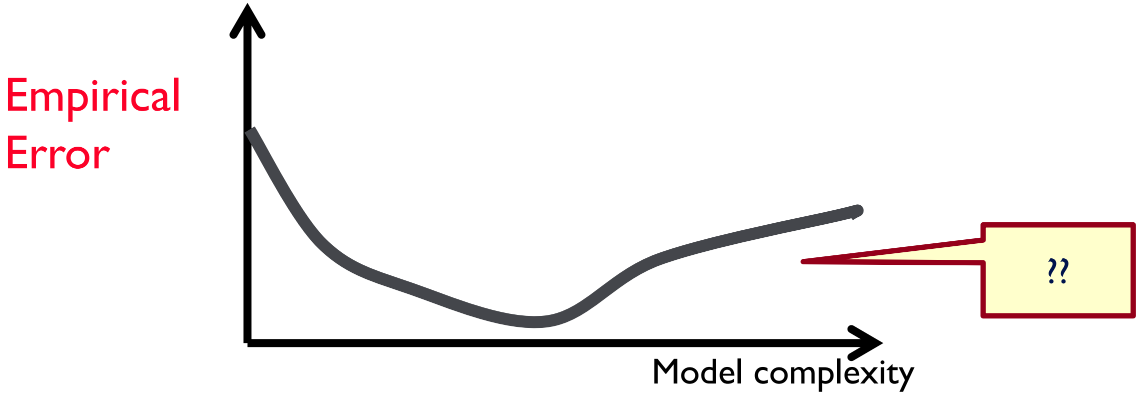
- Training and test items are independently and identically distributed (i.i.d.):
  - There is a distribution $P(\mathbf{X}, Y)$ from which the data $\mathcal{D} = \{(\mathbf{x}, y)\}$ is generated.
    - Sometimes it's useful to rewrite $P(\mathbf{X}, Y)$ as $P(\mathbf{X})P(Y|\mathbf{X})$
      Usually $P(\mathbf{X}, Y)$ is unknown to us (we just know it exists)
  - Training and test data are samples drawn from the *same* $P(\mathbf{X}, Y)$: they are identically distributed
  - Each $(\mathbf{x}, y)$ is drawn independently from $P(\mathbf{X}, Y)$

Overfitting



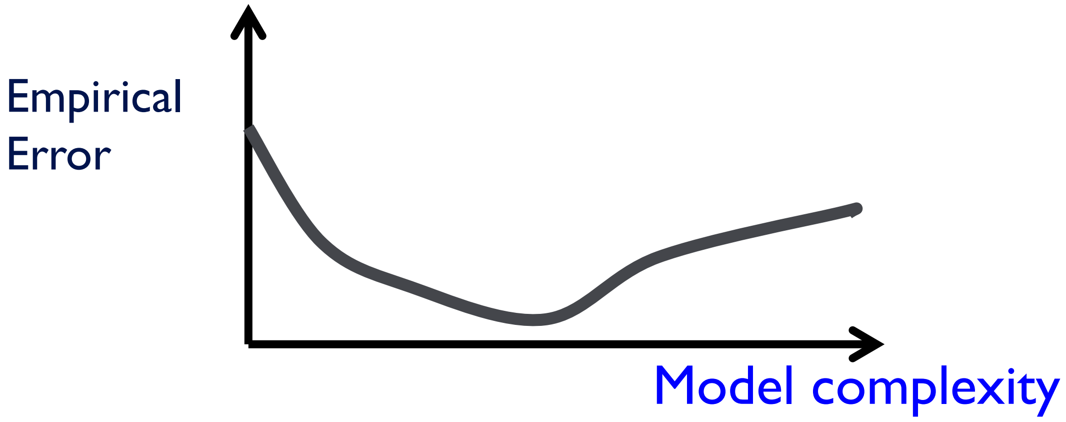
- A decision tree overfits the training data when its accuracy on the training data goes up but its accuracy on unseen data goes down

Overfitting



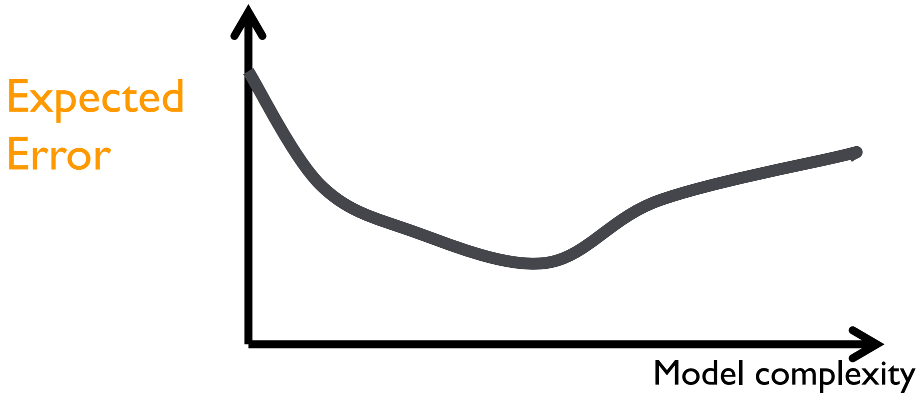
- Empirical error (= on a given data set):
  The percentage of items in this data set are misclassified by the classifier *f*.

Overfitting



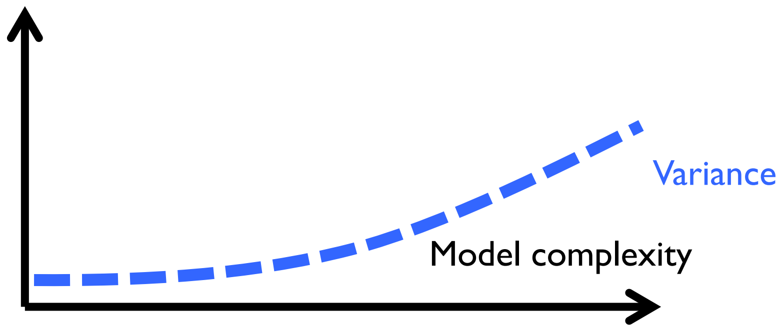
- Model complexity (informally):
  How many parameters do we have to learn?
  - Decision trees: complexity = #nodes

Overfitting



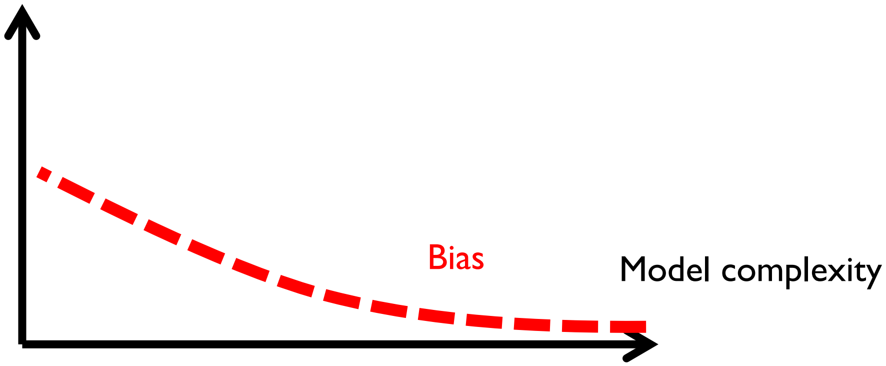
- Expected error:
  What percentage of items drawn from $P(\mathbf{x},y)$ do we expect to be misclassified by f?
- (That’s what we really care about – generalization)

Variance of a learner (informally)



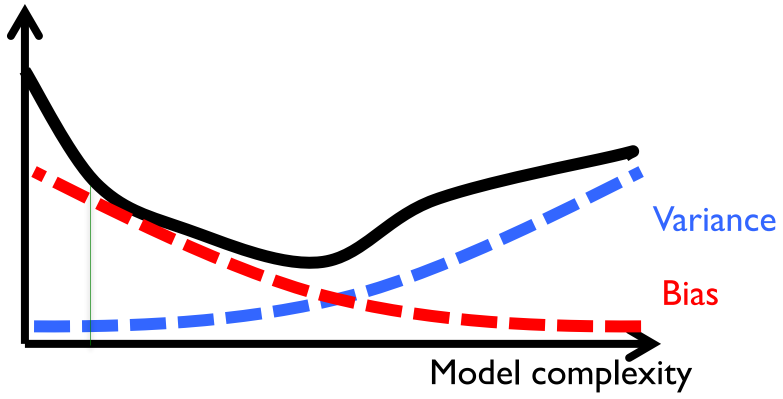
- How susceptible is the learner to minor changes in the training data?
  - (i.e. to different samples from P(**X**, Y))
- Variance increases with model complexity
  - Think about extreme cases: a hypothesis space with one function vs. all functions.
  - Or, adding the "wind" feature in the DT earlier.
  - The larger the hypothesis space is, the more flexible the selection of the chosen hypothesis is as a function of the data.
  - More accurately: for each data set D, you will learn a different hypothesis h(D), that will have a different true error e(h); we are looking here at the variance of this random variable.

Bias of a learner (informally)



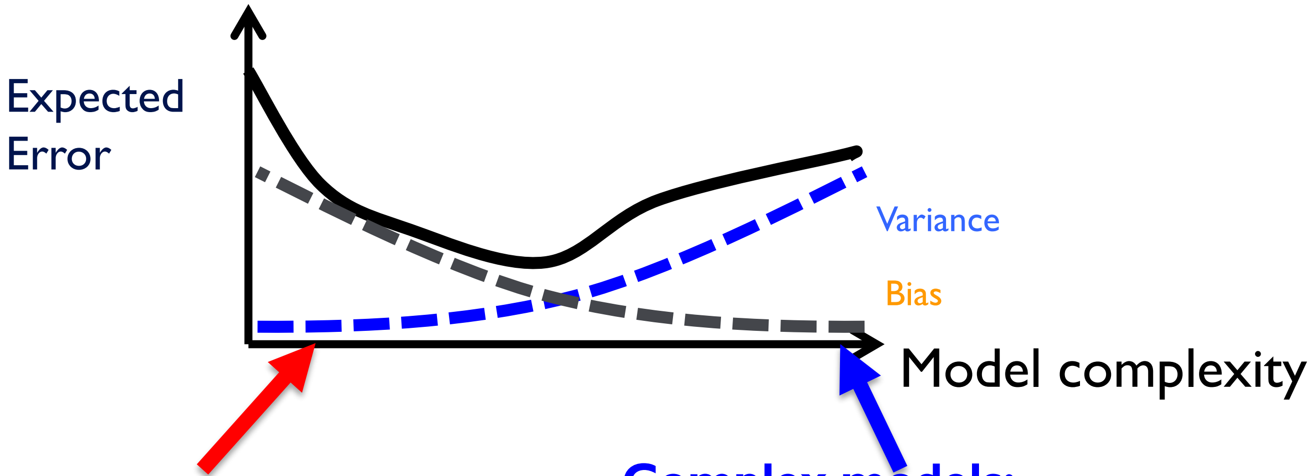
- How likely is the learner to identify the **target** hypothesis?
- Bias is low when the model is expressive (low empirical error)
- Bias is high when the model is (too) simple
  - The larger the hypothesis space is, the easiest it is to be close to the true hypothesis.
  - More accurately: for each data set D, you learn a different hypothesis h(D), that has a different true error e(h); we are looking here at the difference of the mean of this random variable from the true error.

Impact of bias and variance



- Expected error ≈ bias + variance

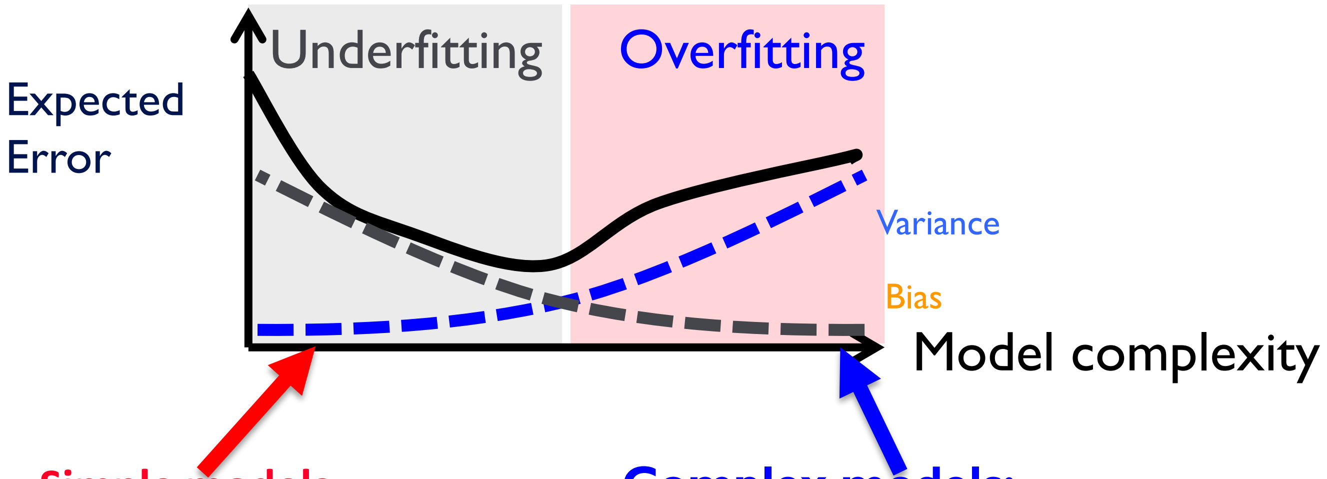
Model complexity



Simple models:
High bias and low variance

Complex models:
High variance and low bias

Underfitting and Overfitting



Simple models:
High bias and low variance

Complex models:
High variance and low bias

- This can be made more accurate for some loss functions.
- We will discuss a more precise and general theory that trades expressivity of models with empirical error

Experimental Machine Learning

- Machine Learning is an Experimental Field and we will spend some time (in Problem sets) learning how to run experiments and evaluate results
  - First hint: be organized; write scripts
- Basics:
  - Split your data into three sets:
    - Training data (often 70-90%)
    - Test data (often 10-20%)
    - Development data (10-20%)
- You need to report performance on test data, but you are not allowed to look at it.
  - You are allowed to look at the development data (and use it to tune parameters)

Metrics
Methodologies
Statistical Significance

Metrics

- We train on our training data Train = $\{x_i, y_i\}_{1,m}$
- We test on Test data.
- We often set aside part of the training data as a development set, especially when the algorithms require tuning.
  - In the HW we asked you to present results also on the Training; why?
- When we deal with binary classification we often measure performance simply using Accuracy:

$$\text{accuracy} = \frac{\#\text{ correct predictions}}{\#\text{ test instances}}$$

$$\text{error} = 1 - \text{accuracy} = \frac{\#\text{ incorrect predictions}}{\#\text{ test instances}}$$

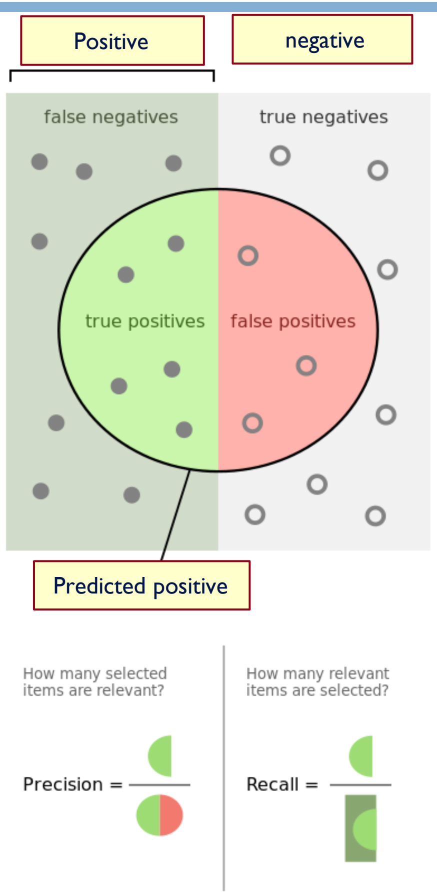
- Any possible problems with it?

Alternative Metrics

- If the Binary classification problem is biased
  - In many problems most examples are negative
- Or, in multiclass classification
  - The distribution over labels is often non-uniform
- Simple accuracy is not a useful metric.
  - Often we resort to task specific metrics
- However one important example that is being used often involves Recall and Precision

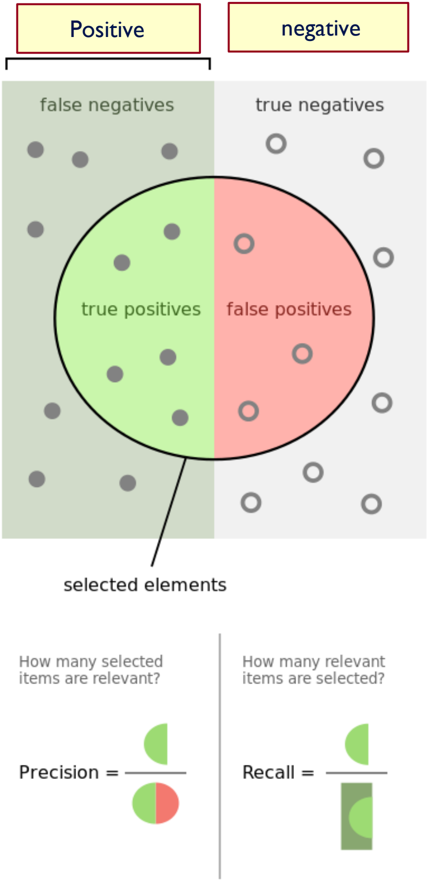
- **Recall:** $\dfrac{\text{\# (positive identified = true positives)}}{\text{\# (all positive)}}$

- **Precision:** $\dfrac{\text{\# (positive identified = true positives)}}{\text{\# (predicted positive)}}$



Example

- 100 examples, 5% are positive.
- Just say NO: your accuracy is 95%
  - Recall = precision = 0
- Predict 4+, 96-; 2 of the +s are indeed positive
  - Recall:2/5; Precision: 2/4



- **Recall:** $\frac{\text{\# (positive identified = true positives)}}{\text{\# (all positive)}}$
- **Precision:** $\frac{\text{\# (positive identified = true positives)}}{\text{\# (predicted positive)}}$

Confusion Matrix

- Given a dataset of P positive instances and N negative instances:

		Predicted Class	
		Yes	No
Actual Class	Yes	TP	FN
	No	FP	TN

$$\text{accuracy} = \frac{TP + TN}{P + N}$$

- Imagine using classifier to identify positive cases (i.e., for information retrieval)

$$\text{precision} = \frac{TP}{TP + FP}$$

Probability that a randomly selected positive prediction is indeed positive

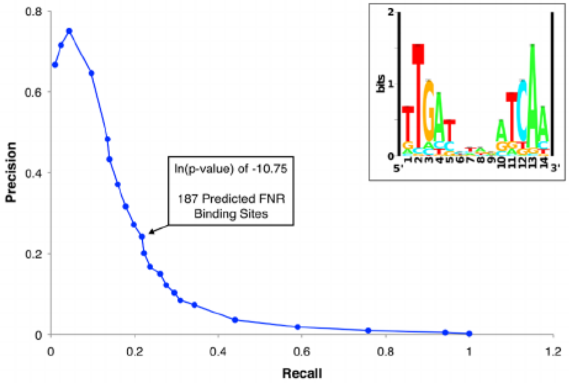
$$\text{recall} = \frac{TP}{TP + FN}$$

Probability that a randomly selected positive is identified

The notion of a confusion matrix can be usefully extended to the multiclass case (i,j) cell indicate how many of the i-labeled examples were predicted to be j

Relevant Metrics

- It makes sense to consider Recall and Precision together or combine them into a single metric.
- Recall-Precision Curve:



- F-Measure:
  - A measure that combines precision and recall is the harmonic mean of precision and recall.

$$F_\beta = (1+\beta^2) \cdot \frac{\text{precision} \cdot \text{recall}}{\beta^2 \cdot \text{precision} + \text{recall}}$$

  - F1 is the most commonly used metric.

Comparing Classifiers

Say we have two classifiers, *C1* and *C2*, and want to choose the best one to use for future predictions

Can we use training accuracy to choose between them?

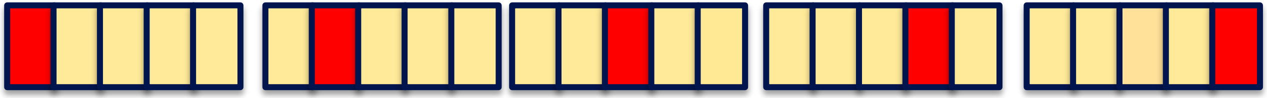
- No!

- What about accuracy on test data?

N-fold cross validation

- Instead of a single test-training split:

- Split data into N equal-sized parts



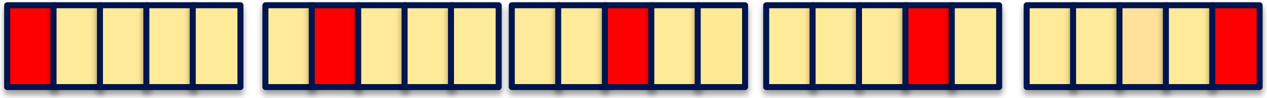
- Train and test N different classifiers
- Report average accuracy and standard deviation of the accuracy

Evaluation: significance tests

- You have two different classifiers, A and B
- You train and test them on the same data set using N-fold cross-validation
- For the n-th fold:

  accuracy(A, n), accuracy(B, n)

  p_n = accuracy(A, n) - accuracy(B, n)
- Is the difference between A and B's accuracies significant?



Hypothesis testing

- You want to show that hypothesis H is true, based on your data
  - (e.g. H = "classifier A and B are different")
- Define a null hypothesis H_0
  - (H_0 is the contrary of what you want to show)
- H_0 defines a distribution $P(m / H_0)$ over some statistic
  - e.g. a distribution over the difference in accuracy between A and B
- Can you refute (reject) H_0?

Rejecting H_0

- H_0 defines a distribution $P(M\ /H_0)$ over some statistic M
  - (e.g. M= the difference in accuracy between A and B)
- Select a significance value S
  - (e.g. 0.05, 0.01, etc.)
  - You can only reject H_0 if $P(m\ /H_0) \leq S$
- Compute the test statistic m from your data
  - e.g. the average difference in accuracy over your N folds
- Compute $P(m\ /H_0)$
- Refute H_0 with $p \leq S$ if $P(m\ /H_0) \leq S$

Paired t-test

- Null hypothesis (H_0; to be refuted):
  - There is no difference between A and B, i.e. the expected accuracies of A and B are the same
- That is, the expected difference (over all possible data sets) between their accuracies is 0:

  $H_0: E[p_D] = 0$
- We don't know the true $E[p_D]$
- N-fold cross-validation gives us N samples of p_D

Paired t-test

- Null hypothesis H_0: $E[diff_D] = \mu = 0$
- *m:* our estimate of μ based on *N* samples of $diff_D$

  $m = 1/N \sum_n diff_n$

- The estimated variance S^2:

  $S^2 = 1/(N-1) \sum_{1,N} (diff_n - m)^2$

- Accept Null hypothesis at significance level *a* if the following statistic lies in $(-t_{a/2,\, N-1}, +t_{a/2,\, N-1})$

$$\frac{\sqrt{N}m}{S} \sim t_{N-1}$$

Decision Trees - Summary

- Hypothesis Space:
  - Variable size (contains all functions)
  - Deterministic; Discrete and Continuous attributes
- Search Algorithm
  - ID3 - batch
  - Extensions: missing values
- Issues:
  - What is the goal?
  - When to stop? How to guarantee good generalization?
- Did not address:
  - How are we doing? (Correctness-wise, Complexity-wise)