Decision Trees

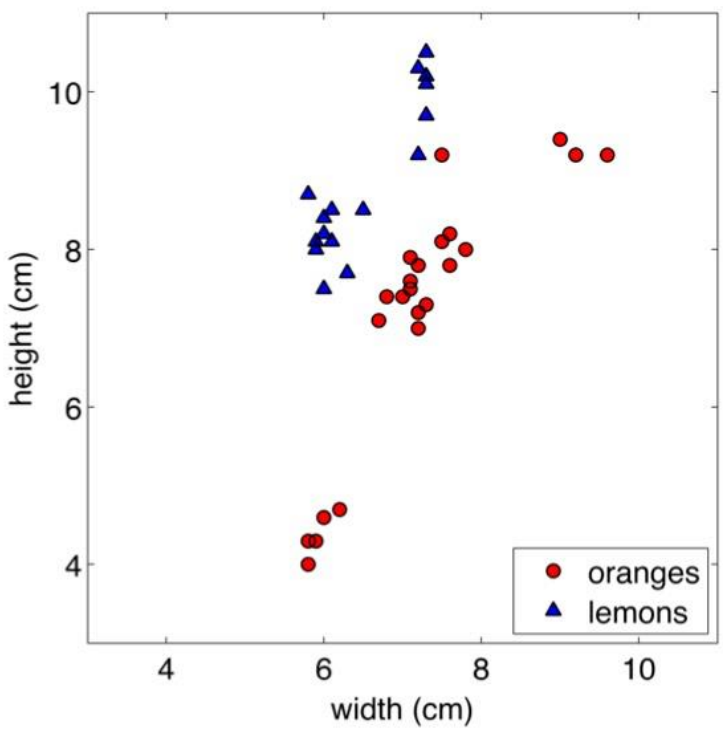
Claude Monet, “The Mulberry Tree”

Slides from Pedro Domingos, Luke Zettlemoyer, Carlos Guestrin, and Andrew Moore

CSC411/2515: Machine Learning and Data Mining, Winter 2018

Michael Guerzhoy and Lisa Zhang

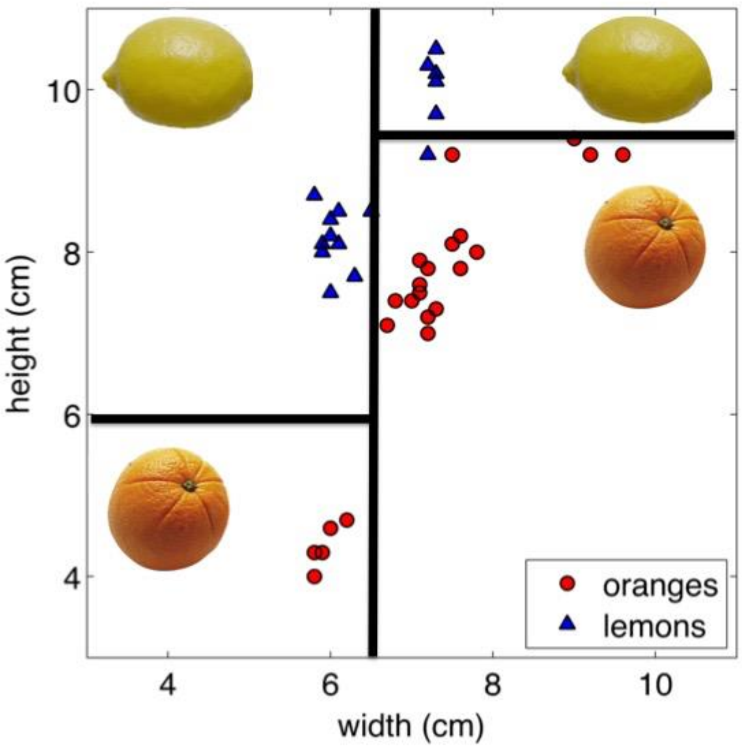
Orange vs Lemon?

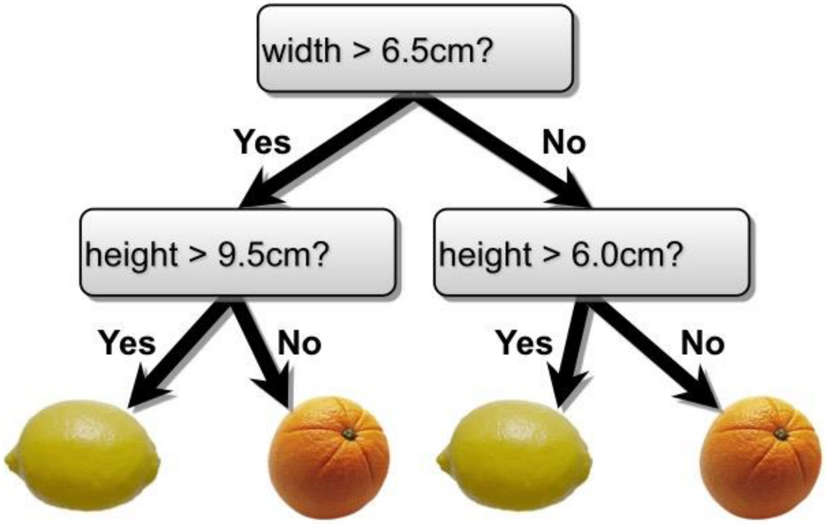


What classifiers can we use to classify fruit as oranges or lemons?

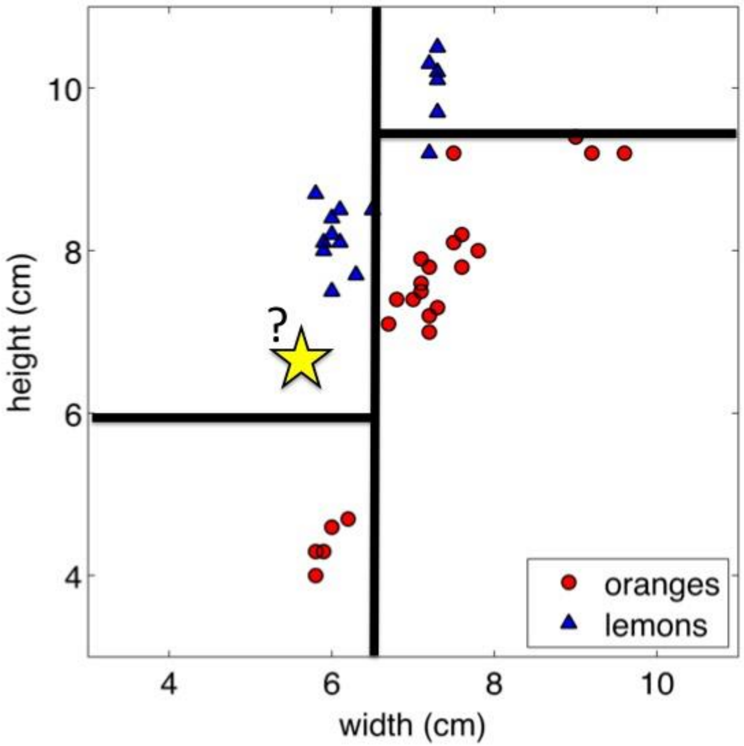
- kNN
- Logistic Regression
- Neural Networks

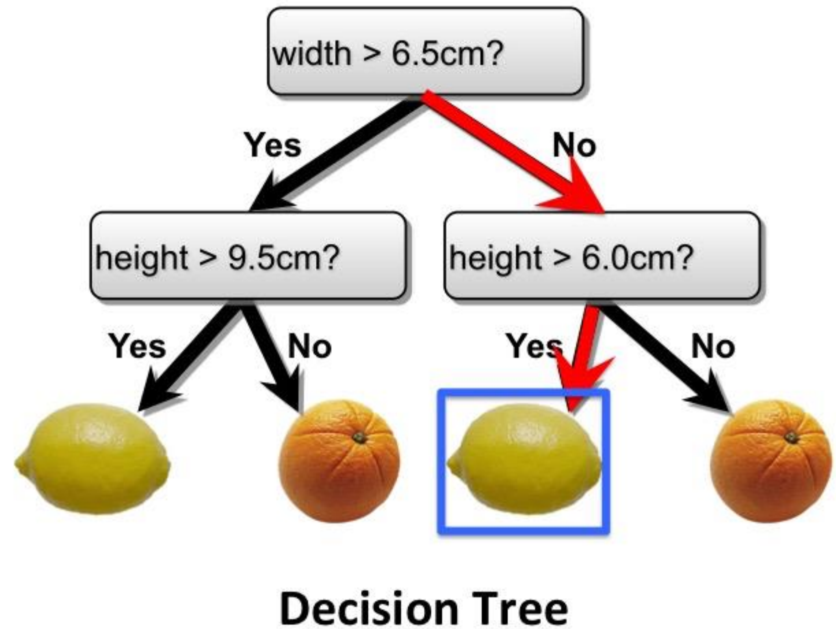
Decision Trees





Decision Trees





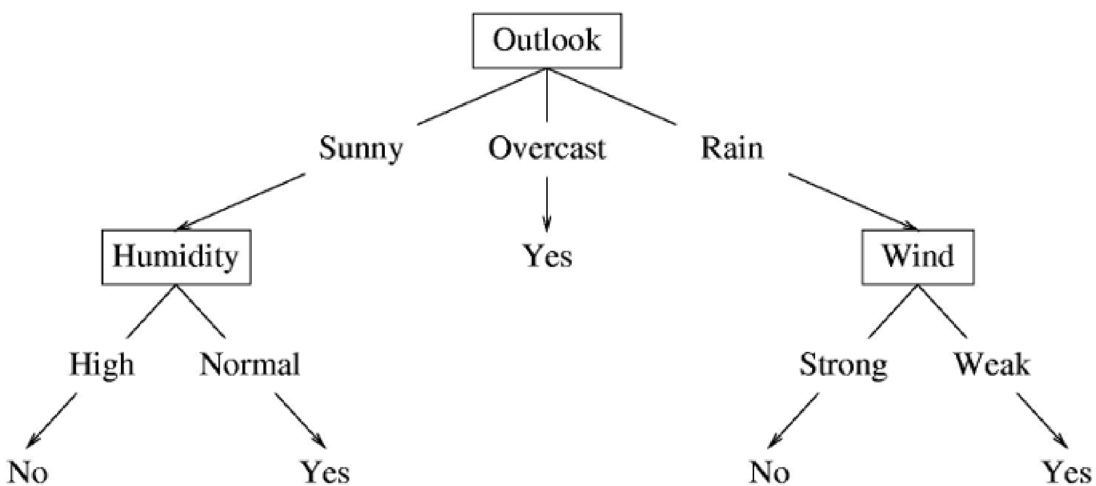
Yes: orange
No: lemon

Decision Trees

- **Internal nodes**

  test the value of particular features x_j

  branch according to the results of the test
- **Leaf nodes** specify the class $h(x)$
- Simpler Example: Predicting whether we'll play tennis (outputs: Yes, No)



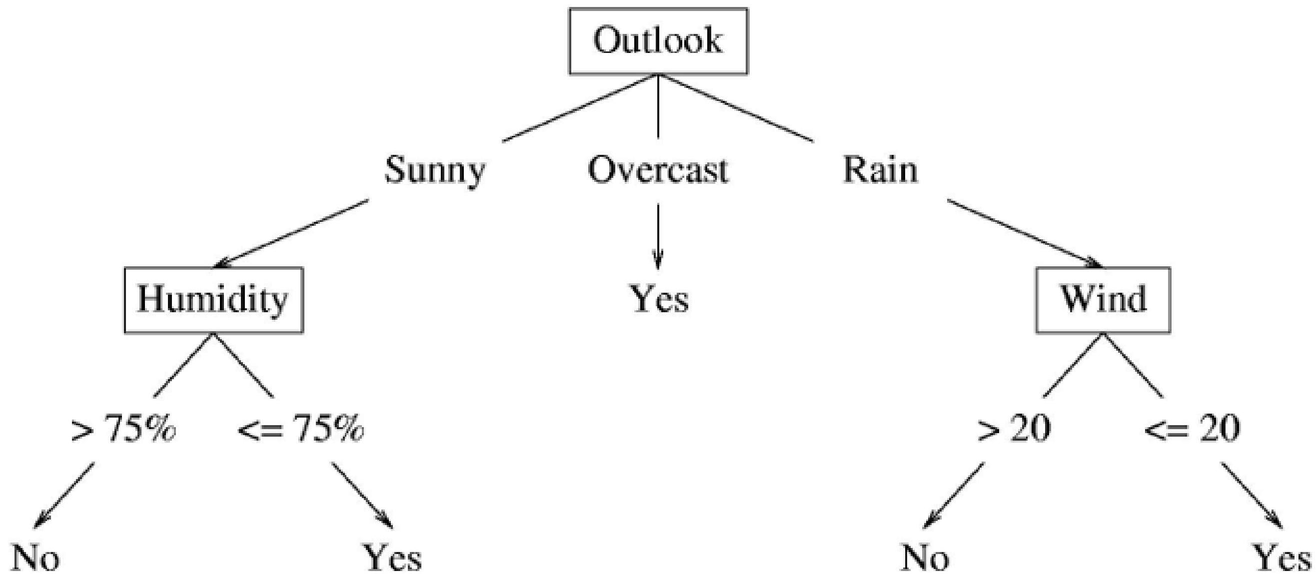
- Features: **Outlook (x_1), Temperature (x_2), Humidity (x_3),** and **Wind (x_4)**.
  - $x = (\mathbf{Sunny}, \mathbf{Hot}, \mathbf{High}, \mathbf{Strong})$ will be classified as **No**
  - The **Temperature** feature is irrelevant

Decision Trees

- As close as it gets to an “off-the-shelf” classifier
- Random forests – averages of multiple decision trees classifiers – often perform the best on Kaggle
  - Kaggle.com: a website that hosts machine learning “bake-offs”
  - Though carefully-engineered neural networks and other methods win as well

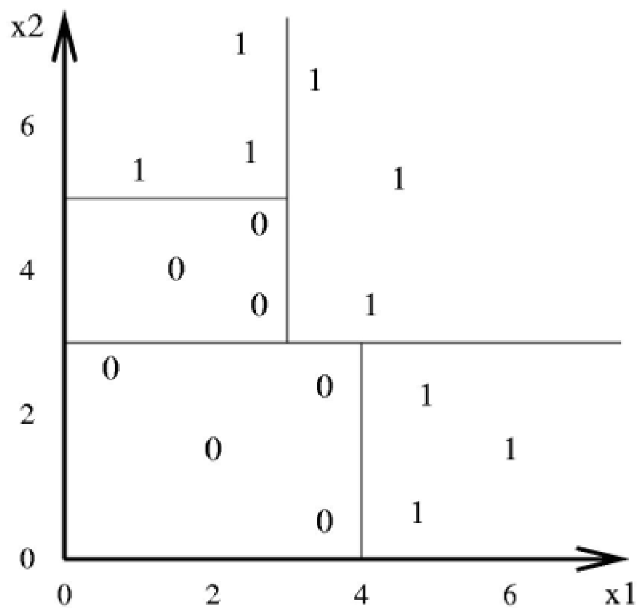
Decision Trees: Continuous Features

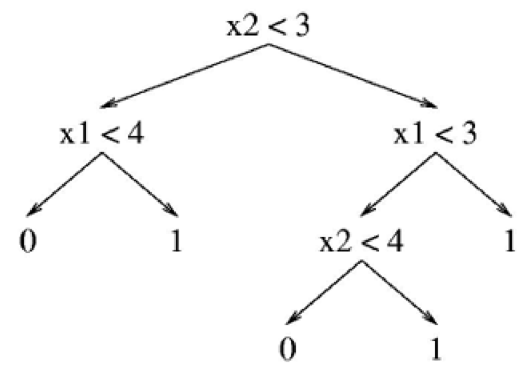
- If the features are continuous, internal nodes may test the value of a feature against a threshold



Decision Trees: Decision Boundaries

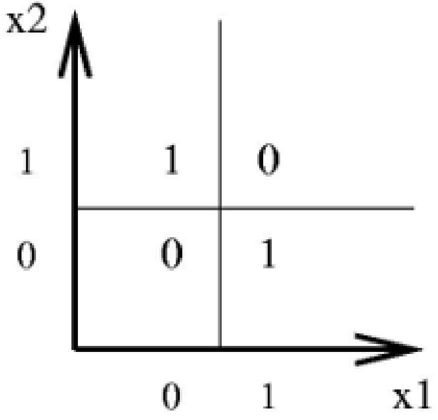
- Decision trees divide the feature space into axis-parallel rectangles
- Each rectangle is labelled as one of the K classes

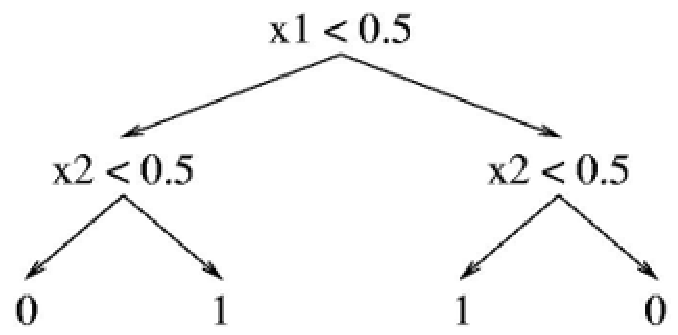




Decision Trees: Model Capacity

- Any Boolean function can be represented
- Might need exponentially many nodes in order to represent the function





Decision Trees: Model Capacity

- As the number of nodes in the tree/the depth of the tree increases, the hypothesis space grows
  - Depth 1 (“decision stump”): can represent any Boolean function of one feature
  - Depth 2: Any Boolean function of two features + some Boolean functions of three features (e.g. $(x_1 \land x_2) \lor (\neg x_1 \land \neg x_3)$)
  - Etc.

Hypothesis space: the set of all possible functions $h_\theta(x)$

Learning the Parity Function

x_1	x_2	x_3	y
0	0	0	0
0	0	1	0
0	1	0	1
0	1	1	1
1	0	0	1
1	0	1	1
1	1	0	0
1	1	1	0

- Suppose we want to learn to distinguish strings of parity 0 and strings of parity 1
  - # of 1's in the string mod 2
- All splits will look equally good!
- Need 2^n examples to learn the function correctly
- If there are extra random features, cannot do anything

Learning Decision Trees

- Learning the simplest (smallest) decision tree is an NP-complete problem
  - See Hyafil and Rivest, “Constructing Optimal Binary Decision Trees is NP-complete,” *Information Processing Letters* Vol 5(1), 1976
- So use a greedy heuristic to construct the tree
  - Start from an empty decision tree
  - Select the **best** attribute/feature to split on
  - Recurse

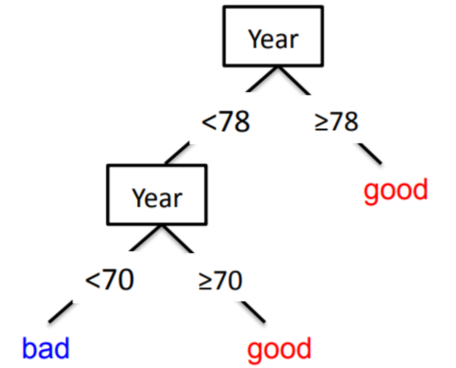
But what does “best” mean?
We’ll come back to this.

Learning Decision Trees (Binary Features)

```
GrowTree(S)
  if (y=0 for all < x, y >∈ S)
    return new leaf(0)
  else if (y=1 for all < x, y >∈ S)
    return new leaf(1)
  else
    choose the best attribute x_j
    S_0 = {< x, y >∈ S s.t. x_j = 0}
    S_1 = {< x, y >∈ S s.t. x_j = 1}
    return new node(x_j, GrowTree(S_0), GrowTree(S_1))
```

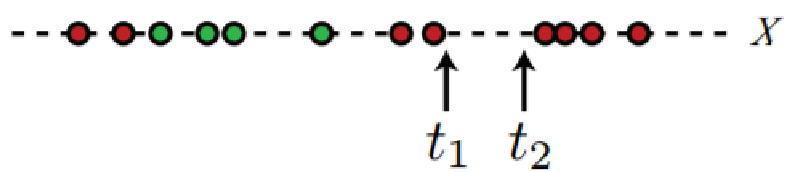
Threshold splits

- For continuous features, need to decide on a threshold t
  - Branches: $(x_j < t), (x_j \geq t)$
- Want to allow repeated splits along a path
  - Why?

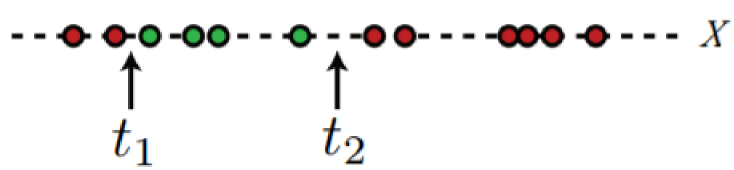


Set of all possible thresholds

- Branches: $(x_j < t), (x_j \geq t)$
- Can't try all real t
- But only a finite number of t's are important



- Sort the values of x_j into $z_1, \dots, z_m$, consider split points of the form $z_i + (z_{i+1} - z_i)/2$
- Only splits between different examples of different classes matter



Choosing the Best Attribute

- Most straightforward idea: do a 1-step lookahead, and choose the attribute such that if we split on it, we get the lowest error rate on the training data
  - Do a majority vote if not all y's agree at a leaf

```
ChooseBestAttribute(S)
 Choose j  s.t. J_j is minimized
```

$S_o =< x, y >\in S\ s.t.\ x_j = 0$

$S_1 =< x, y >\in S\ s.t.\ x_j = 1$

y_0: the most common value of y in S_0

y_1: the most common value of y in S_1

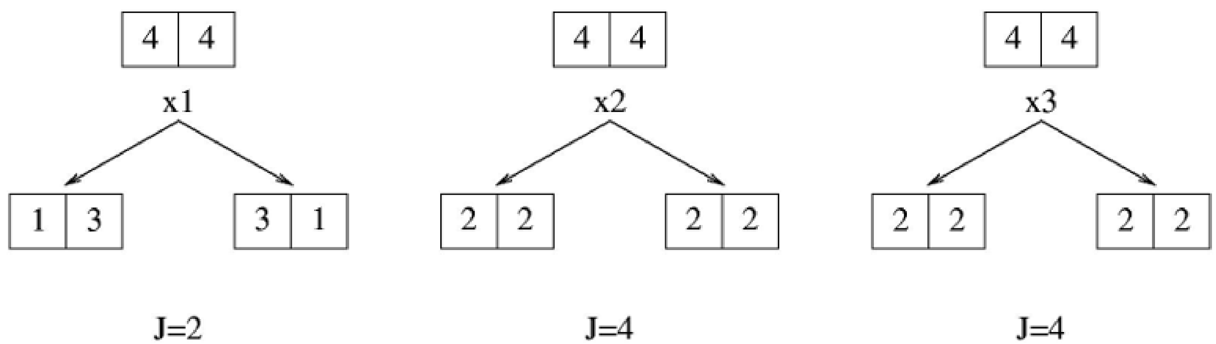
J_0=#$\{< x.y >\in S_0, y \neq y_0\}$, J_1=#$\{< x.y >\in S_1, y \neq y_1\}$

$J_j = J_0 + J_1$ #total number of errors if we split on x_j

Choosing the Best Attribute (example)

x_1	x_2	x_3	y
0	0	0	1
0	0	1	0
0	1	0	1
0	1	1	1
1	0	0	0
1	0	1	1
1	1	0	0
1	1	1	0

Four 0's,
four 1's

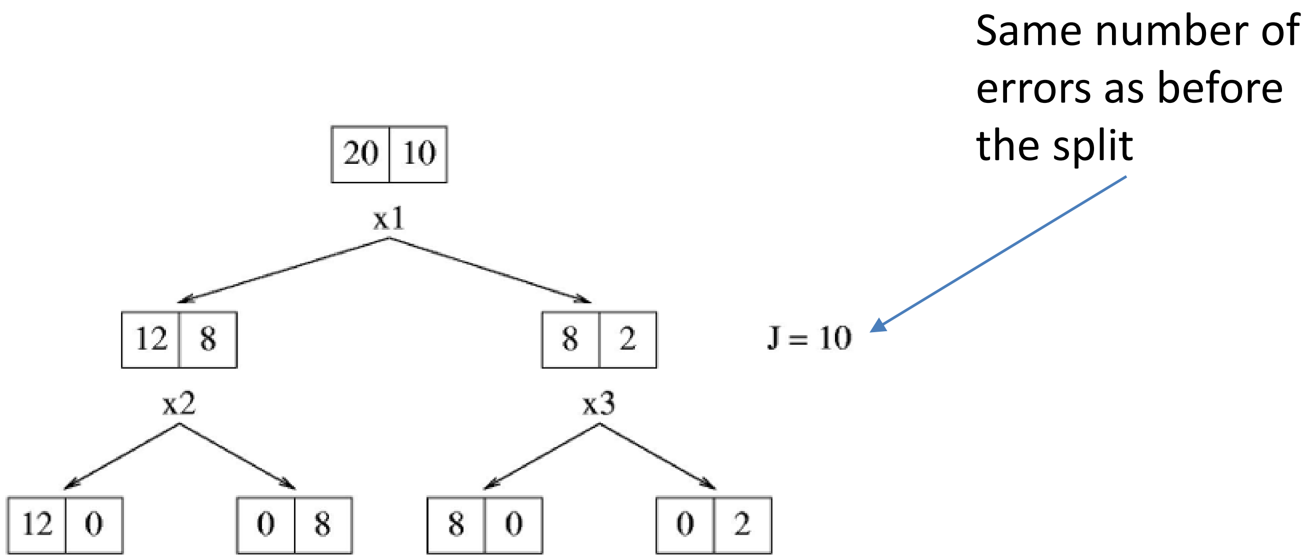


One 0, three 1's

Splitting on x_1 produces just two errors, splitting on other attributes produces four errors

Choosing the Best Attribute

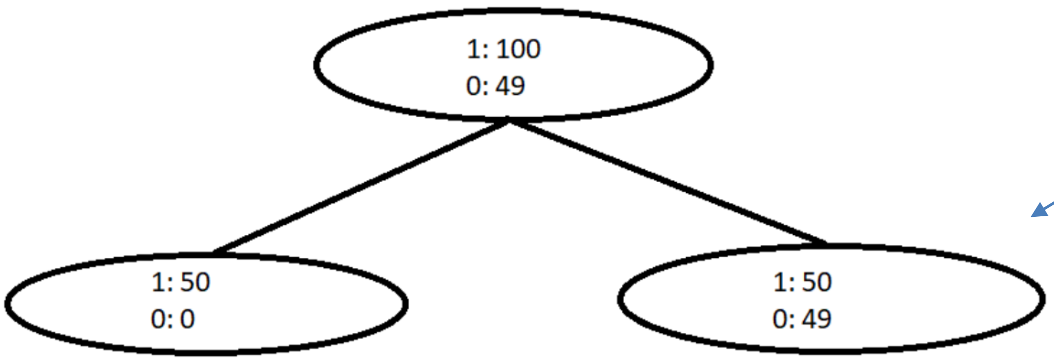
- The number of errors won't always tell us that we're making progress



Choosing the Best Attribute

- The number of errors won't always tell us that we're making progress

Same number of errors as before the split



A digression on Information Theory

- Suppose V is a random variable with the probability distribution

$P(v = 0)$	$P(v = 1)$	$P(v = 2)$	$P(v = 3)$	$P(v = 4)$	$P(v = 5)$	$P(v = 6)$
0.1	0.002	0.52	…	…	…	…

- The *surprise* $S(V = v)$ for each value of v is defined as

$$S(V = v) = -\log_2 P(V = v)$$

  - The smaller the probability of the event, the larger the surprise if we observe the event
  - 0 surprise for events with probability 1
  - Infinite surprise for events with probability 0

Surprise and Message Length

- Suppose we want to communicate the value of v to a receiver. It makes sense to use longer binary codes for rarer values of V
  - Can use $-\log_2 P(V=v)$ bits to communicate v
    - Check that this makes sense if $P(V=0)=1$ (no need to transmit any information) and $P(V=0)=P(V=1)=\frac{1}{2}$ (need one bit to transmit v)
    - Fractional bits only make sense for longer messages
    - Example: UTF-8 uses more bytes for rare symbols
    - "Amount of information"
    - We won't go into this in further detail. We need to make sure that the receiver can decode the message even though different symbols take up different amounts of bits, for example

Entropy: Average/Expected Surprise

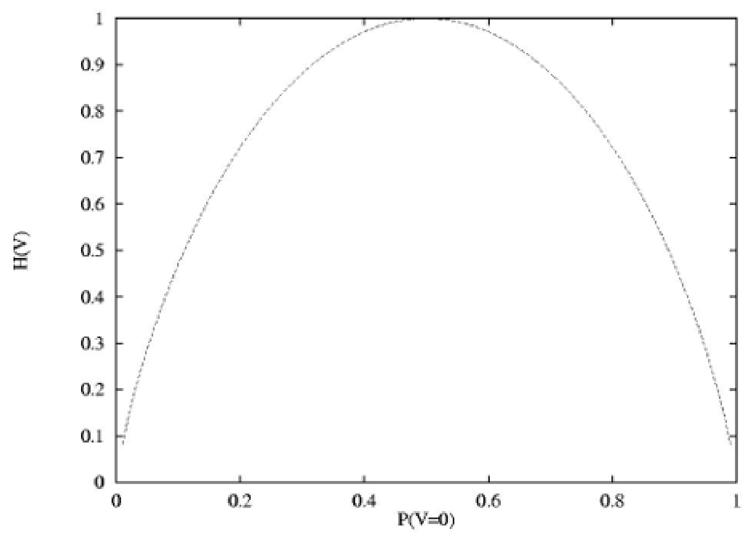
- The entropy of V, $H(V)$ is defined as

$$H(V) = \sum_{v} -P(V = v) \log_2 P(V = v)$$

- The average surprise for one "trial" of V
  - The average message length when communicating the outcome v
- The average amount of information we get by seeing one value of V (in bits)

Entropy: How "Spread Out" the distribution is

- High entropy of V means we cannot predict what the value of V might be
- Low entropy means we are pretty sure we know what the value of V is every time

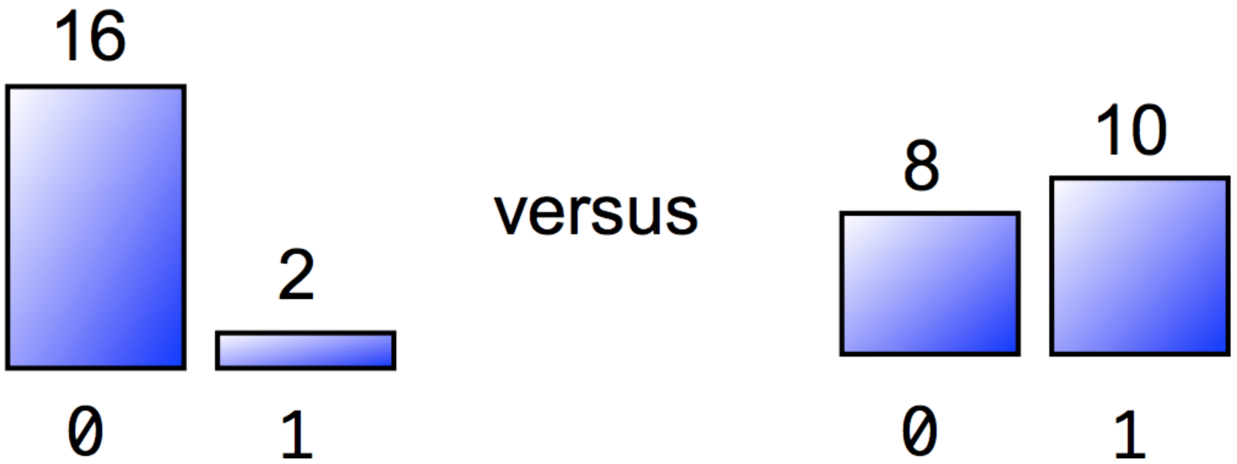


The entropy of a Bernoulli variable is maximized when $p = 0.5$

Entropy of Coin Flips

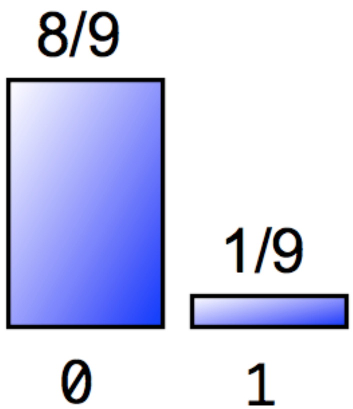
Sequence 1:
0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 1 0 0 ... ?

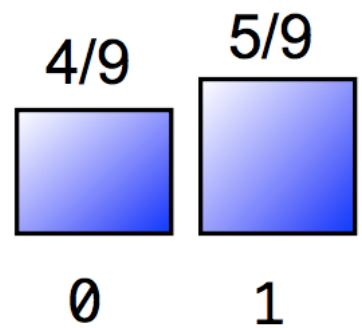
Sequence 2:
0 1 0 1 0 1 1 1 0 1 0 0 1 1 0 1 0 1 ... ?



Entropy of Coin Flips

$$H(V) = \sum_{v} -P(V = v) \log_2 P(V = v)$$





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

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

Higher Entropy; more uncertainty about the outcome

Three views of Entropy

We are considering a random variable V, and a sample v from it

The Entropy is

1. Average Surprise at v
2. Average message length when transmitting v in an efficient way
3. Measure of the ”spread-out”-ness of the distribution V

Conditional Entropy

- The amount of information needed to communicate the outcome of B given that we know A

$$H(B|A) = \sum_a P(A = a)H(B|A = a)$$

$$= \sum_a P(A = a)[-\sum_b P(B = b|A = a) \log_2 P(B = b|A = a)]$$

$H(B)$ if A and B are indep.
0 if $A = B$ always.

Mutual Information

- The amount of information we learn about the value of B by knowing the value of A

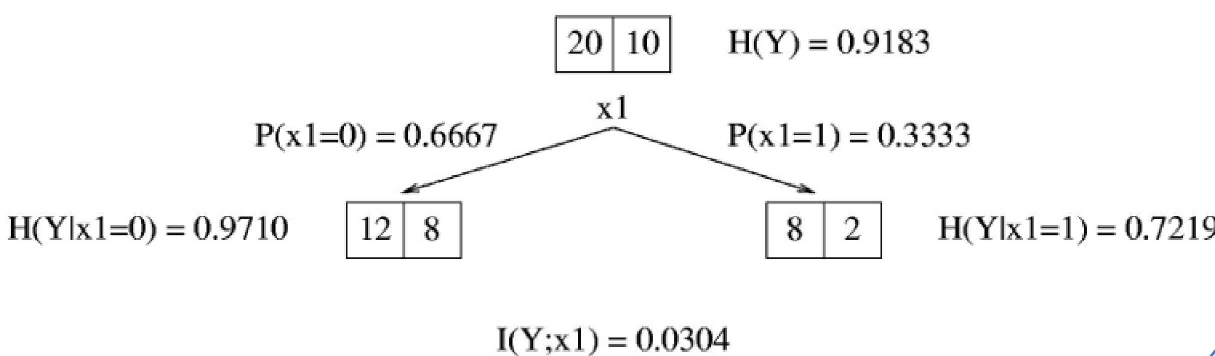
$$I(A;B) = H(B) - H(B|A) = H(A) - H(A|B)$$

# of bits of information we know about B if we know A = # of bits need to communicate the value of B - # of extra bits need to communicate the value of B if we know A

Also called "Information Gain"

Mutual Information

- Suppose the class Y of each training example and the value of feature x_1 are random variables. The mutual information quantifies how much x_1 tells us about the value of Y

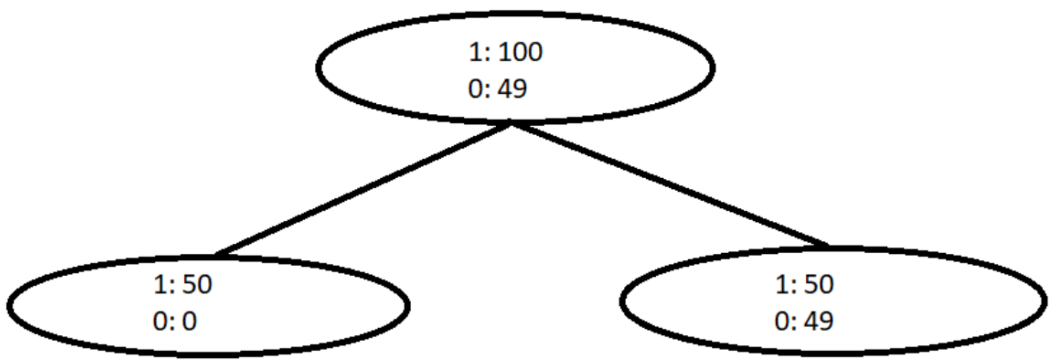


Lower is better for higher I(Y;X)

$$I(Y;X) = H(Y) - H(Y|X) = H(Y) - \sum_{x} P(X=x)H(Y|X=x)$$

Mutual Information

- What is the mutual information of this split? (Exercise)

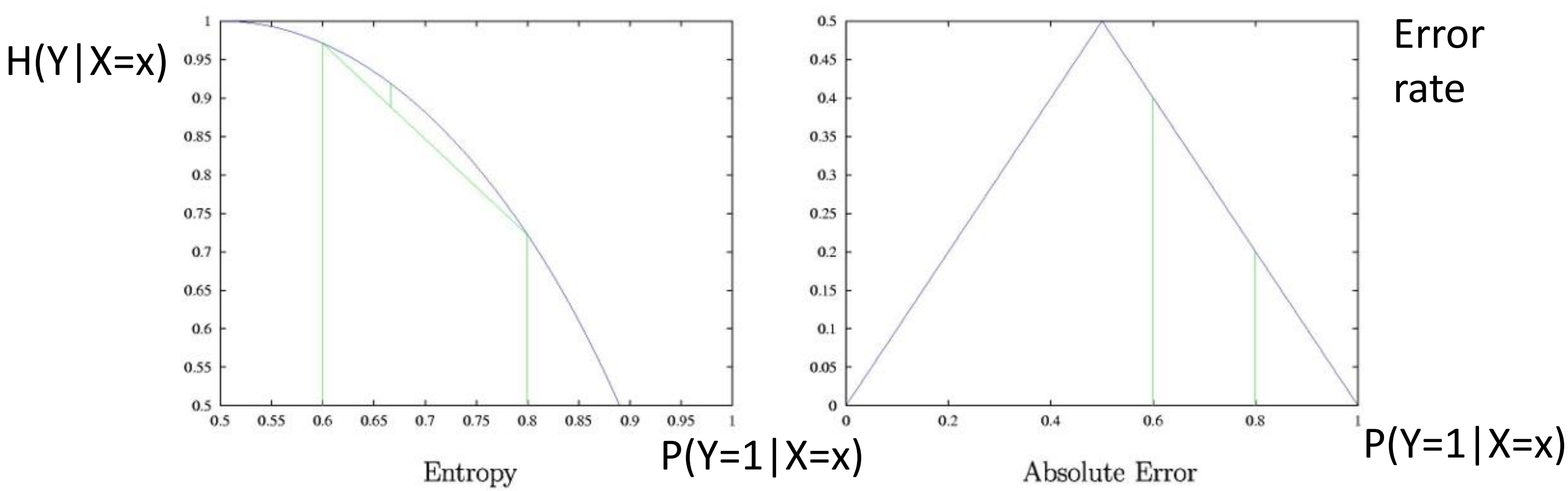


Mutual Information Heuristic

- Pick the attribute x_j such that $I(x_j; Y)$ is as high as possible

Mutual Information Heuristic

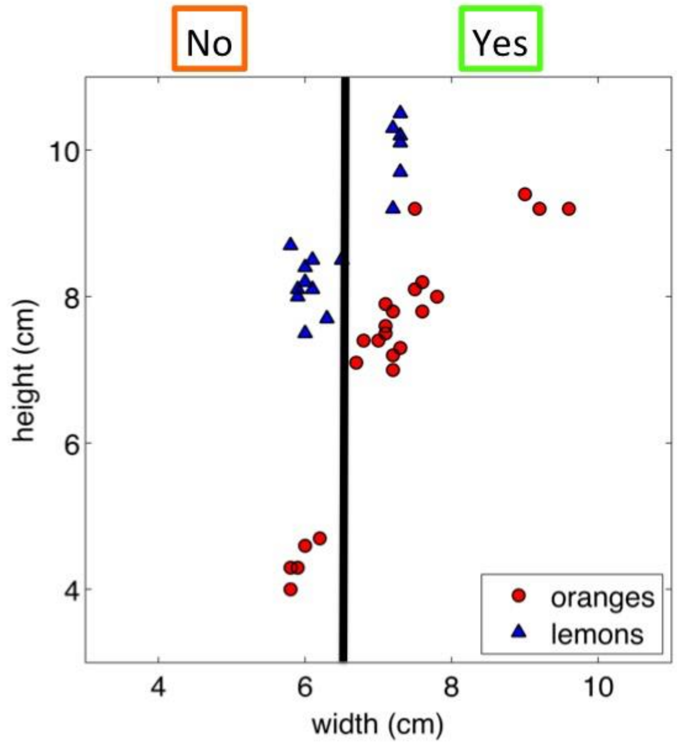
- If we had a correct rate of 0.7, and split the data into two groups where the correct rates were 0.6 and 0.8, we will not make progress on the number of errors, but we will make progress on the average $H(Y|X)$

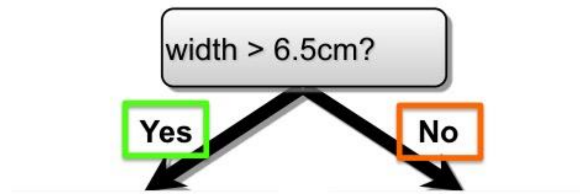


- We could use any concave function of p instead of computing the conditional entropy in

$$I(Y;X) = H(Y) - H(Y|X) = H(Y) - \sum_x P(X=x)H(Y|X=x)$$

Learning Decisions Trees: Summary





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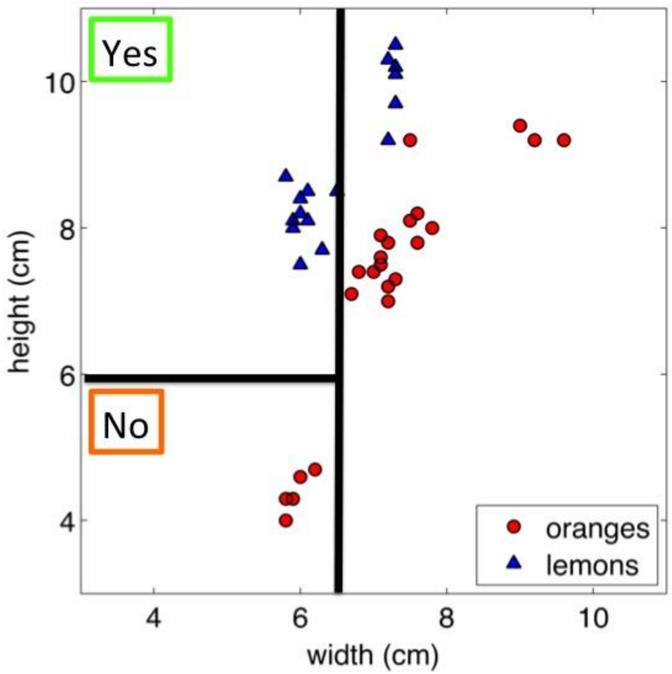

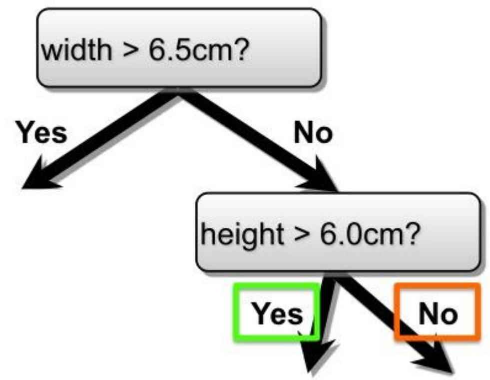

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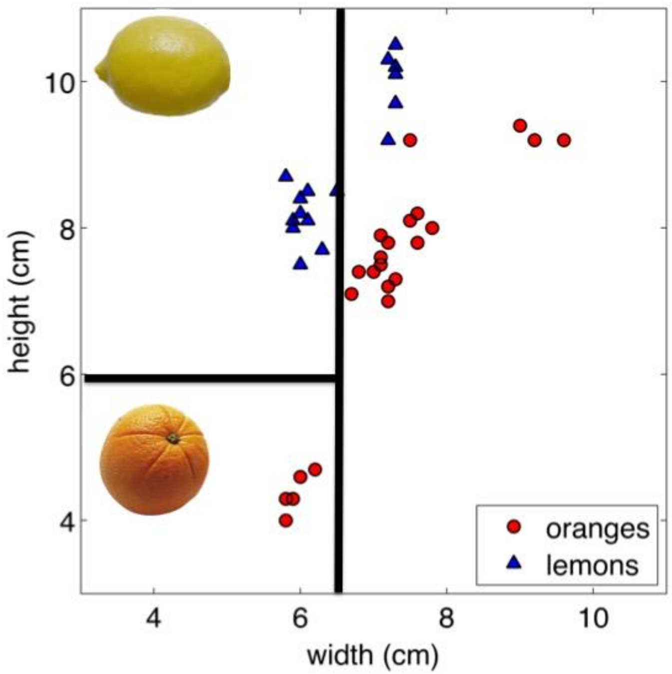

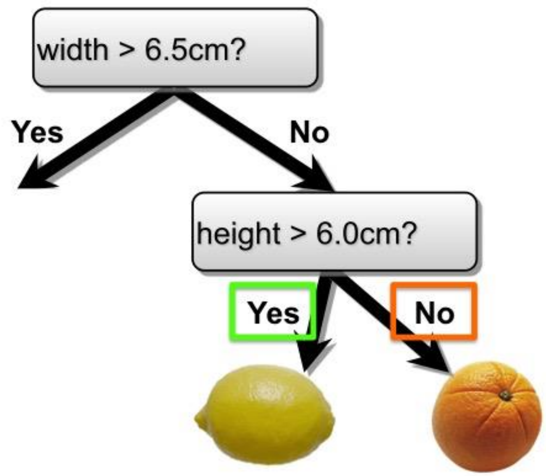

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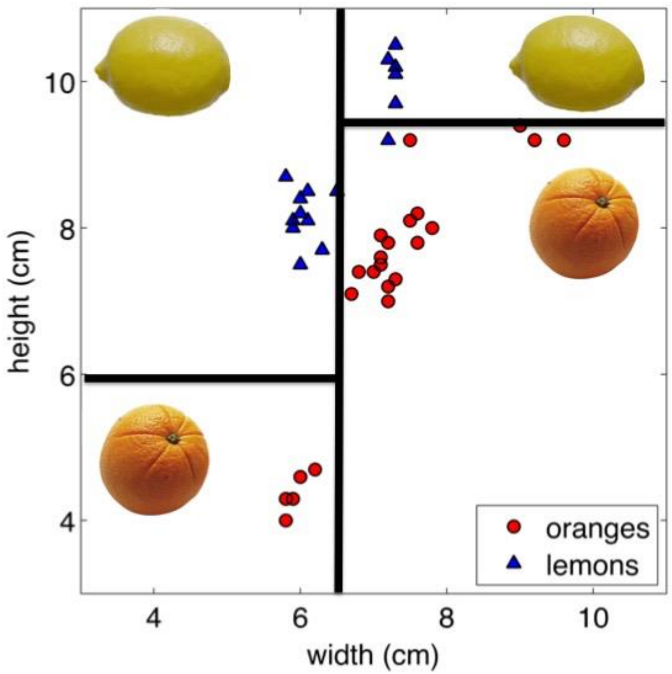
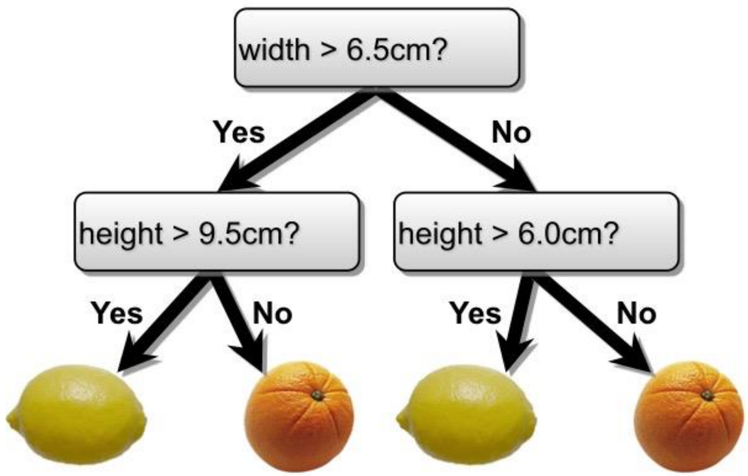




Aside: Cross Entropy

- The cost function we used when training classifiers was called the Cross Entropy

$$H(P, Q) = -\sum_v P(V = v) \log Q(V = v)$$

With this probability

Transmit this many bits

- The amount of information we need to transmit if we are using a coding scheme optimized for distribution Q, when the actual distribution over V is P

Aside: Cross Entropy

Change of notation: the random variable is y

- $H(P, Q) = -\sum_y P(X = y) \log Q(X = y)$
- When used as a cost function:
  - P: the observed distribution (we know the answer)

Y = 0	Y=1	Y=2	Y=3
$P(Y^{(0)} = 0 \mid x^{(0)}) = 0$	$P(Y^{(0)} = 1 \mid x^{(0)}) = 1$	$P(Y^{(0)} = 2 \mid x^{(0)}) = 0$	$P(Y^{(0)} = 3 \mid x^{(0)}) = 0$

  - Q: what the classifier actually outputs

Y = 0	Y=1	Y=2	Y=3
$P(Y^{(0)} = 0 \mid x^{(0)}) = 0.1$	$P(Y^{(0)} = 1 \mid x^{(0)}) = .7$	$P(Y^{(0)} = 2 \mid x^{(0)}) = .15$	$P(Y^{(0)} = 3 \mid x^{(0)}) = .15$

  - Smaller $H(P, Q)$ means the distributions P and Q are more similar
    - Different conditional distribution for every value of $x^{(i)}$!
  - Note: we previously explained the function as the negative log-likelihood of the datapoint. That also works

Missing Attribute Values

- Can use examples with missing attribute values
  - If node n tests missing attribute A, assign the most common value of attribute A among the other examples in node n
  - Assign the most common value of A among examples with the same target value
  - Assign probability p_i to each possible value v_i of A. Assign fraction p_i of example to each descendent in the tree

Avoiding Overfitting

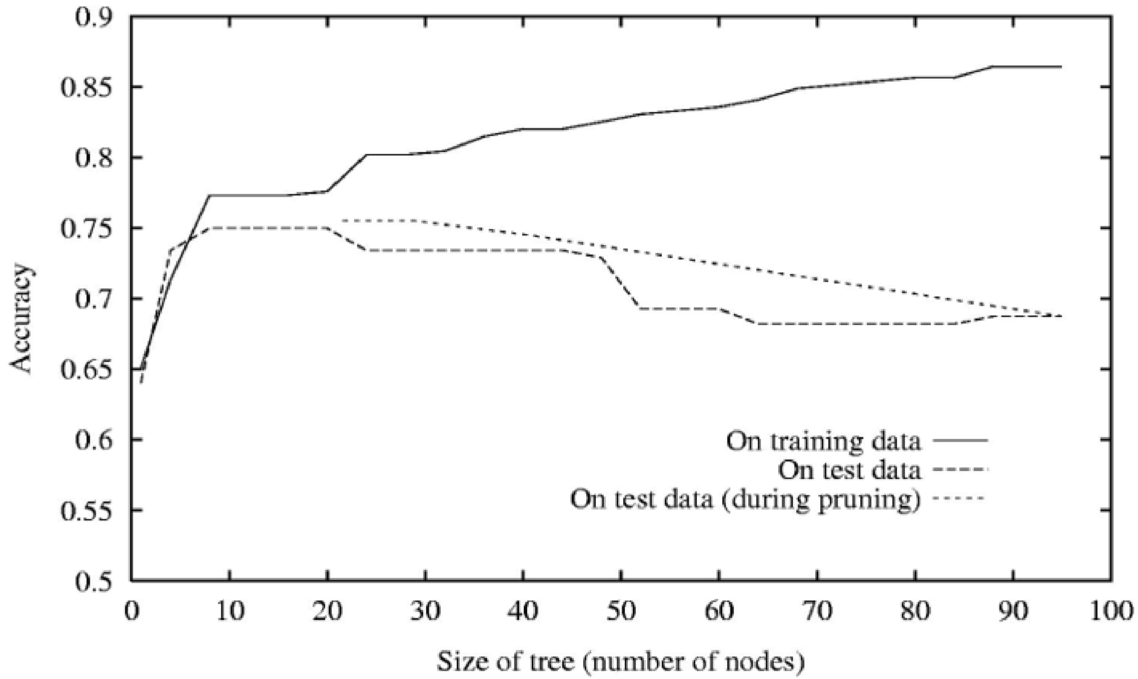
- Stop growing the tree early
- Or grow full tree, then prune

- The “best” tree:
  - Measure performance on the validation set
  - Measure performance on the training data, but add a penalty term that grows with the size of the tree

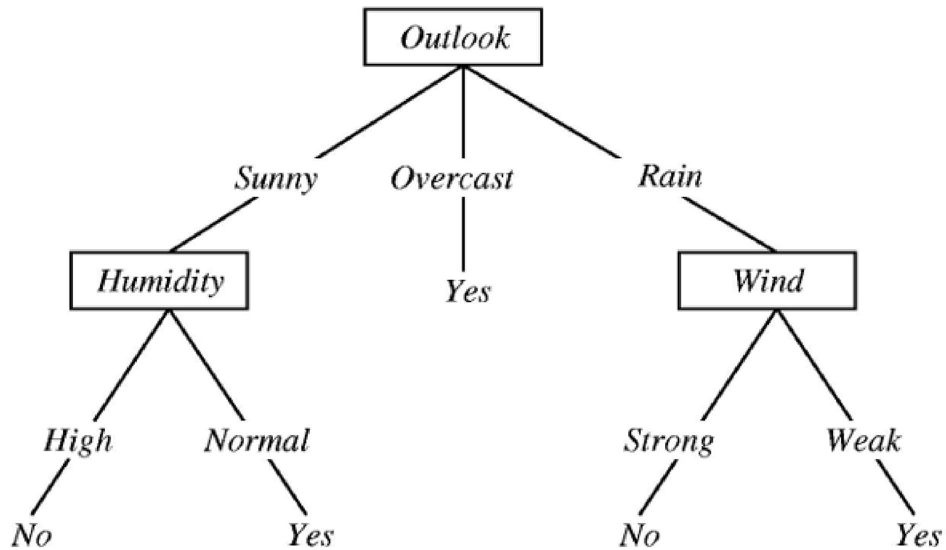
Reduced-Error Pruning

- Repeat
  - Evaluate the impact on the *validation set* of pruning each possible node (and all those below it)
  - Greedily remove the node such that removing the node improves validation set accuracy the most

Effect of Reduced-Error Pruning



Converting a Tree to Rules



IF $(Outlook = Sunny)\ AND\ (Humidity = High)$
THEN $PlayTennis = No$

IF $(Outlook = Sunny)\ AND\ (Humidity = Normal)$
THEN $PlayTennis = Yes$

...

Rule Post-Pruning

- Convert the tree into an equivalent set of rules
  - “If sunny and warm, there will be a tennis match”
  - “If rainy, there will not be a tennis match”
  - …
- Prune each rule independently of the others
  - Is removing the rule improving validation performance
- Sort the rules into a good sequence for use

Scaling Up

- Decision trees algorithms like ID3 and C4.5 assume random access to memory is fast
  - Good for up to hundreds of thousands of examples
- SPRINT, SLIQ: multiple sequential scans of data
  - OK for millions of examples
- VDFT: at most one sequential scan
  - “stream mode”