Recap of Probability and Decision Trees

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Slides adapted from Nick Rouzzi, Sriraam Natarajan and Vibhav Gogate

Roadmap of this Lecture

- **Part I: Recap of Probability, Random Variables and Entropy**

- Part II: Decision Trees

Discrete Probability

- **Sample space** specifies the set of possible outcomes
  - For example, $\Omega = \{\mathrm{H}, \mathrm{T}\}$ would be the set of possible outcomes of a coin flip
- Each element $\omega \in \Omega$ is associated with a number $\mathrm{p}(\omega) \in [0,1]$ called a **probability**

$$\sum_{\omega \in \Omega} p(\omega) = 1$$

  - For example, a biased coin might have $p(H) = .6$ and $p(T) = .4$

Discrete Probability

- An **event** is a subset of the sample space
  - Let $\Omega = \{1, 2, 3, 4, 5, 6\}$ be the 6 possible outcomes of a dice role
  - $A = \{1, 5, 6\} \subseteq \Omega$ would be the event that the dice roll comes up as a one, five, or six
- The probability of an event is just the sum of all of the outcomes that it contains
  - $p(A) = p(1) + p(5) + p(6)$

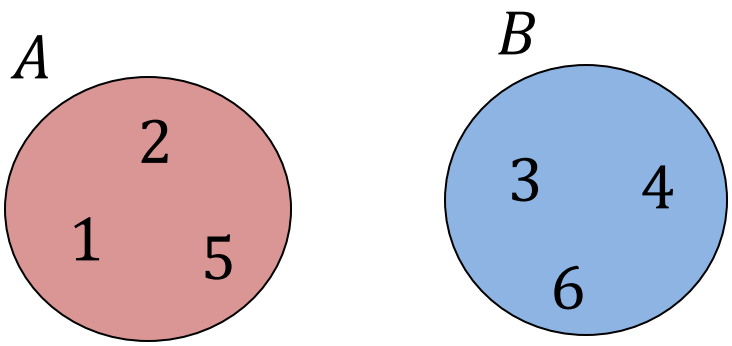
Independence

- Two events A and B are **independent** if

$$p(A \cap B) = p(A)P(B)$$

Let's suppose that we have a fair die: $p(1) = \ \ldots = p(6) = 1/6$

If $A = \{1, 2, 5\}$ and $B = \{3, 4, 6\}$ are A and B indpendent?



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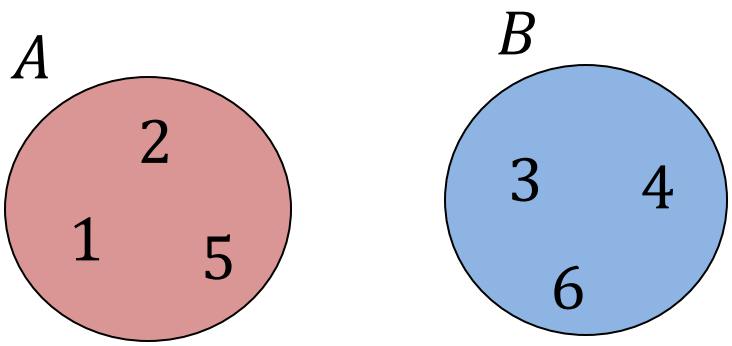
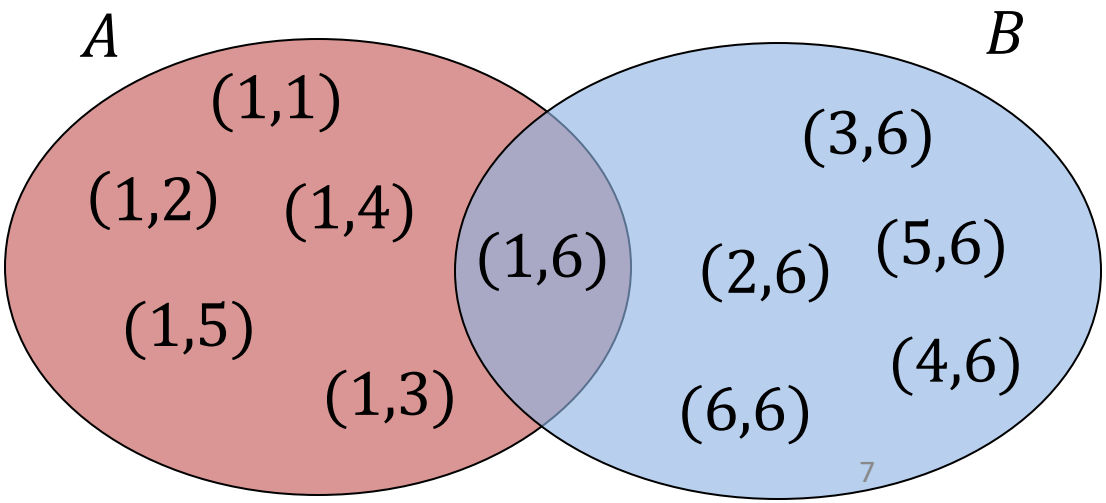


No!

$$p(A \cap B) = 0 \neq \frac{1}{4}$$

Independence

- Now, suppose that $\Omega = \{(1,1), (1,2), \dots, (6,6)\}$ is the set of all possible rolls of two **unbiased** dice
- Let $A = \{(1,1), (1,2), (1,3), \dots, (1,6)\}$ be the event that the first die is a one and let $B = \{(1,6), (2,6), \dots, (6,6)\}$ be the event that the second die is a six
- Are A and B independent?



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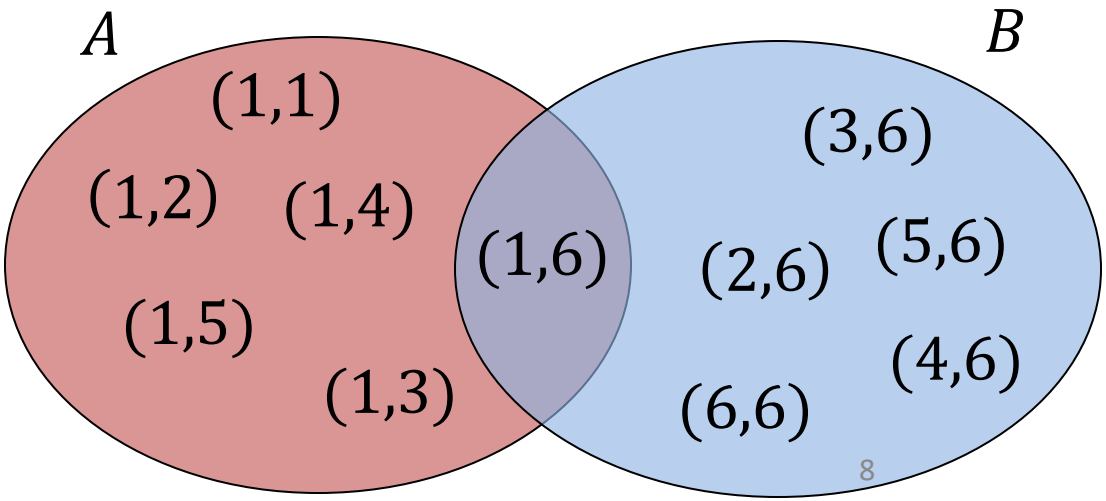

Yes!

$$p(A \cap B) = \frac{1}{36} = \frac{1}{6} * \frac{1}{6}$$

Conditional Probability

- The **conditional probability** of an event A given an event B with $p(B) > 0$ is defined to be

$$p(A|B) = \frac{p(A \cap B)}{P(B)}$$

- This is the probability of the event $A \cap B$ over the sample space $\Omega' = B$

- Some properties:
  - $\sum_{\omega \in \Omega} p(\omega|B) = 1$
  - If A and B are independent, then $p(A|B) = p(A)$

Discrete Random Variables

- A discrete **random variable**, X, is a function from the state space Ω into a discrete space D
  - For each $x \in D$,

$$p(X = x) \equiv p(\{\omega \in \Omega : X(\omega) = x\})$$

    is the probability that X takes the **value** x

  - $p(X)$ defines a probability distribution
    - $\sum_{x \in D} p(X = x) = 1$
- Random variables partition the state space into disjoint events

Example: Pair of Dice

- Let Ω be the set of all possible outcomes of rolling a pair of dice
- Let p be the uniform probability distribution over all possible outcomes in Ω
- Let $X(\omega)$ be equal to the sum of the value showing on the pair of dice in the outcome ω
  - $p(X = 2) = ?$
  - $p(X = 8) = ?$

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  - $p(X = 8) = \mathbf{\frac{5}{36}}$

Discrete Random Variables

- We can have vectors of random variables as well

$$X(\omega) = [X_1(\omega), \ldots, X_n(\omega)]$$

- The **joint distribution** is $p(X_1 = x_1, \ldots, X_n = x_n)$ is

$$p(X_1 = x_1 \cap \cdots \cap X_n = x_n)$$

  typically written as

$$p(x_1, \ldots, x_n)$$

- Because $X_i = x_i$ is an event, all of the same rules from basic probability apply

Entropy

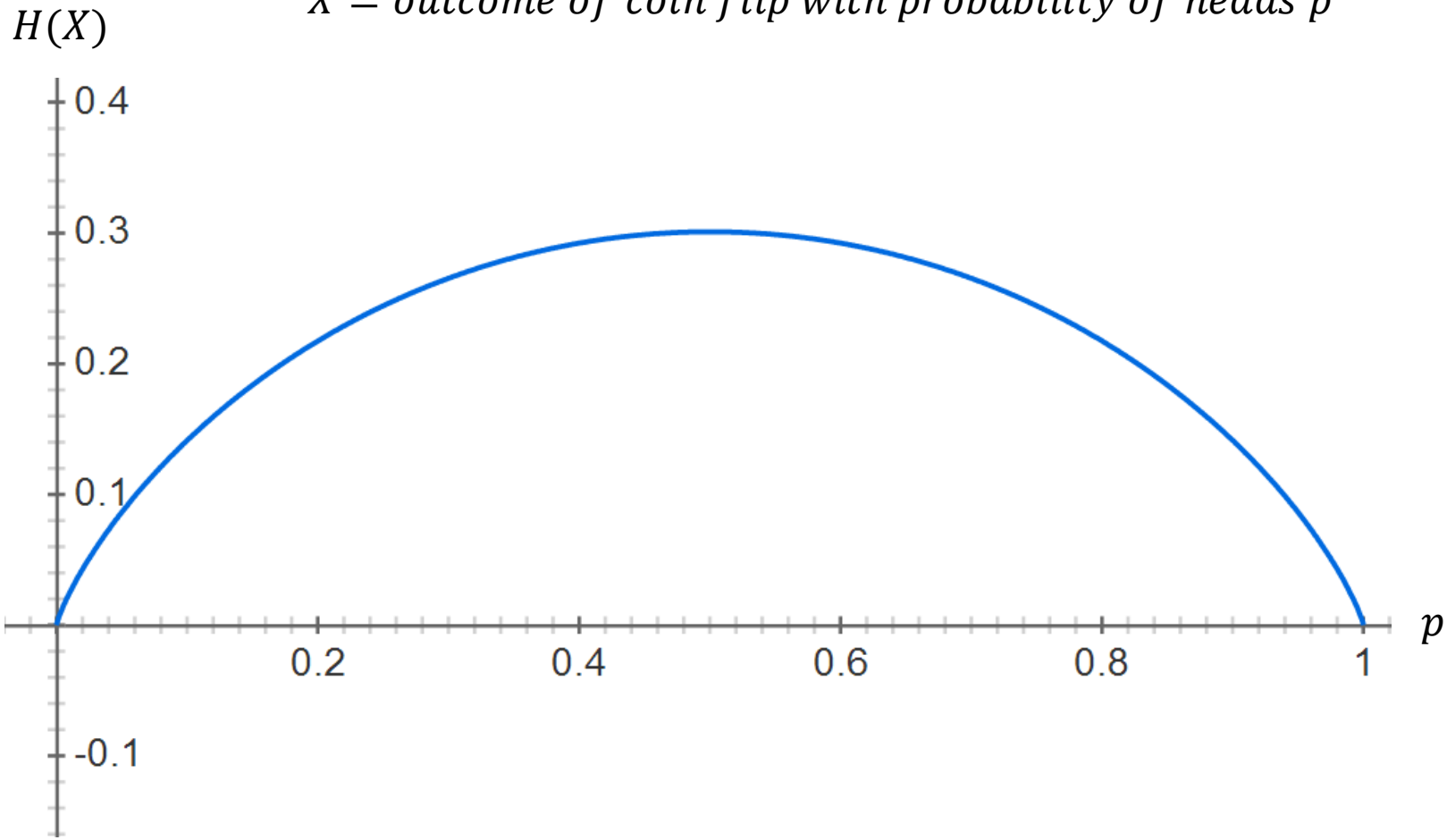
- A standard way to measure uncertainty of a random variable is to use the entropy

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

- Entropy is maximized for uniform distributions
- Entropy is minimized for distributions that place all their probability on a single outcome

Entropy of a Coin Flip

$X = outcome\ of\ coin\ flip\ with\ probability\ of\ heads\ p$



Conditional Entropy

- We can also compute the entropy of a random variable conditioned on a different random variable

$$H(Y|X) = -\sum_{x} p(X = x) \sum_{y} p(Y = y|X = x) \log p(Y = y|X = x)$$

  - This is called the conditional entropy
  - This is the amount of information needed to quantify the random variable Y given the random variable X

Information Gain

- Using entropy to measure uncertainty, we can greedily select an attribute that guarantees the largest expected decrease in entropy (with respect to the empirical partitions)

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

  - Called information gain
  - Larger information gain corresponds to less uncertainty about Y given X
    - Note that $H(Y|X) \leq H(Y)$

Roadmap of this Lecture

- Part I: Recap of Probability, Random Variables and Entropy
- **Part II: Decision Trees**

Supervised Learning

- Input: labeled training data
  - i.e., data plus desired output
- Assumption: there exists a function f that maps data items x to their correct labels
- Goal: construct an approximation to f

Until Now

We've been focusing on linear separators

- Relatively easy to learn (using standard techniques)
- Easy to picture, but not clear if data will be separable

This lecture and the previous lecture: non-parametric approaches

- Decision trees
- Nearest neighbor classification

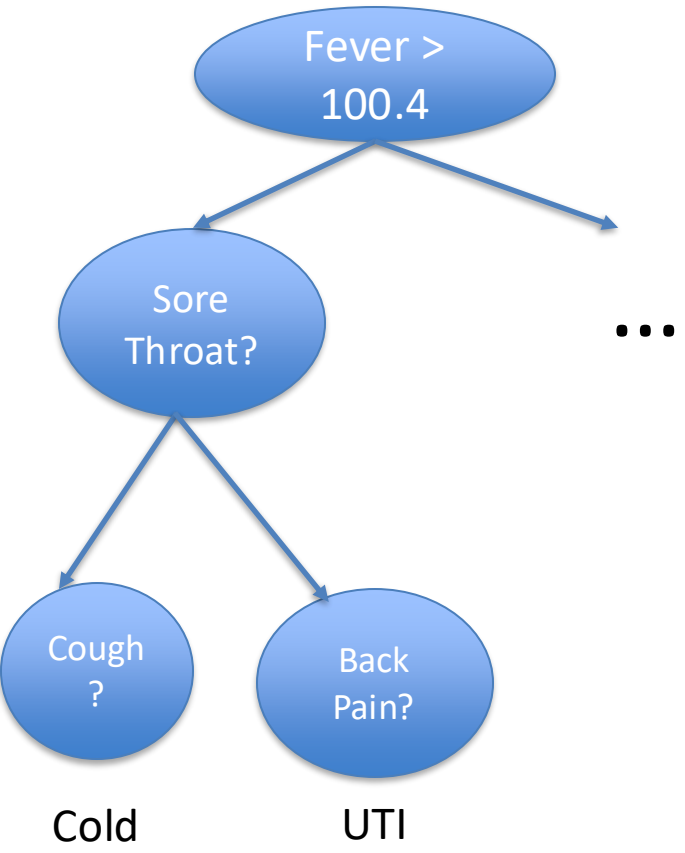
Application: Medical Diagnosis

- Suppose that you go to your doctor with flu-like symptoms
  - How does your doctor determine if you have a flu that requires medical attention?

Application: Medical Diagnosis

- Suppose that you go to your doctor with flu-like symptoms
  - How does your doctor determine if you have a flu that requires medical attention?
  - Check a list of symptoms:
    - Do you have a fever over 100.4 degrees Fahrenheit?
    - Do you have a sore throat or a stuffy nose?
    - Do you have a dry cough?

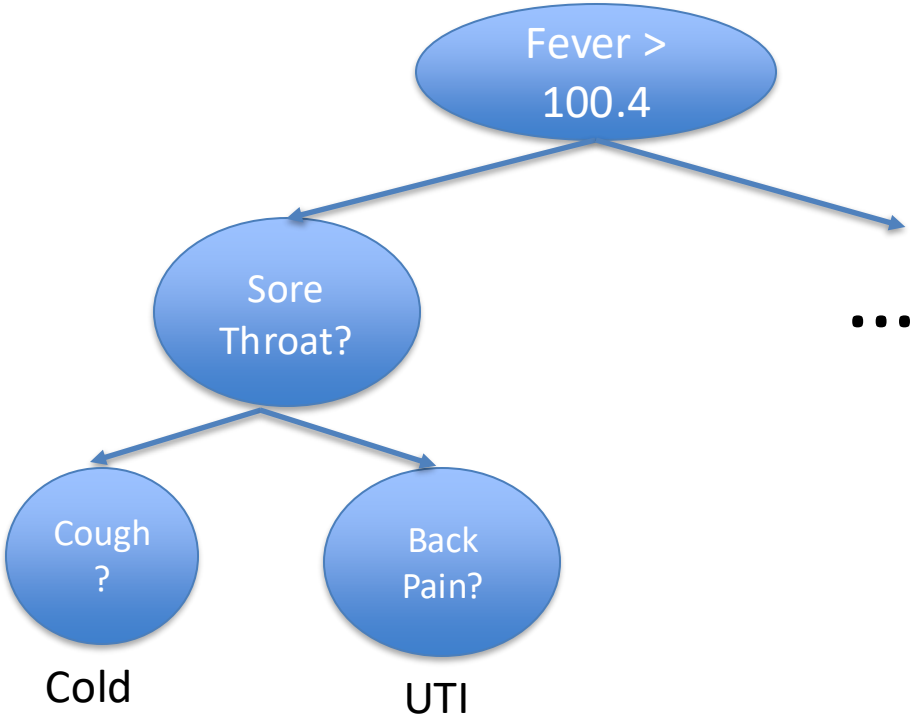
Application: Medical Diagnosis



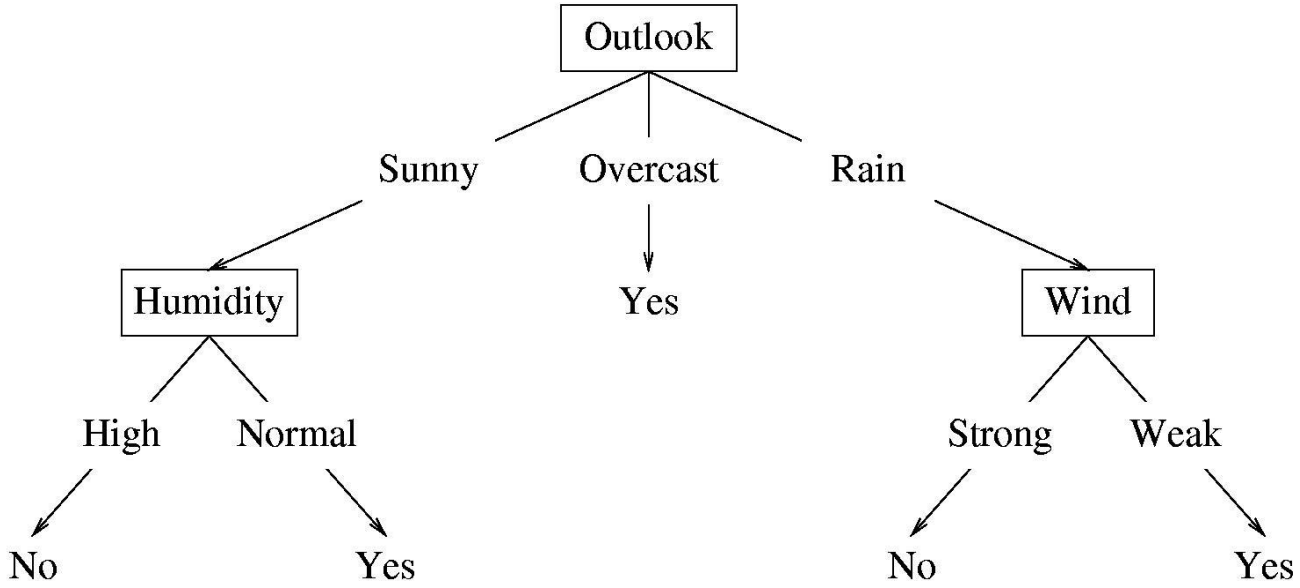
- Just having some symptoms is not enough, you should also not have symptoms that are not consistent with the flu
- For example,
  - If you have a fever over 100.4 degrees Fahrenheit?
  - And you have a sore throat or a stuffy nose?
  - You probably do not have the flu (most likely just a cold)

Application: Medical Diagnosis

- In other words, your doctor will perform a series of tests and ask a series of questions in order to determine the likelihood of you having a severe case of the flu
- This is a method of coming to a diagnosis (i.e., a classification of your condition)

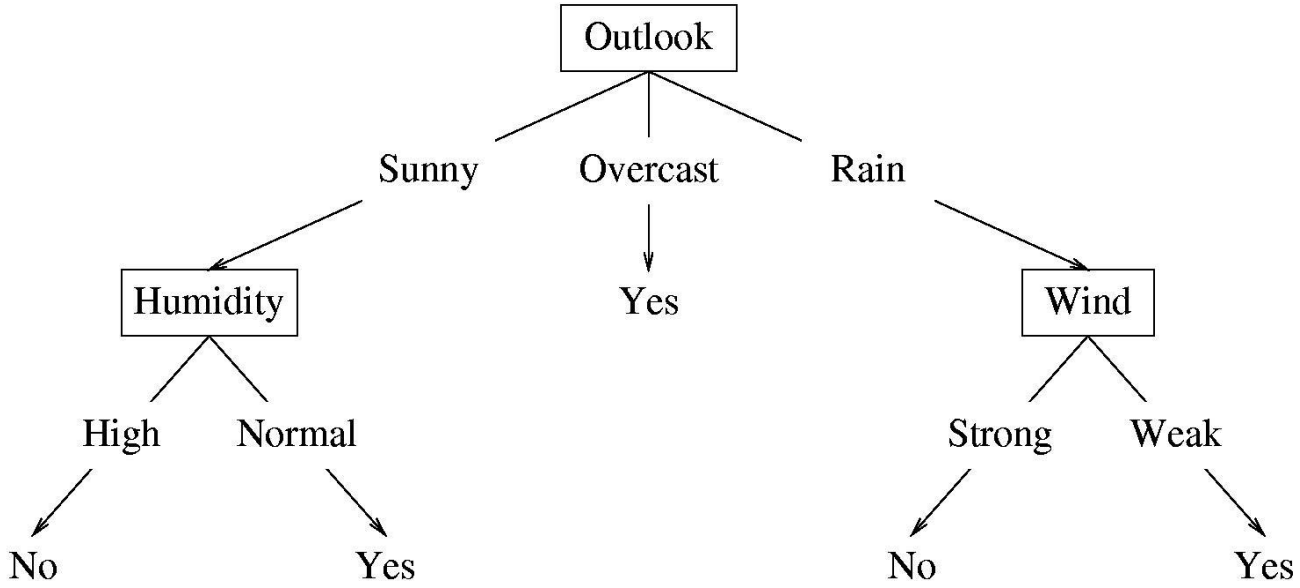


Decision Trees



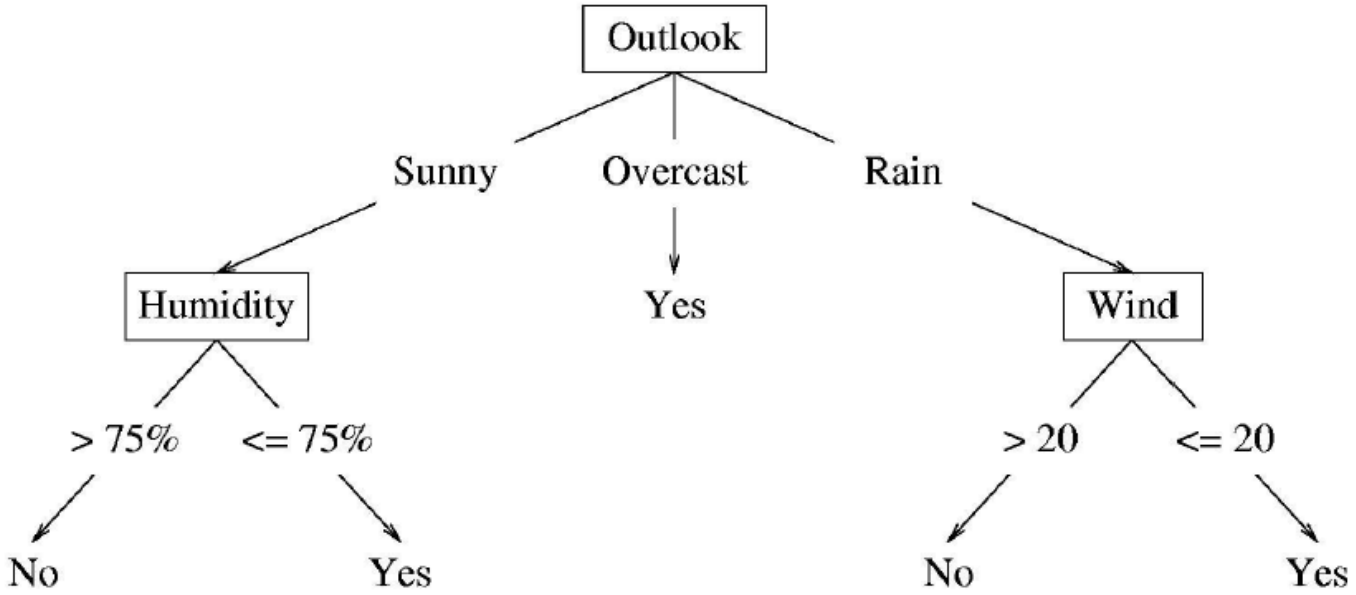
- A tree in which each internal (non-leaf) node tests the value of a particular feature
- Each leaf node specifies a class label (in this case whether or not you should play tennis)

Decision Trees



- Features: (Outlook, Humidity, Wind)
- Classification is performed root to leaf
  - The feature vector (Sunny, Normal, Strong) would be classified as a yes instance

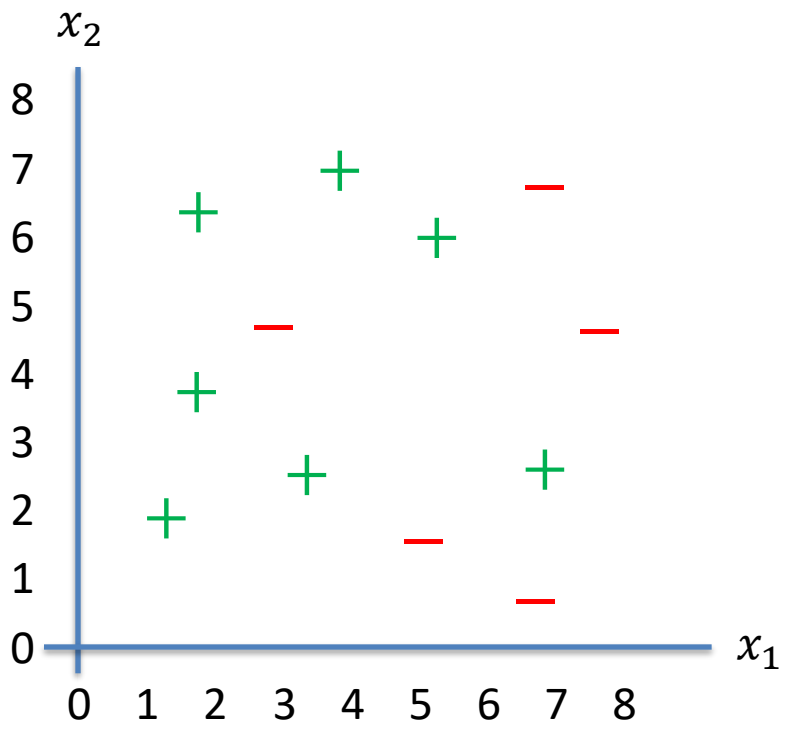
Decision Trees

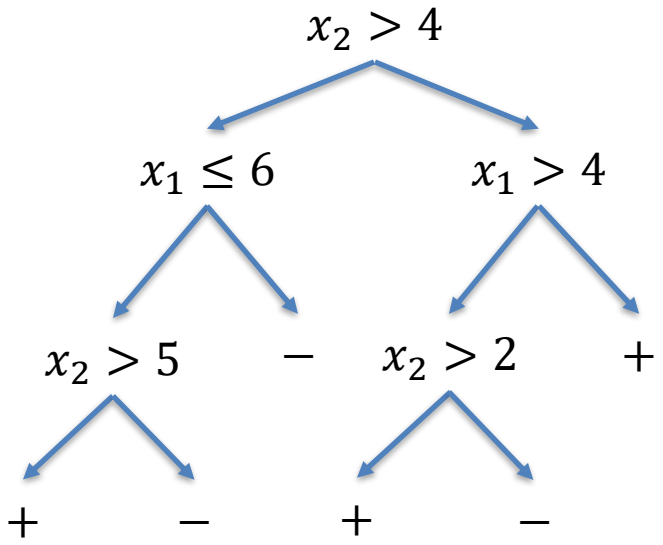


- Can have continuous features too
  - Internal nodes for continuous features correspond to thresholds

Decision Trees

- Decision trees divide the feature space into axis parallel rectangles





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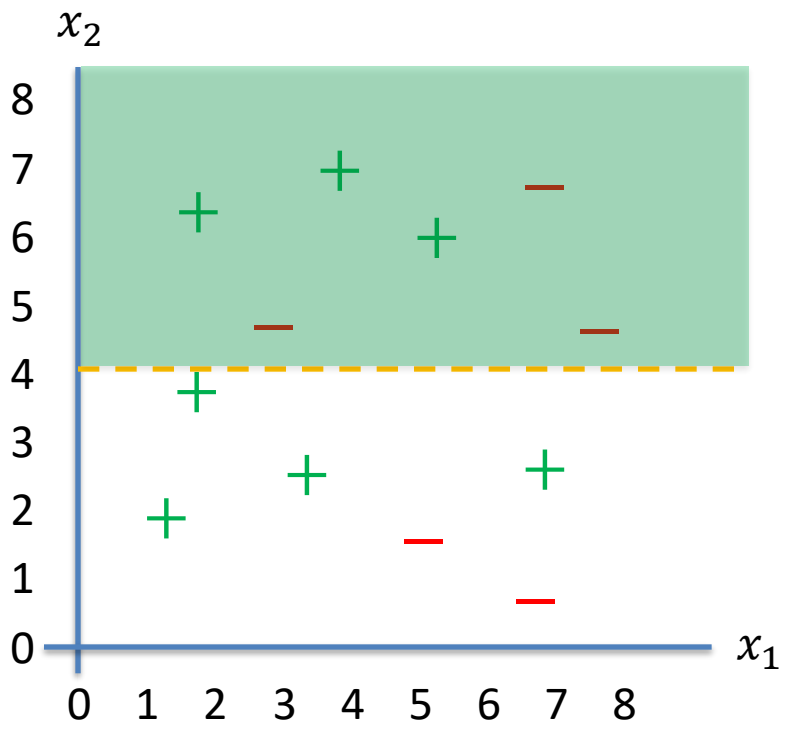

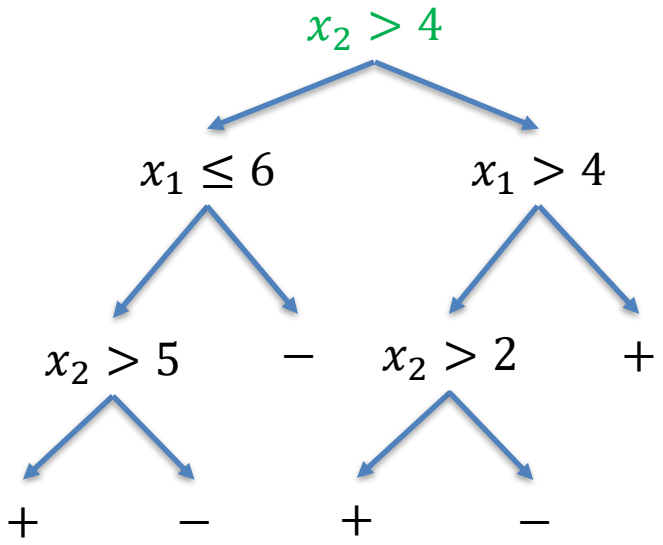

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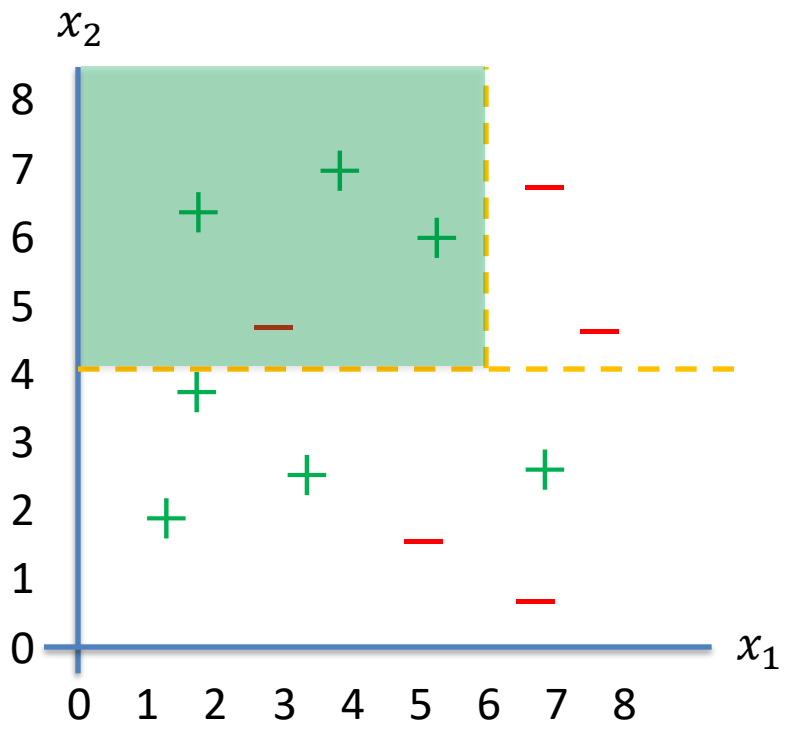

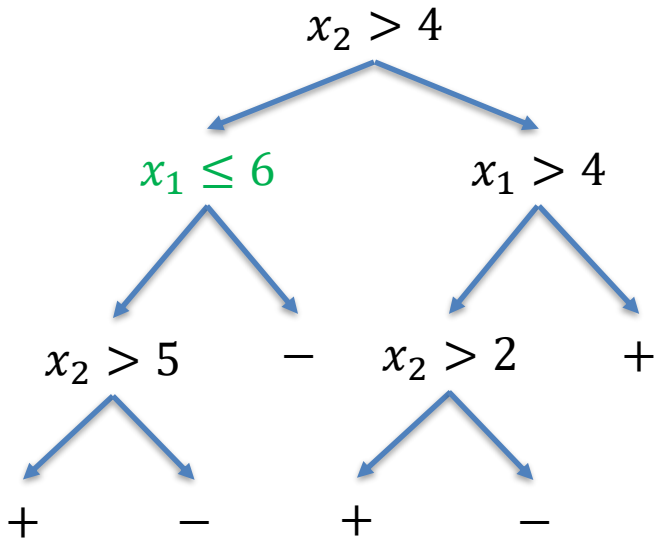

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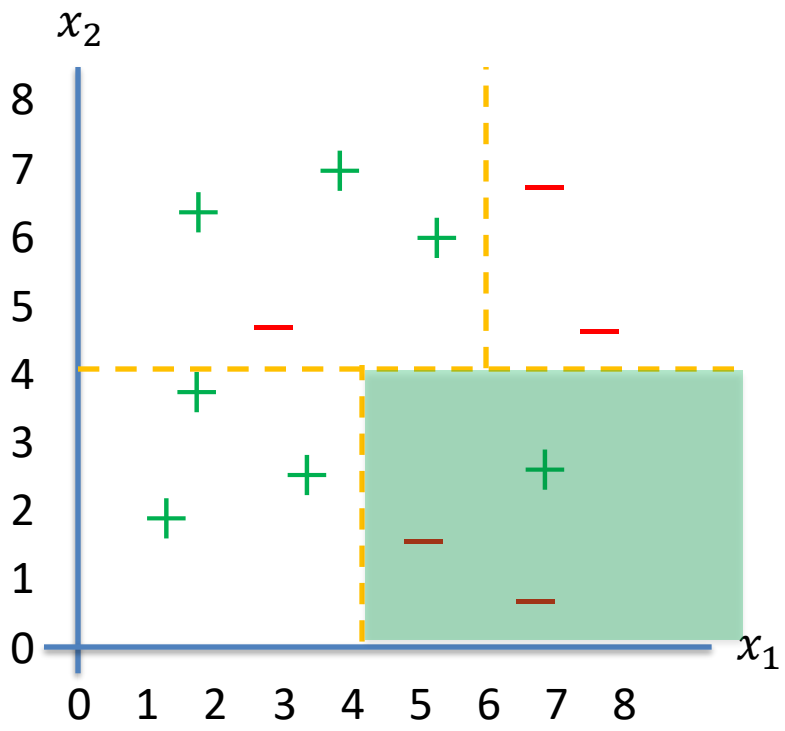

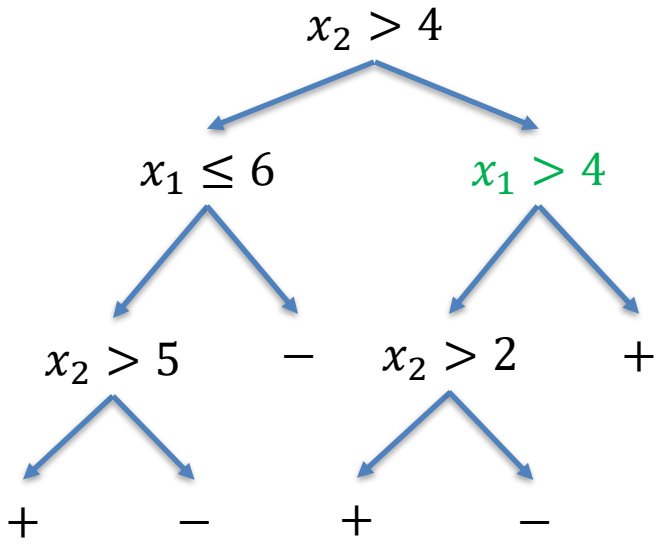

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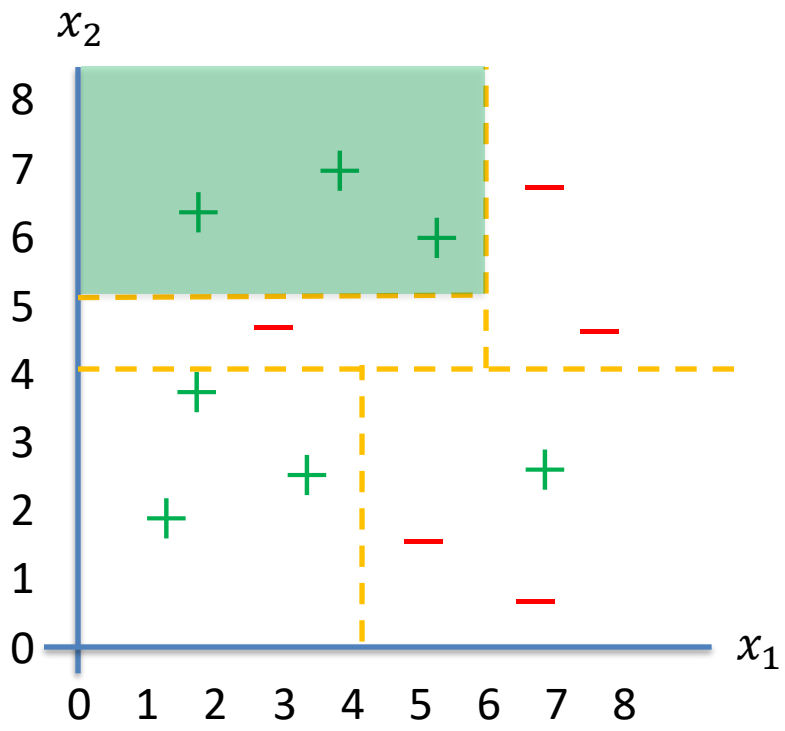

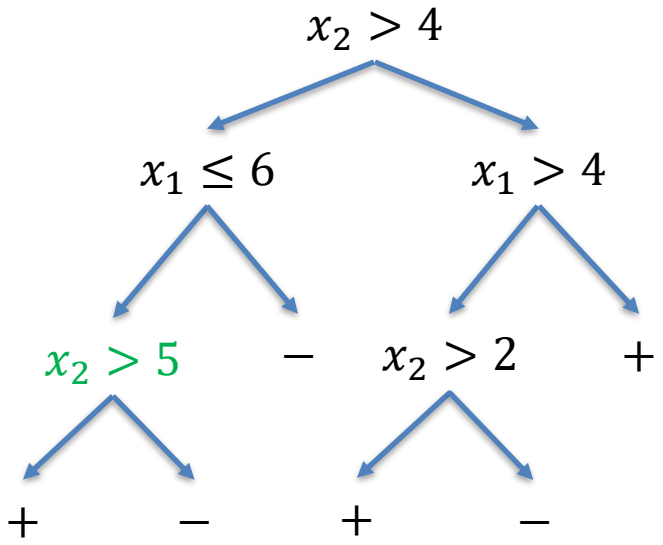

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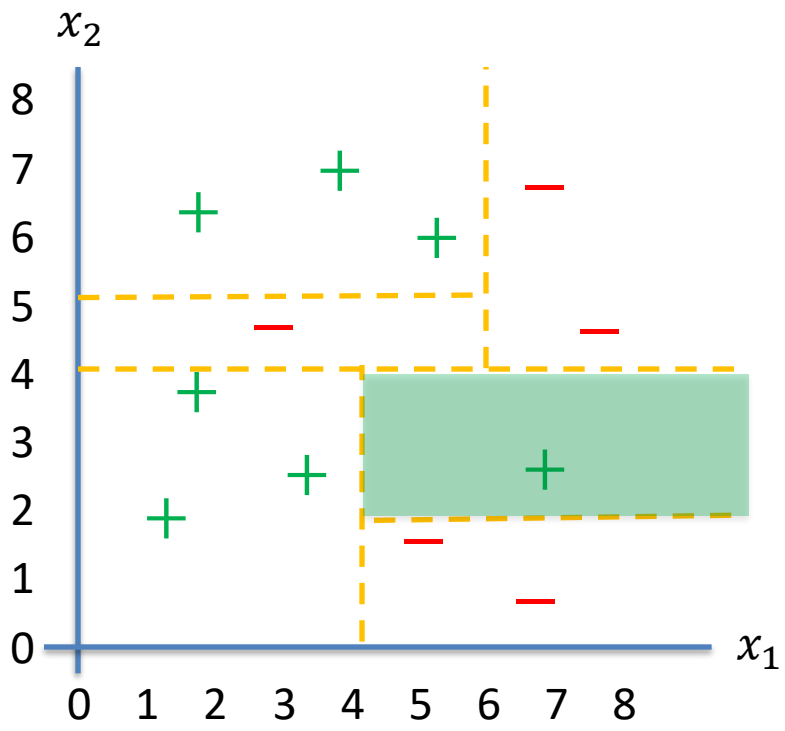

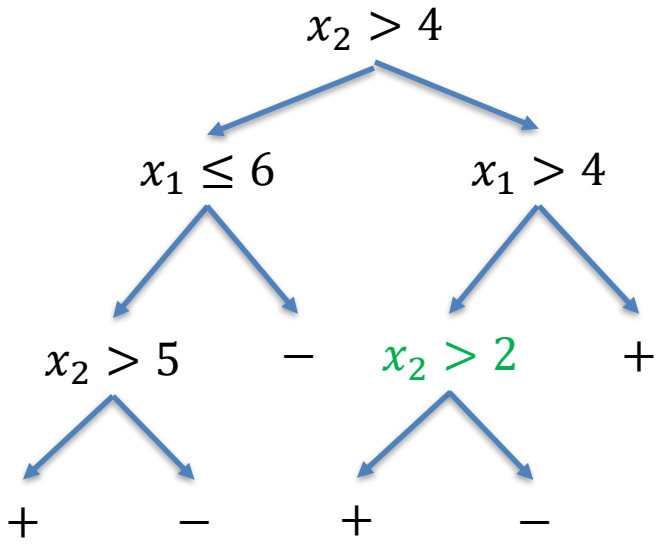

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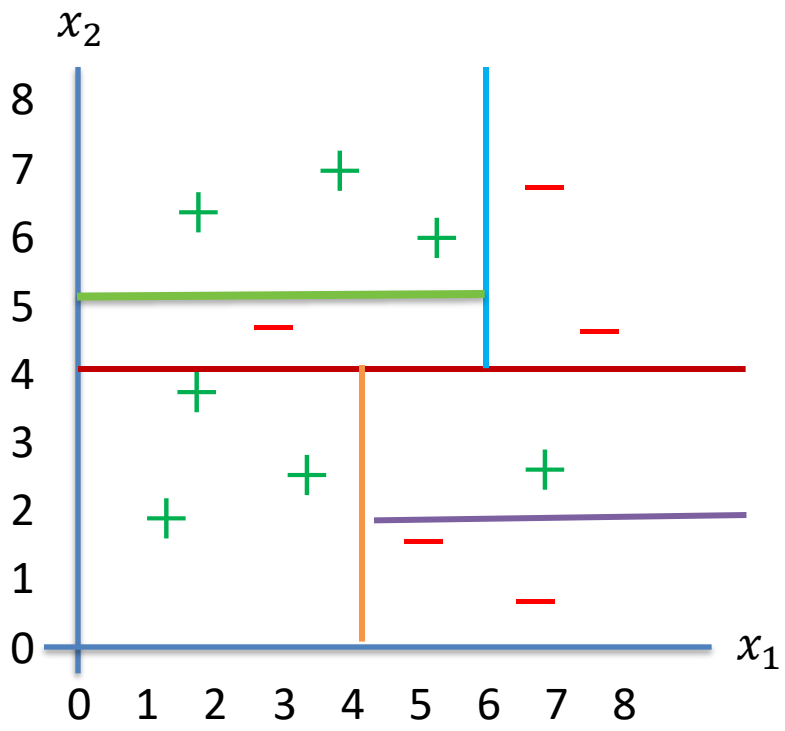

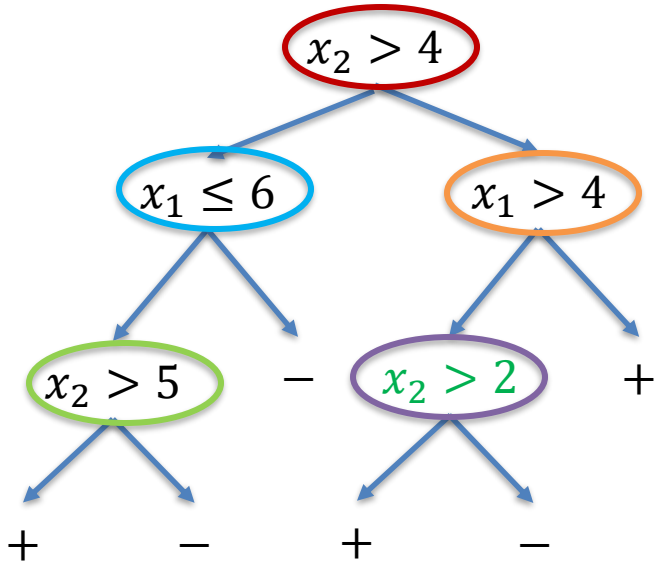

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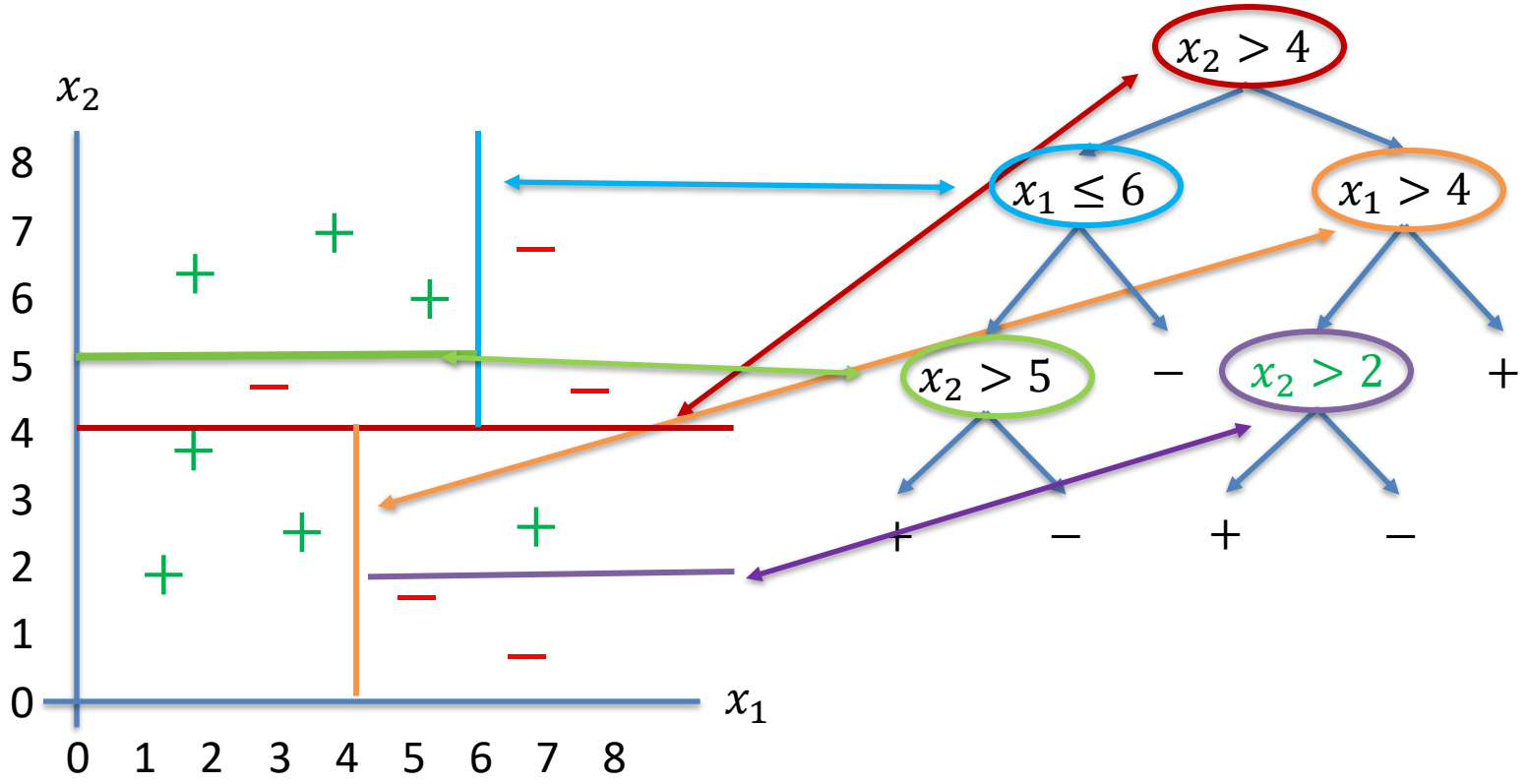
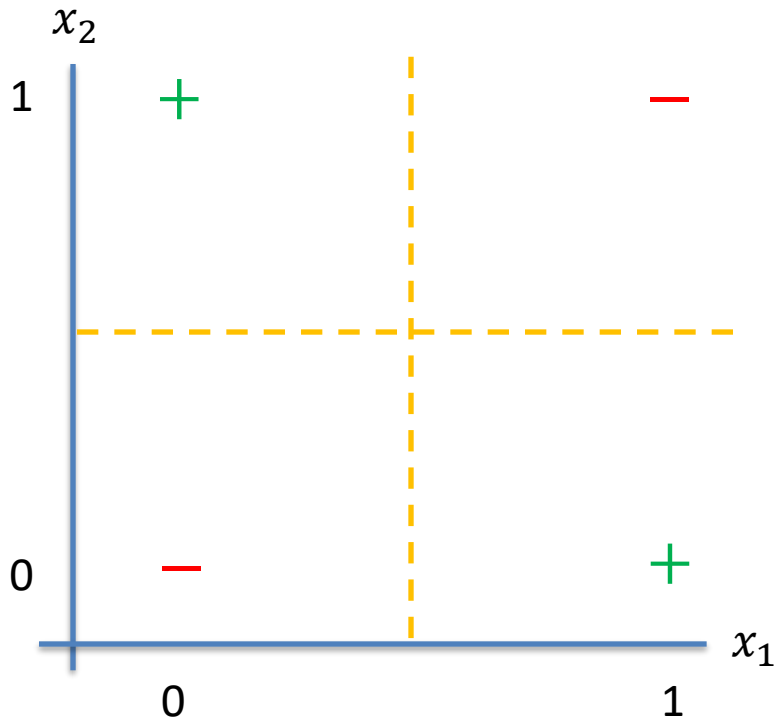
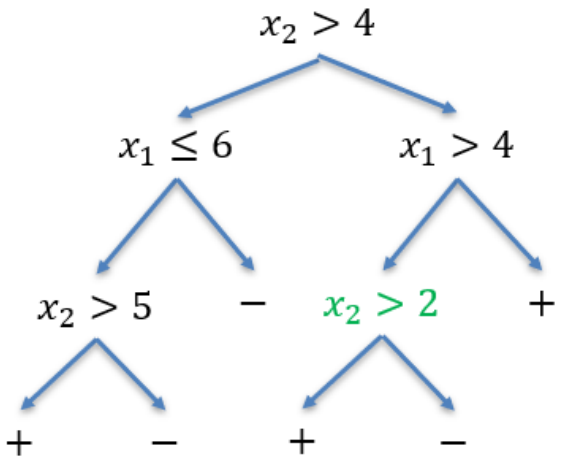


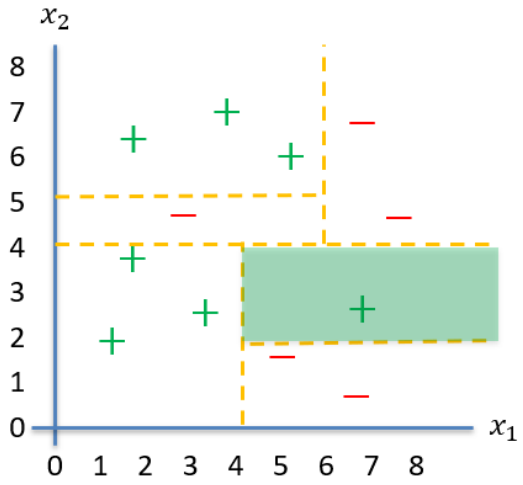
Decision Trees

- Worst case decision tree may require exponentially many nodes



Decision Tree Learning





Basic decision tree building algorithm:

Pick some feature/attribute (how to pick the "best"?)	Partition the data based on the value of this attribute	Recurse over each new partition (when to stop?)

We'll focus on the discrete case first (i.e., each feature takes a value in some finite set)

Decision Trees

What functions can be represented by decision trees?

- Every function can be represented by a sufficiently complicated decision tree

Are decision trees unique?

Decision Trees

What functions can be represented by decision trees?

- Every function of +/- can be represented by a sufficiently complicated decision tree

Are decision trees unique?

- No, many different decision trees are possible for the same set of labels

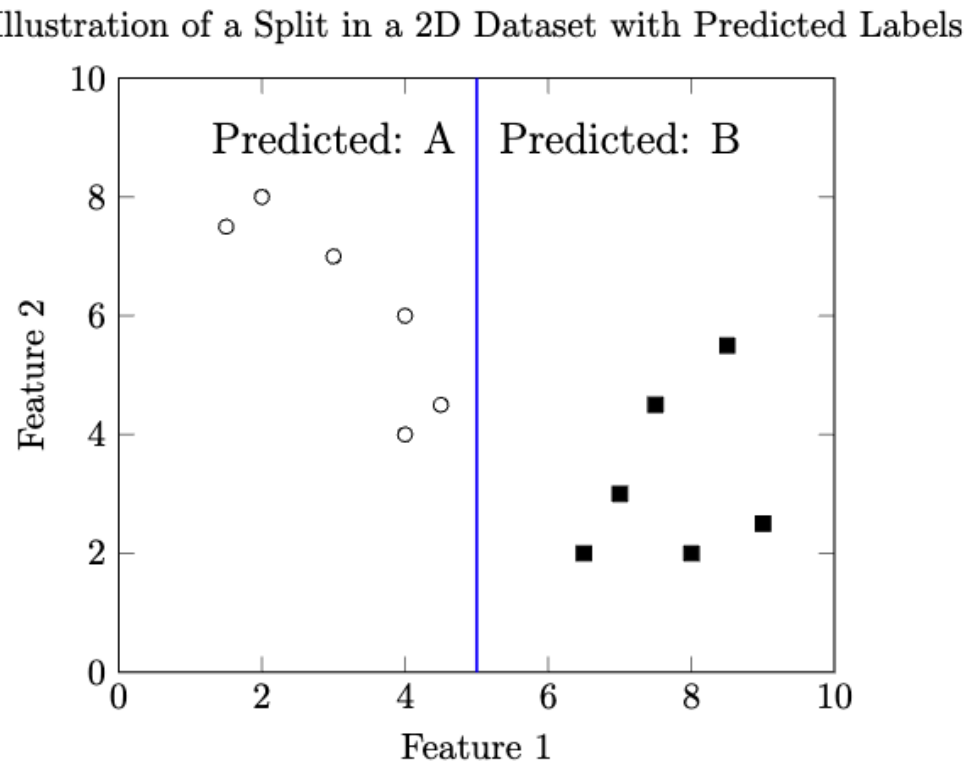
Choosing the Best Attribute

- Because the complexity of storage and classification increases with the size of the tree, should prefer smaller trees
  - Simplest models that explain the data are usually preferred over more complicated ones
  - Finding the smallest tree is an NP-hard problem
  - Instead, use a greedy heuristic based approach to pick the best attribute at each stage

Choosing the Best Attribute

- The selected attribute is a good split if we are more "certain" about the classification after the split
  - If each partition with respect to the chosen attribute has a distinct class label, we are completely certain about the classification after partitioning
  - If the class labels are evenly divided between the partitions, the split isn't very good (we are very uncertain about the label for each partition)
  - What about other situations? How do you measure the uncertainty of a random process?

Choosing the Best Attribute to Split

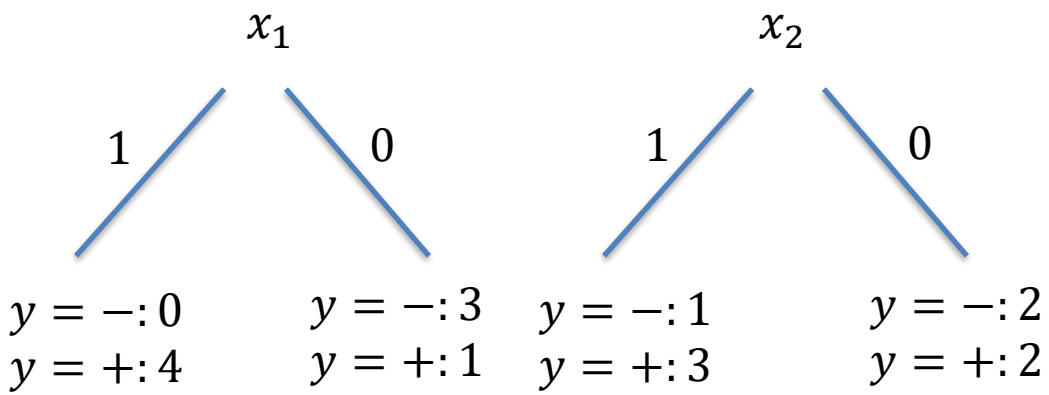


- Splitting on Feature 1 results in homogeneous datasets (i.e., the same label in the two child datasets after the split).
- No split on Feature 2 would achieve this!

Choosing the Best Attribute

$$x_1, x_2 \in \{0,1\}$$

Which attribute should you split on?

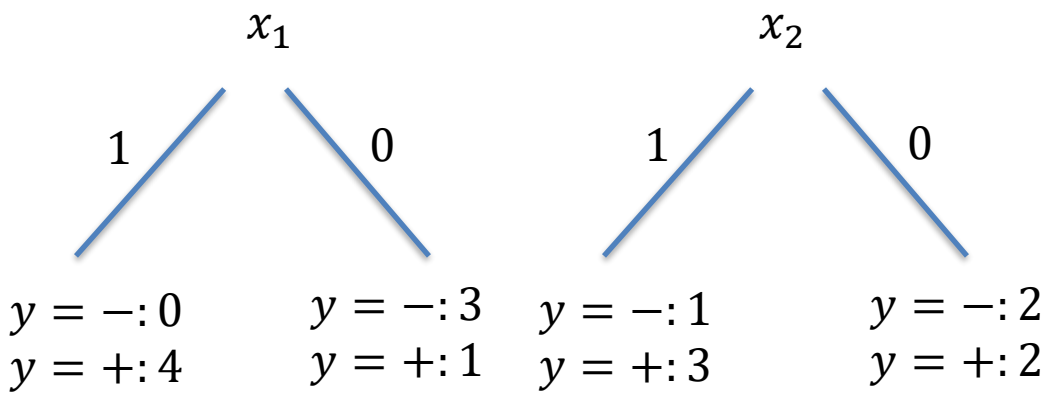


x_1	x_2	y
1	1	+
1	0	+
1	1	+
1	0	+
0	1	+
0	0	−
0	1	−
0	0	−

Choosing the Best Attribute

$x_1, x_2 \in \{0,1\}$

Which attribute should you split on?



x_1	x_2	y
1	1	+
1	0	+
1	1	+
1	0	+
0	1	+
0	0	−
0	1	−
0	0	−

Can think of these counts as probability distributions over the labels: if $x = 1$, the probability that $y = +$ is equal to 1

Recap: Information Gain

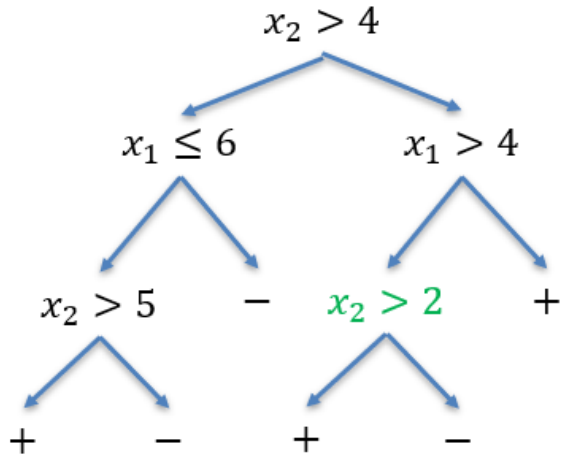
- Using entropy to measure uncertainty, we can greedily select an attribute that guarantees the largest expected decrease in entropy (with respect to the empirical partitions)

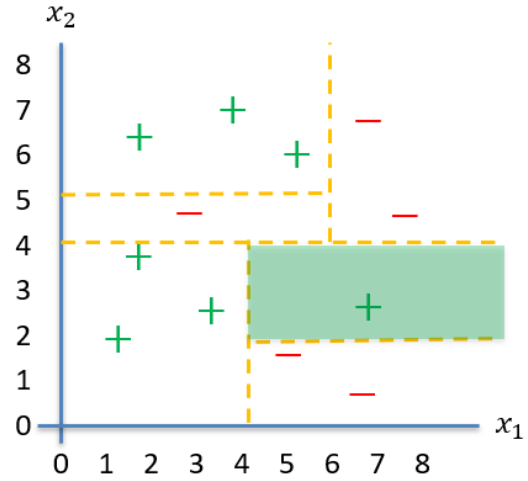
$$IG(X) = H(Y) - H(Y|X)$$

  - Called information gain
  - Larger information gain corresponds to less uncertainty about Y given X
    - Note that $H(Y|X) \leq H(Y)$

Decision Tree Learning

- Basic decision tree building algorithm:
  - Pick the feature/attribute with the highest information gain
  - Partition the data based on the value of this attribute
  - Recurse over each new partition

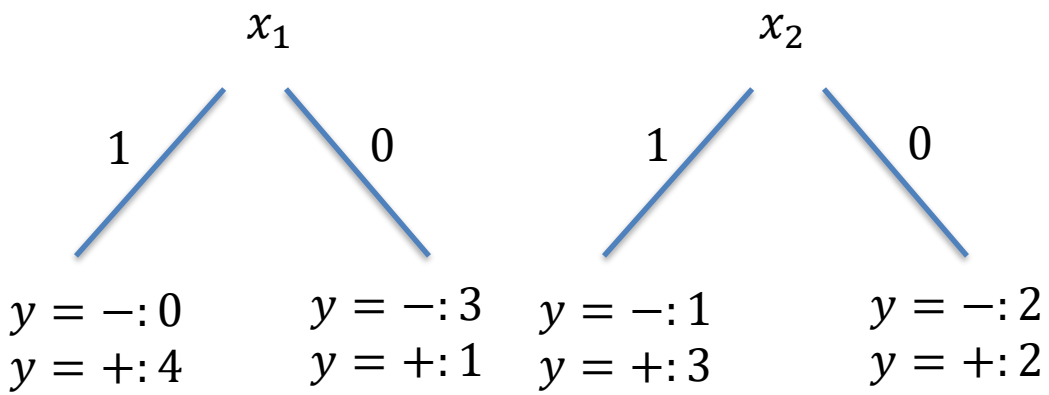




Choosing the Best Attribute

$$x_1, x_2 \in \{0,1\}$$

Which attribute should you split on?



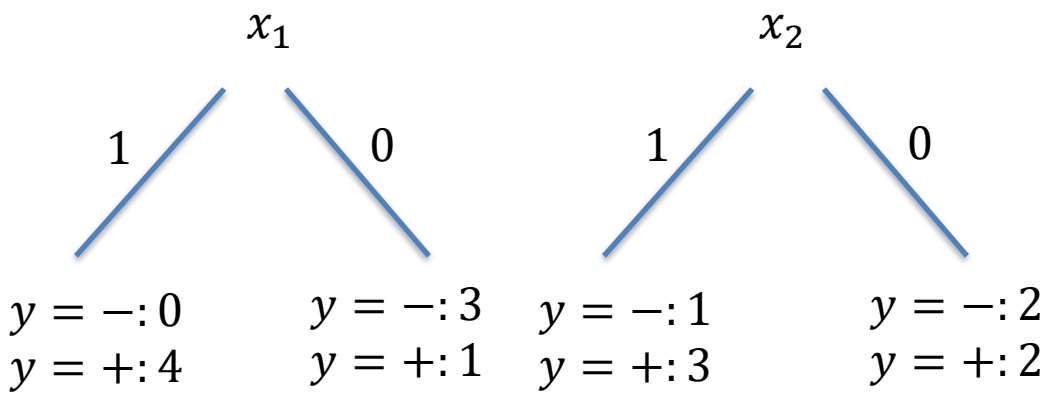
x_1	x_2	y
1	1	+
1	0	+
1	1	+
1	0	+
0	1	+
0	0	−
0	1	−
0	0	−

What is the information gain in each case?

Choosing the Best Attribute: Information Gain

$$x_1, x_2 \in \{0,1\}$$

Which attribute should you split on?



x_1	x_2	y
1	1	+
1	0	+
1	1	+
1	0	+
0	1	+
0	0	−
0	1	−
0	0	−

$$H(Y) = -\frac{5}{8}\log\frac{5}{8} - \frac{3}{8}\log\frac{3}{8}$$

$$H(Y|X_1) = .5[-0\log 0 - 1\log 1] + .5[-.75\log .75 - .25\log .25]$$

$$H(Y|X_2) = .5[-.5\log .5 - .5\log .5] + .5[-.75\log .75 - .25\log .25]$$

$$H(Y) - H(Y|X_1) - H(Y) + H(Y|X_2) = -.5\log .5 > 0$$

Should split on x_1

The Gini Coefficient

- The Gini coefficient is another popular measure used to evaluate splits, focusing on minimizing the probability of misclassification. It is defined for a set S as:

$$Gini(S) = 1 - \sum_{i=1:N} p_i^2$$

- Once a dataset is split into two sets S_1 and S_2, the Gini-split is defined as:

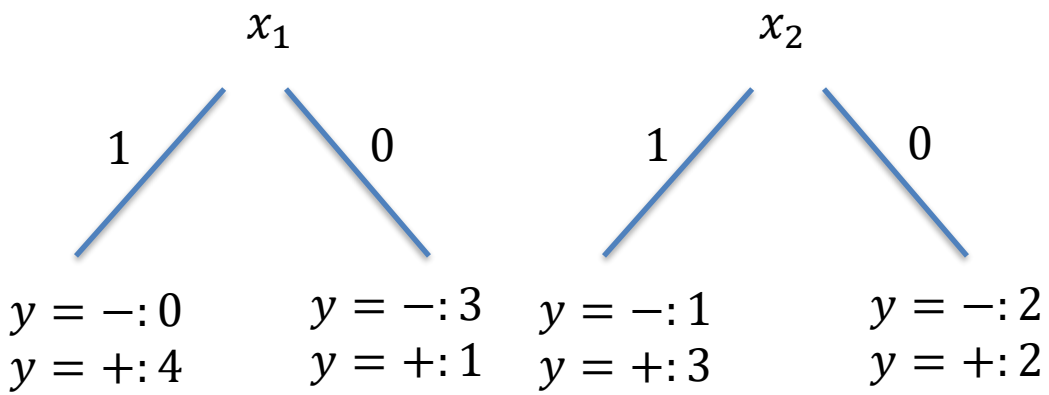
$$GiniSplit = \frac{|S_1|}{|S|} Gini(S_1) + \frac{|S_2|}{|S|} Gini(S_2)$$

- The goal is to find the split that **minimizes the Gini Split.**

Choosing the Best Attribute: Gini Coefficient

$$x_1, x_2 \in \{0,1\}$$

Which attribute should you split on?



x_1	x_2	y
1	1	+
1	0	+
1	1	+
1	0	+
0	1	+
0	0	–
0	1	–
0	0	–

$GiniSplit(X_1) = ½ (1 – 1- 0) + ½(1 – 9/16 – 1/16) = 5/32$
$GiniSplit(X_2) = ½ (1 – ¼ – ¼) + ½(1 – 9/16 – 1/16) = 13/32$

Gini-Split of X_1 is lower than the the Gini-Split of X_2

Should split on x_1

When to Stop

If the current set is “pure” (i.e., has a single label in the output), stop

If you run out of attributes to recurse on, even if the current data set isn’t pure, stop and use a majority vote

If a partition contains no data points, use the majority vote at its parent in the tree

If a partition contains no data items, nothing to recurse on

For fixed depth decision trees, the final label is determined by majority vote

Handling Real-Valued Attributes

- For continuous attributes, use threshold splits
  - Split the tree into $x_k < t$ and $x_k \geq t$
  - Can split on the same attribute multiple times on the same path down the tree
- How to pick the threshold t?

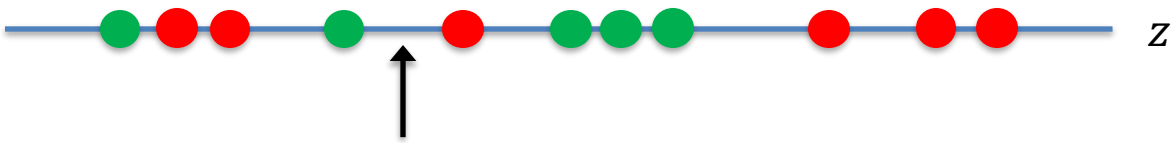
Handling Real-Valued Attributes

- For continuous attributes, use threshold splits
  - Split the tree into $x_k < t$ and $x_k \geq t$
  - Can split on the same attribute multiple times on the same path down the tree
- How to pick the threshold t?
  - Try every possible t

How many possible t are there?

Handling Real-Valued Attributes

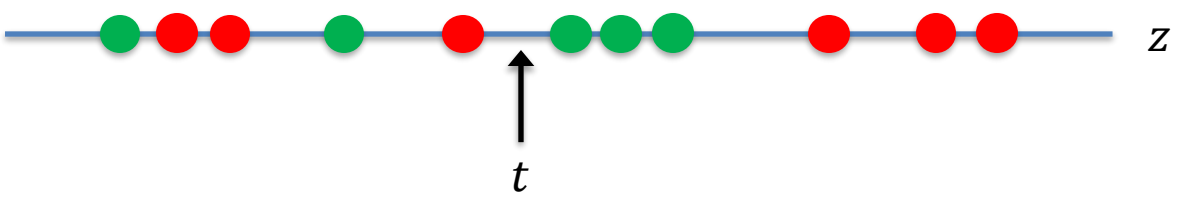
- Sort the data according to the k^{th} attribute: $z_1 > z_2 > \cdots > z_n$



- Only a finite number of thresholds make sense

Handling Real-Valued Attributes

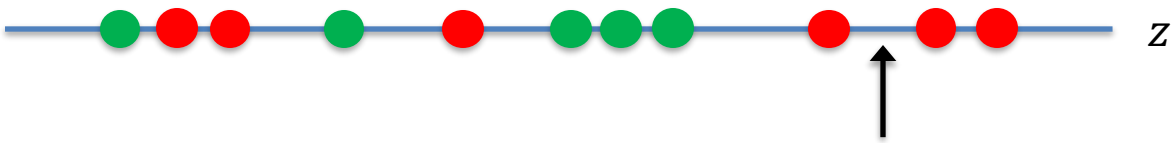
- Sort the data according to the k^{th} attribute: $z_1 > z_2 > \cdots > z_n$



- Only a finite number of thresholds make sense
  - Just split in between each consecutive pair of data points (e.g., splits of the form $t = \frac{z_i + z_{i+1}}{2}$)

Handling Real-Valued Attributes

- Sort the data according to the k^{th} attribute: $z_1 > z_2 > \cdots > z_n$



Does it make sense for a threshold to appear between two x's with the same class label?

- Only a finite number of thresholds make sense
  - Just split in between each consecutive pair of data points (e.g., splits of the form $t = \frac{z_i + z_{i+1}}{2}$)

Handling Real-Valued Attributes

- Compute the information gain of each threshold
- Let $X: t$ denote splitting with threshold t and compute

$$H(Y|X:t) = -p(X < t) \sum_y p(Y = y|X < t) \log p(Y = y|X < t) +$$
$$-p(X \geq t) \sum_y p(Y = y|X \geq t) \log p(Y = y|X \geq t)$$

- In the learning algorithm, maximize over all attributes and all possible thresholds of the real-valued attributes

$$\max_t H(Y) - H(Y|X:t), \text{ for real-valued } X$$

$$H(Y) - H(Y|X), \text{ for discrete } X$$

Regression Decision Trees

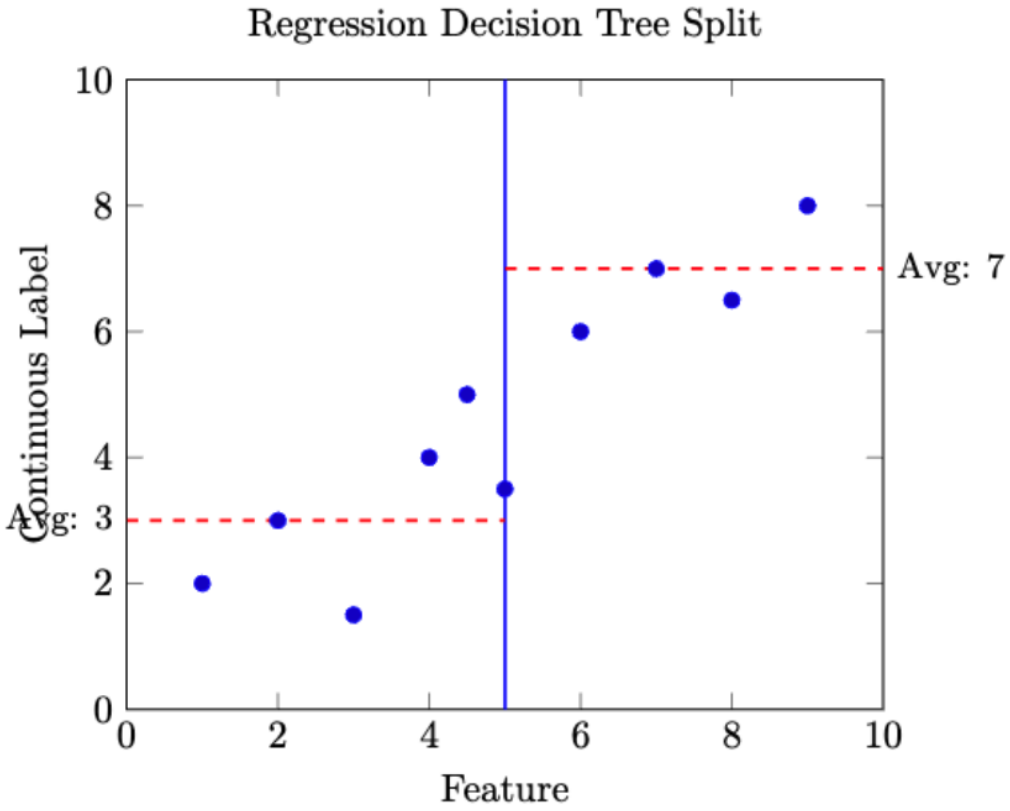


Figure 5: Illustration of a regression decision tree split with a single feature. The dataset is split at Feature = 5, with horizontal dashed lines representing the average label value for each partition.

Regression Splitting Criteria

- MSE Reduction: Calculate the Mean Squared Error of each dataset (i.e. parent dataset and the two children dataset)
- Given a dataset S, the predicted label y_S is the mean of the labels in that set.
- The MSE is then defined as:

$$MSE(S) = \frac{1}{|S|}\sum_{i \in S}(y_i - y_S)^2$$

- We can then define the MSE Reduction as:

$$MSERed = MSE(S) - \frac{|S_1|}{|S|}MSE(S_1) - \frac{|S_2|}{|S|}MSE(S_2)$$

- The goal is to find the split that minimizes the MSE Reduction.

Decision Trees

Because of speed/ease of implementation, decision trees are quite popular

Can be used for regression too

Decision trees will **always** overfit!

It is always possible to obtain zero training error on the input data with a deep enough tree (if there is no noise in the labels)

Solution?