



# Recap of Probability and Decision Trees

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# Roadmap of this Lecture

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- **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,  $\Omega = \{H, T\}$  would be the set of possible outcomes of a coin flip
  - Each element  $\omega \in \Omega$  is associated with a number  $p(\omega) \in [0,1]$  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 roll
  - $A = \{1, 5, 6\} \subseteq \Omega$  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
  - $p(A) = p(1) + p(5) + p(6)$

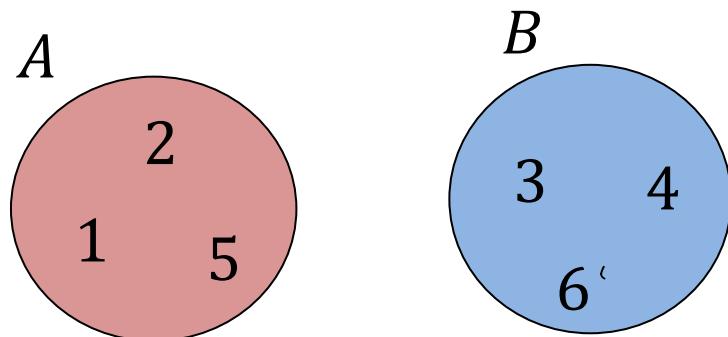
# Independence

- 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:  $p(1) = \dots = p(6) = 1/6$

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



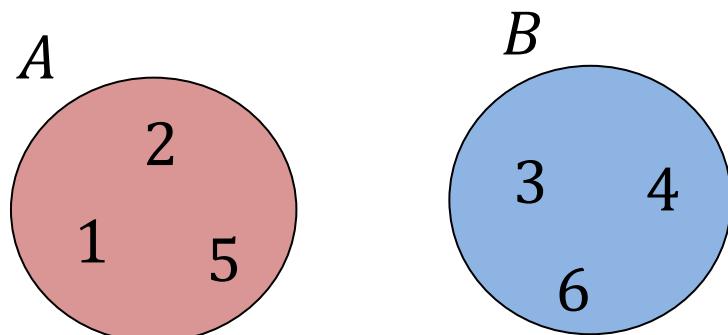
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No!

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

$$A = \{1, 2, 3\} \Rightarrow P(A) = \frac{1}{2}$$

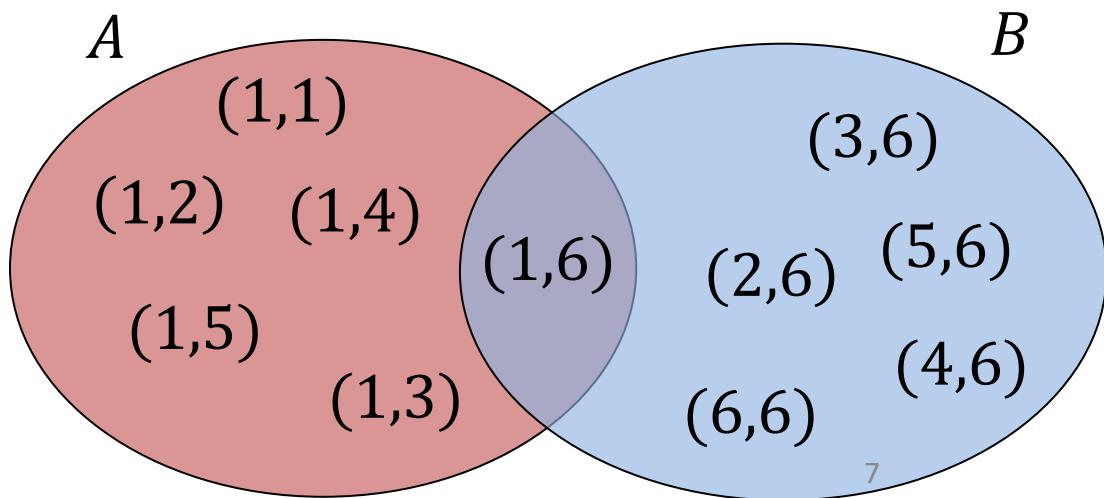
$$B = \{1, 4\} \Rightarrow P(B) = \frac{1}{3}$$

Are A & B independent?

$$P(A \cap B) = P(1) = \frac{1}{6}$$

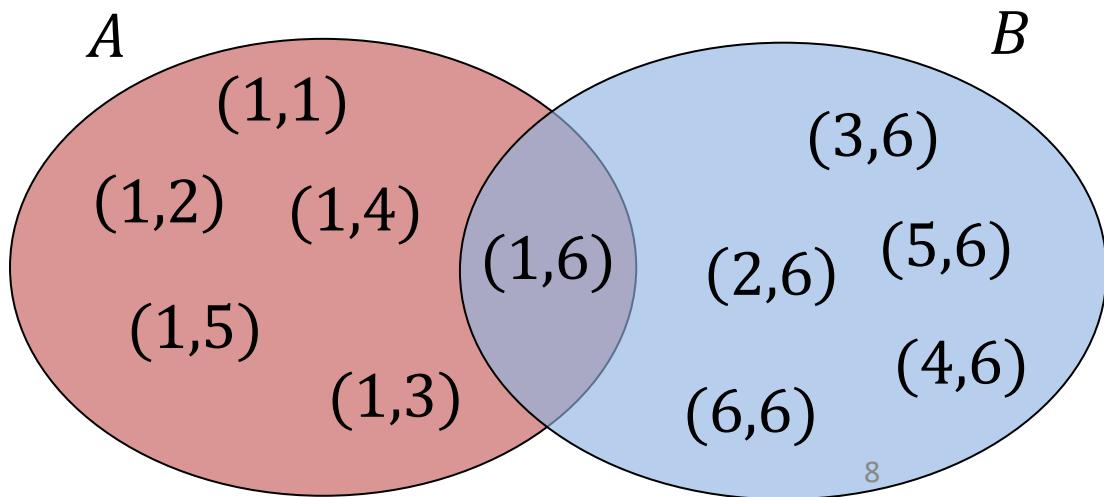
# Independence

- 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?



# Independence

- Now, suppose that  $\Omega = \{(1,1), (1,2), \dots, (6,6)\}$  is the set of all possible rolls of two **unbiased** dice
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- Are  $A$  and  $B$  independent?



*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

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

If  $A \cap B$   
 $\geq p(A)p(B)$   
 $\quad\quad\quad p(B)$

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

- Some properties:

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

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

- If  $A$  and  $B$  are independent, then  $p(A|B) = p(A)$

# Discrete Random Variables



- A discrete **random variable**,  $\underline{X}$ , is a function from the state space  $\Omega$  into a discrete space  $D$

- For each  $x \in D$ ,

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

Dice throw

$x = 1 \rightarrow \{ \begin{matrix} \text{Dice face} \\ \# \text{ on top} \end{matrix} \}$

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

$$D = \{1, 6\}$$

$n$

- $p(X)$  defines a probability distribution

$$\sum_{x \in D} p(X = \underline{x}) = 1$$

- Random variables partition the state space into disjoint events

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

# Example: Pair of Dice

- Let  $\underline{\Omega}$  be the set of all possible outcomes of rolling a pair of dice
- Let  $\underline{p}$  be the uniform probability distribution over all possible outcomes in  $\underline{\Omega}$
- Let  $\underline{X}(\omega)$  be equal to the sum of the value showing on the pair of dice in the outcome  $\omega$

$$\cdot p(\underline{X} = 2) = ? \quad \frac{1}{36}$$

$$\cdot p(X = 8) = ?$$

$x_1, x_2$   
 $X = D_1 + D_2$   
 $x_1 \rightarrow$  Dice throw 1  
 $x_2 \rightarrow$  Dice throw 2  
 outcome of

$$X = X_1 + X_2$$

# Example: Pair of Dice

- Let  $\Omega$  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  $\Omega$
- Let  $X(\omega)$  be equal to the sum of the value showing on the pair of dice in the outcome  $\omega$ 
  - $p(X = 2) = \frac{1}{36}$
  - $p(X = 8) = ?$

# Example: Pair of Dice

- Let  $\Omega$  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  $\Omega$
- Let  $X(\omega)$  be equal to the sum of the value showing on the pair of dice in the outcome  $\omega$ 
  - $p(X = 2) = \frac{1}{36}$
  - $p(X = 8) = \frac{5}{36}$

# Discrete Random Variables

- We can have vectors of random variables as well

$$X(\omega) = [\underbrace{X_1(\omega)}, \dots, \underbrace{X_n(\omega)}]$$

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

$$\underbrace{p(X_1 = x_1 \cap \dots \cap X_n = x_n)}$$

typically written as

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

- 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

$$H(X) = - \sum_{i=1}^n p(X = x_i) \log p(X = x_i)$$

$$H(X) \leq \log |M|$$

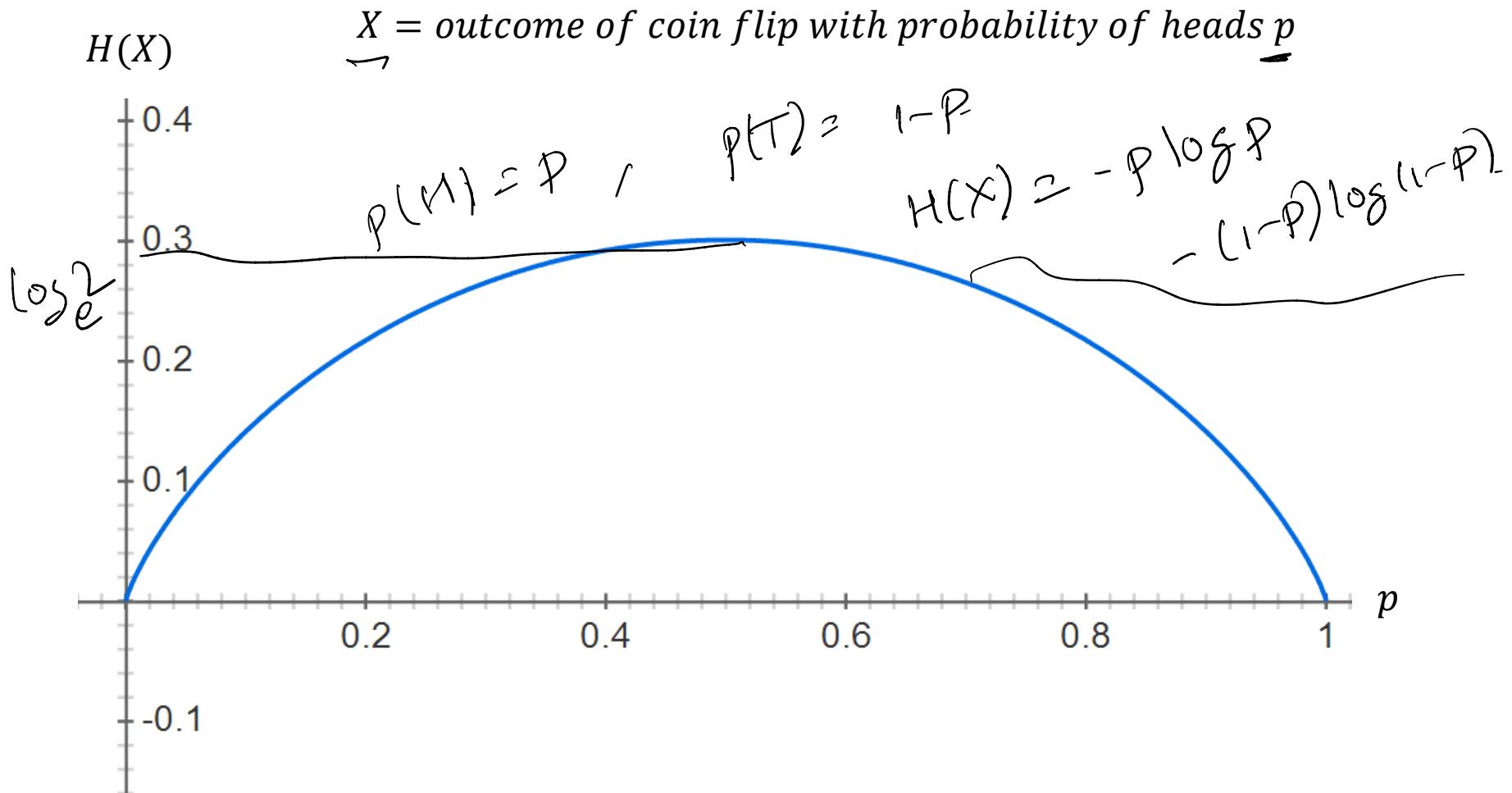
## Coin Flip

$$P_1 = 1/2$$

$$P_2 = 1/2$$

$$\begin{aligned} & -P_1 \log P_1 - P_2 \log P_2 \\ &= \frac{1}{2} \log 2 + \frac{1}{2} \log 2 = \log 2 \end{aligned}$$

# Entropy of a Coin Flip



# Conditional Entropy

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

$$\underbrace{H(Y|X)}_{\text{ }} = - \sum_x p(X=x) \sum_y \underbrace{p(Y=y|X=x) \log p(Y=y|X=x)}_{\text{ }}$$

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

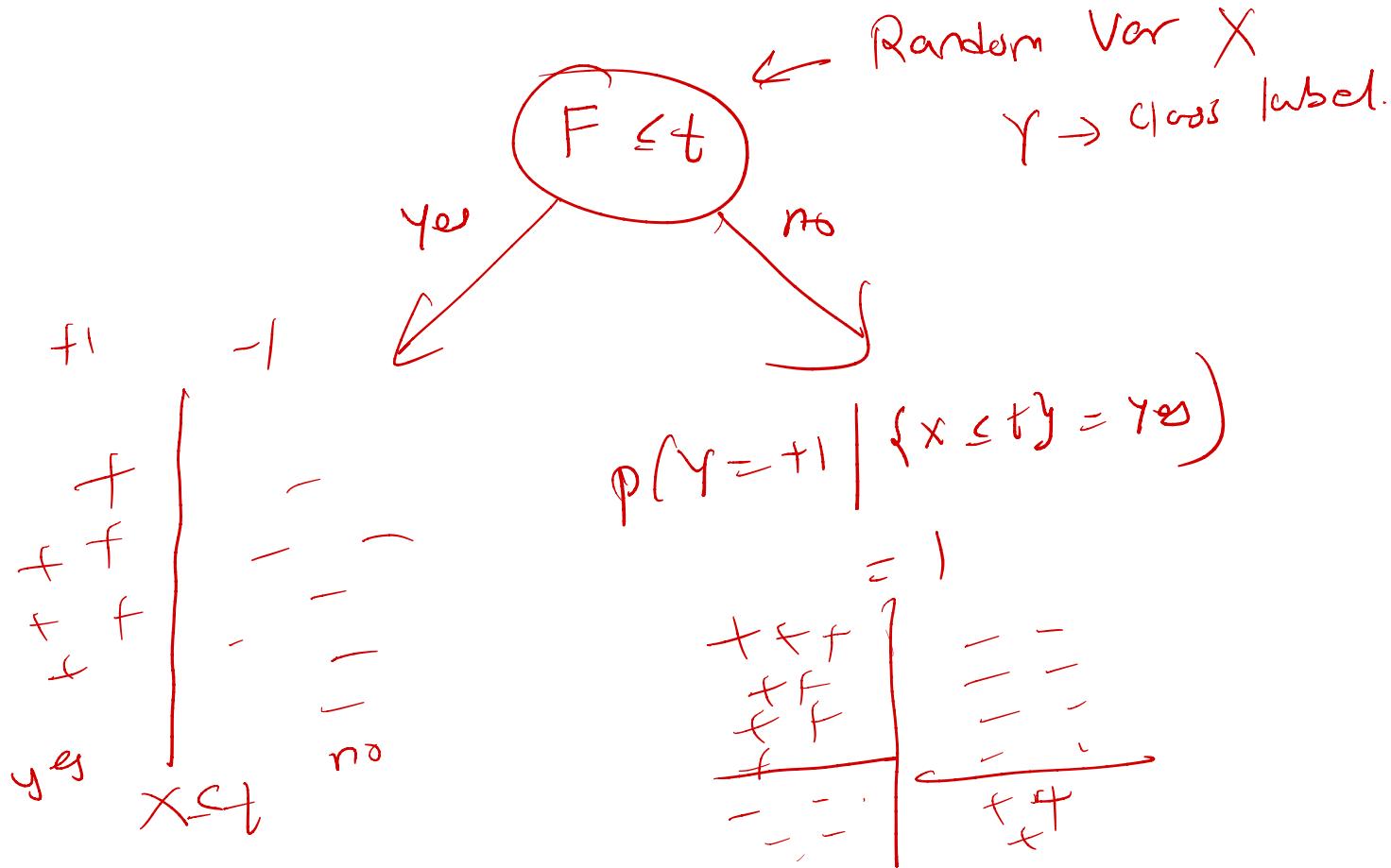
$$\begin{aligned} H(Y|X) &= - \sum_n p(X=n) H(Y|X=n) \\ &= - \sum_n p(X=n) \sum_j p(Y=j|X=n) \log \dots \end{aligned}$$

## Cond. Entropy

$$H(Y|X) = \sum_{x \in X} p(x=x) \underbrace{H(Y|X=x)}$$

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

## Why Cond. Entropy for DT



# Information Gain $Y = \text{Class}, X = \text{feature}$



- 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  $H(Y|X) \leq H(Y)$

$$\begin{aligned} IG(X) &= I(X; Y) \geq 0 \\ H(Y|X) &= H(Y) - I(X; Y) \end{aligned}$$

$$I(X;Y) = H(X) - H(X|Y)$$
$$= H(Y) - H(Y|X).$$

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

$$H(Y|X) = H(X,Y) - H(X).$$

$$I(X;Y) = H(X) + H(Y) - H(X,Y)$$

# Roadmap of this Lecture

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

# Supervised Learning



- Input: labeled training data  $\{(x_1, y_1), (x_2, y_2), \dots, (x_M, y_M)\}$ 
  - i.e., data plus desired output
- Assumption: there exists a function  $f$  that maps data items  $x$  to their correct labels  
 $f$
- Goal: construct an approximation to  $f$

$$f^*(x_i) = y_i$$

Learn a  $f \approx f^*$

# Until Now

$$h(x) = \underline{\underline{w^T x + b}}$$
$$h_{\phi}(x) = \underline{\underline{w^T \phi(x) + b}}$$



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



Next two lectures we'll  
focus on other hypothesis  
spaces

Decision trees

Nearest neighbor  
classification

(*Last  
lecture*)

Non-parametric



# Application: Medical Diagnosis

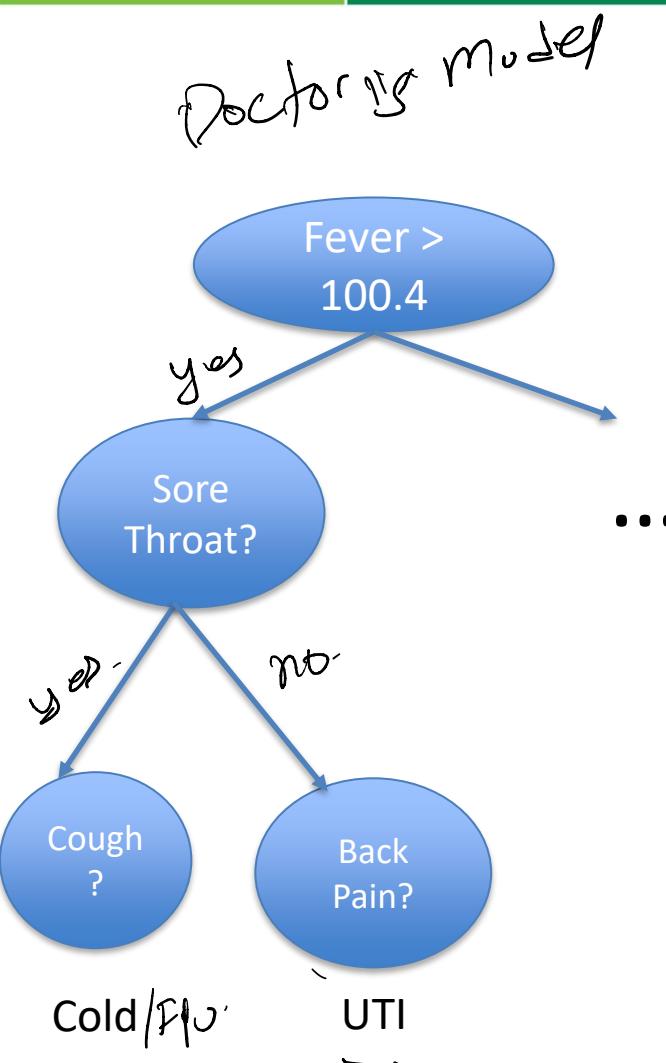
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- Suppose that you go to your doctor with flu-like symptoms
  - How does your doctor determine if you have a flu that requires medical attention?

# 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

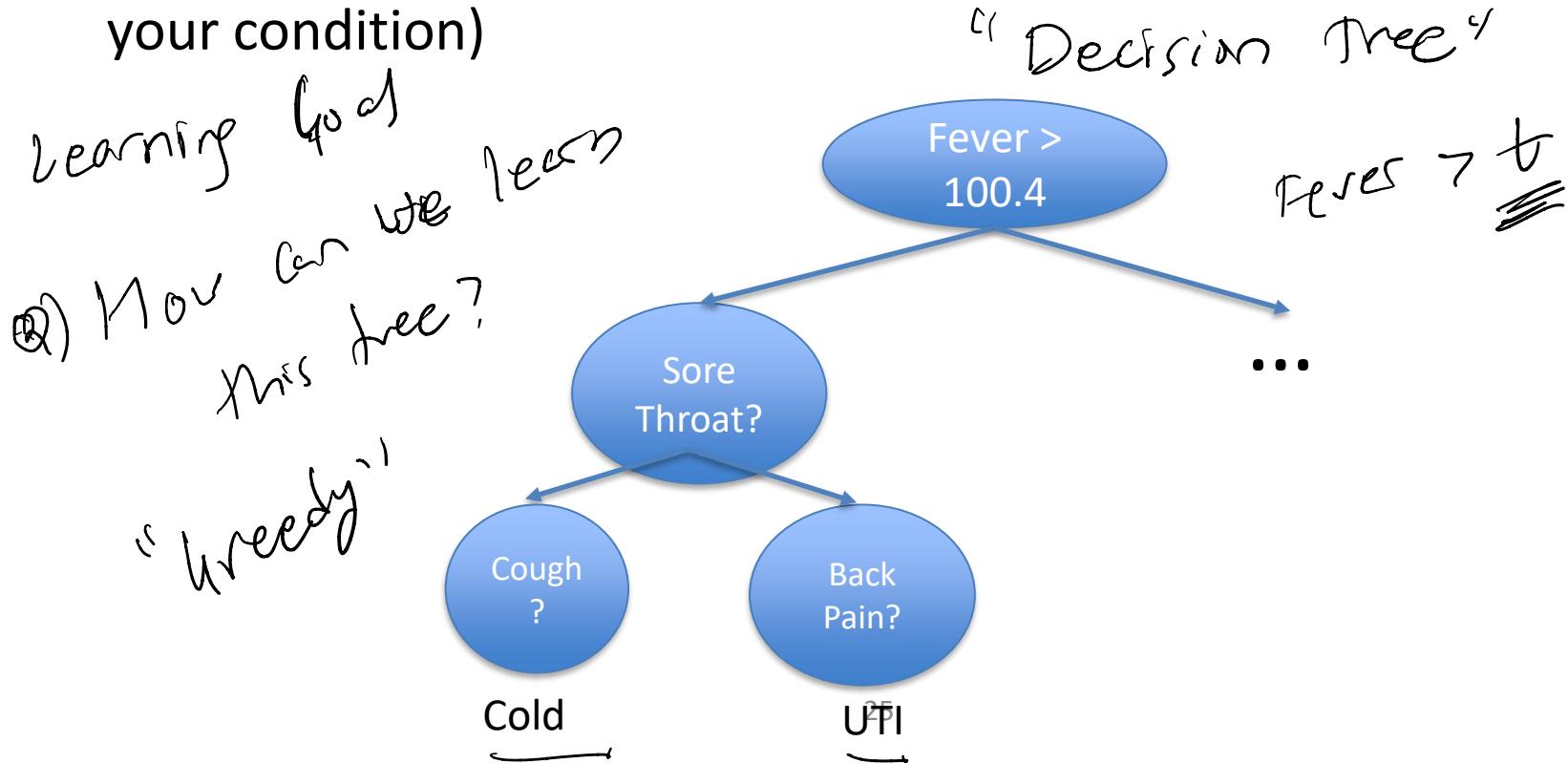


- Just having some symptoms is not enough, you should also not have symptoms that are not consistent with the flu
- For example,
  - If you have a fever over 100.4 degrees Fahrenheit?
  - And you have a sore throat or a stuffy nose?
  - You probably do not have the flu (most likely just a cold)

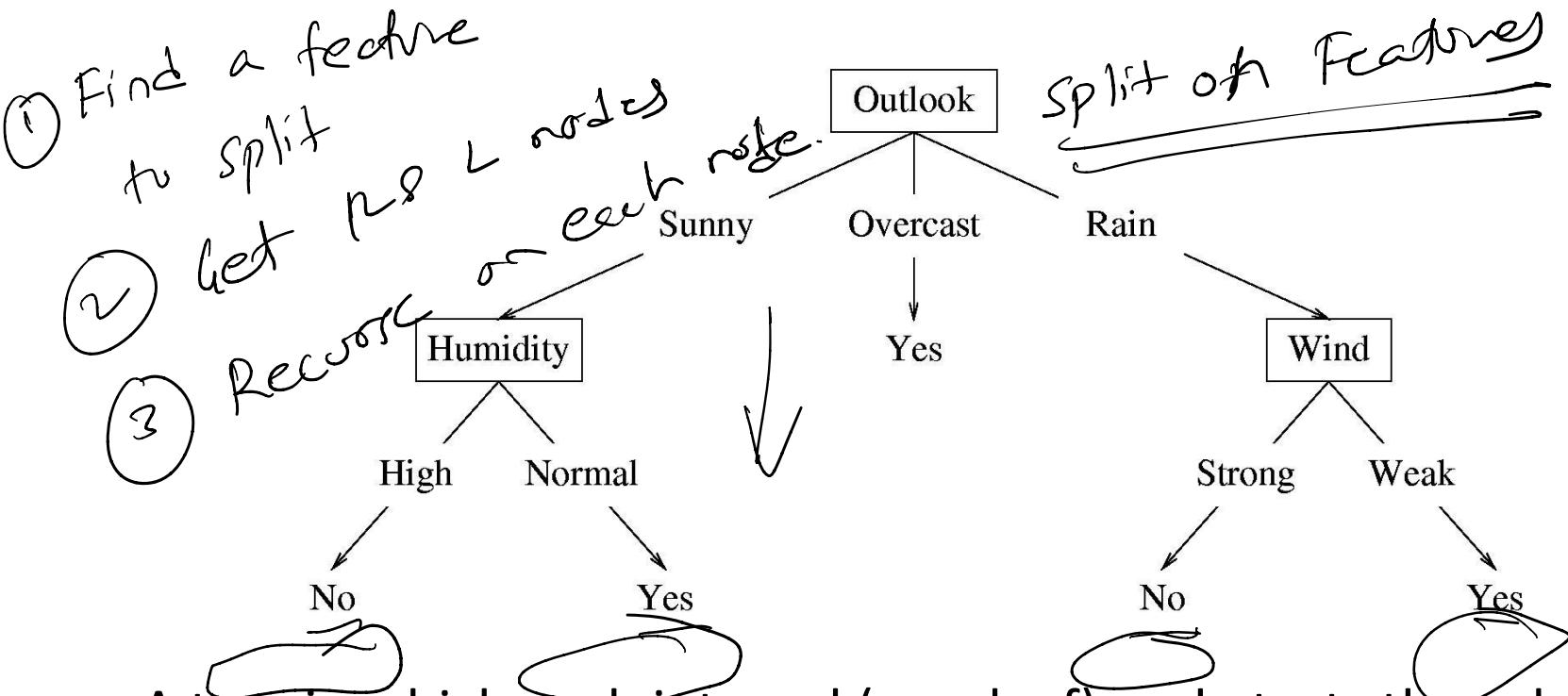
# Application: Medical Diagnosis



- 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)



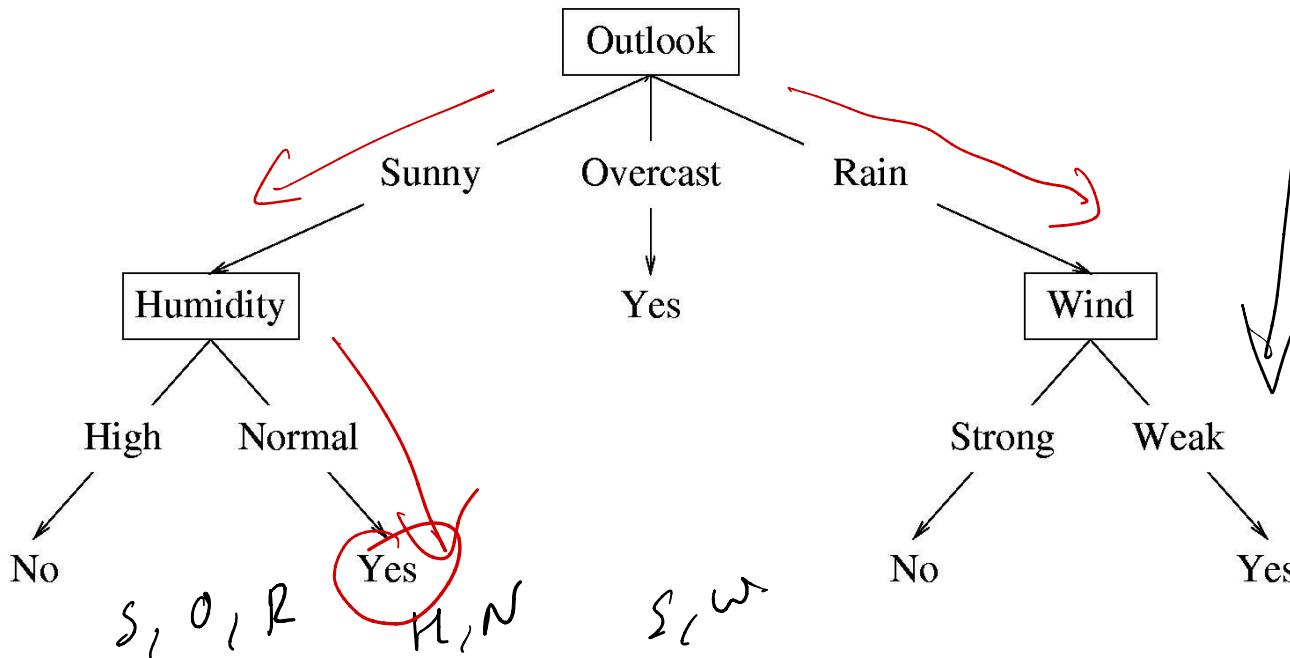
# Decision Trees



- 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)

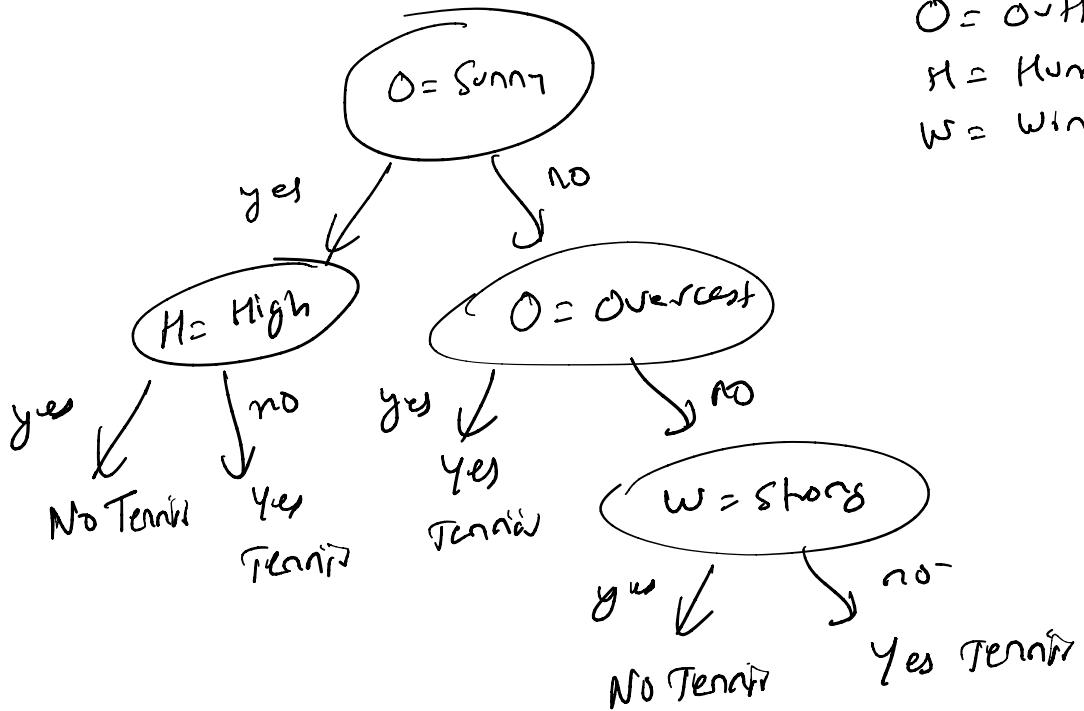
# Decision Trees

"Tree Inference"

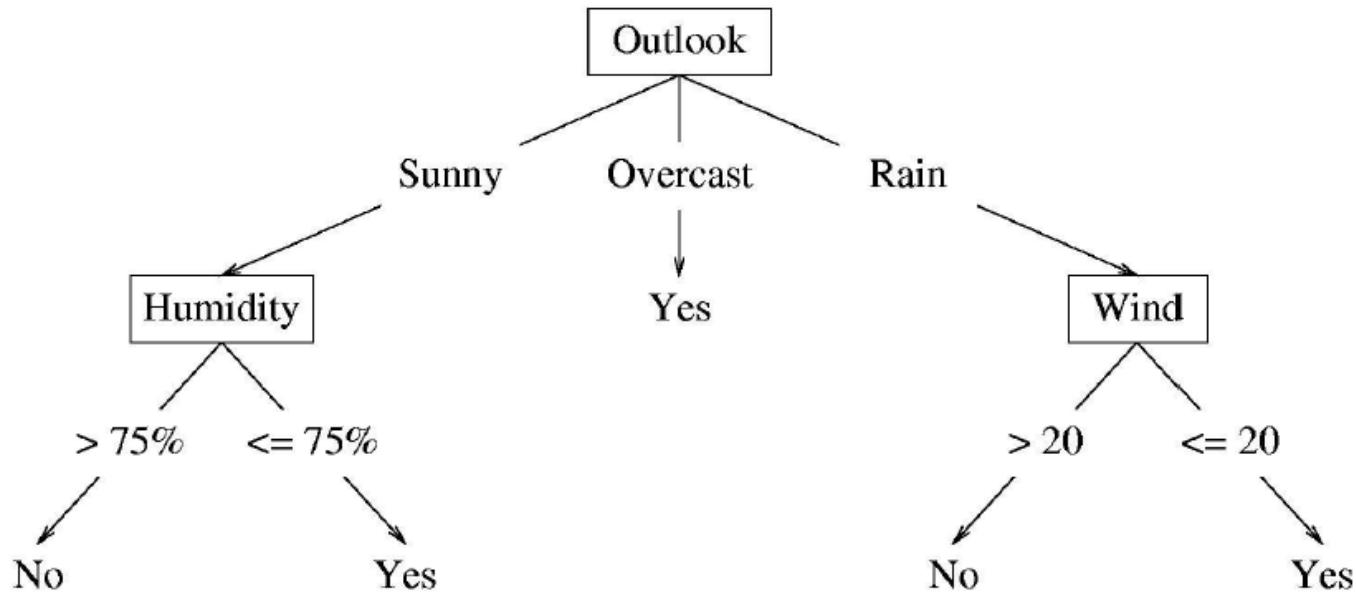


- Features: (Outlook, Humidity, Wind)
- Classification is performed root to leaf
  - The feature vector (Sunny, Normal, Strong) would be classified as a yes instance

O = Outlook  
H = Humidity  
W = Wind.



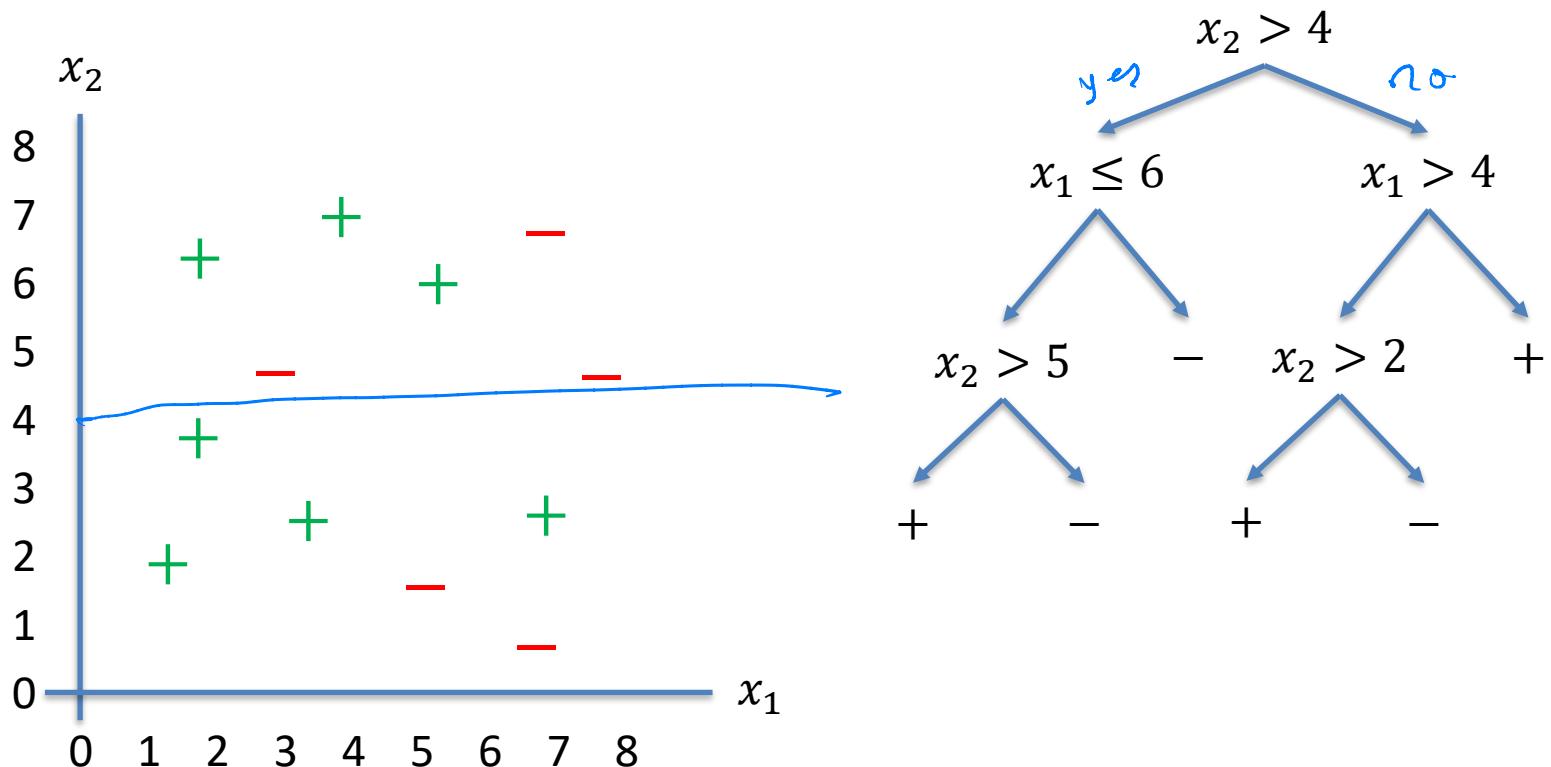
# Decision Trees



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

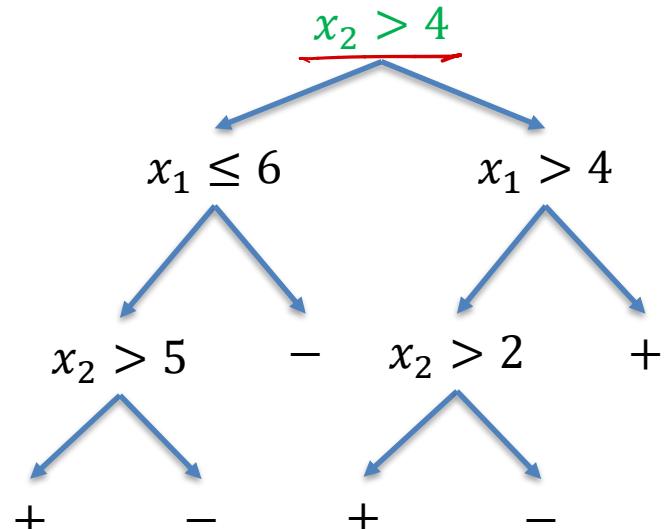
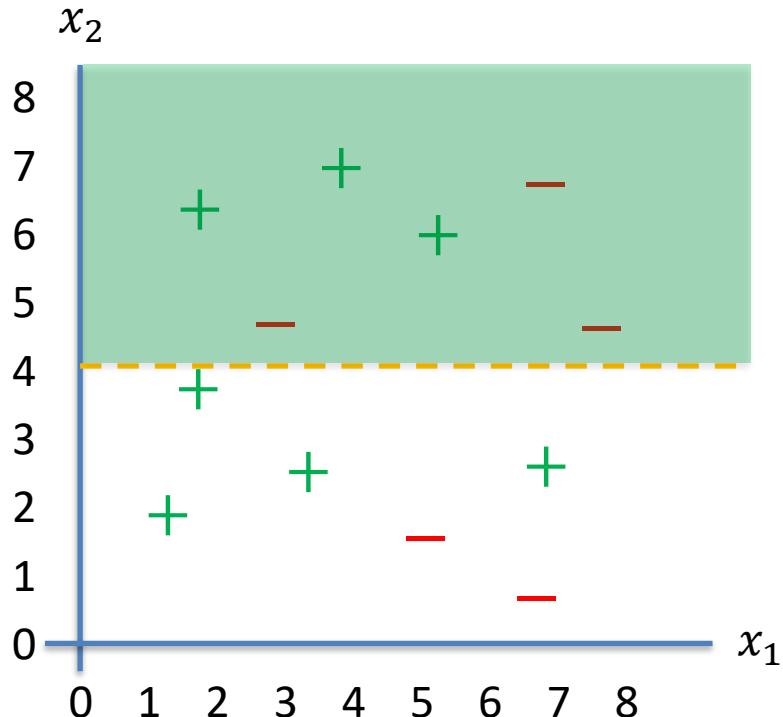
# Decision Trees

- Decision trees divide the feature space into axis parallel rectangles



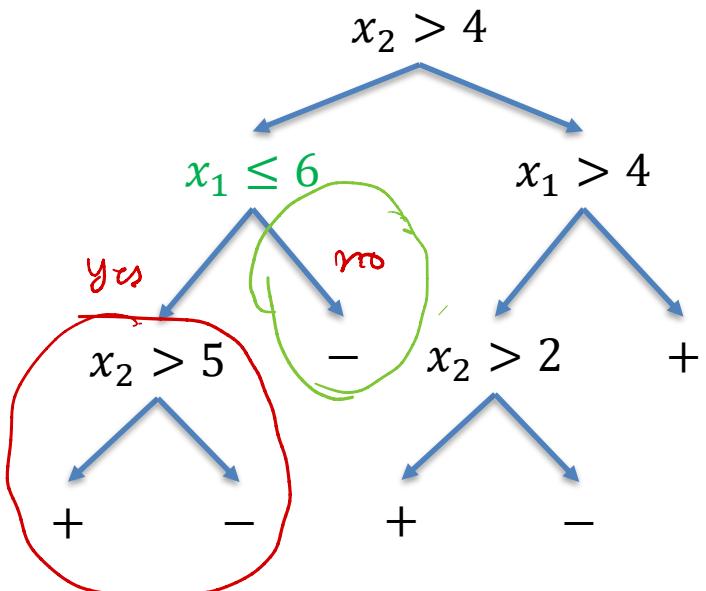
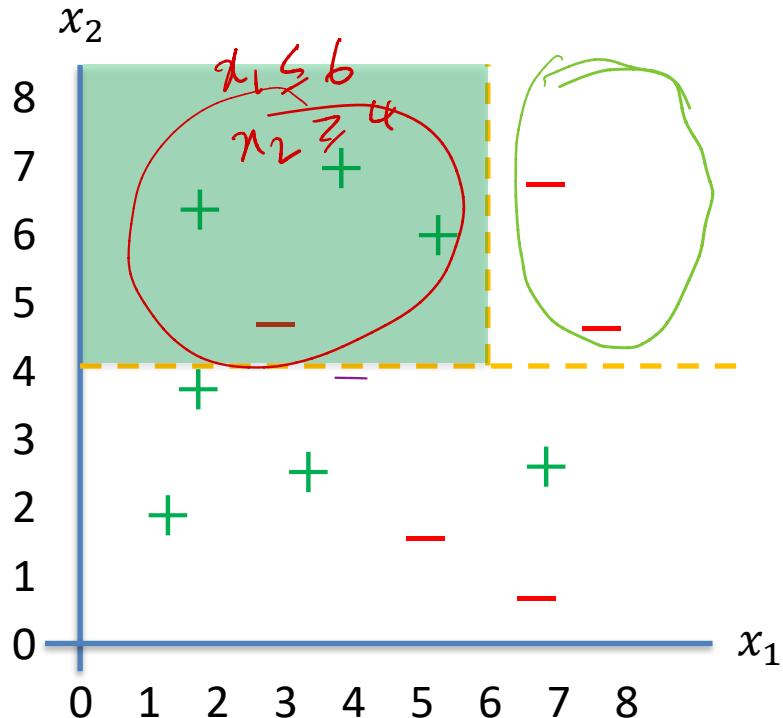
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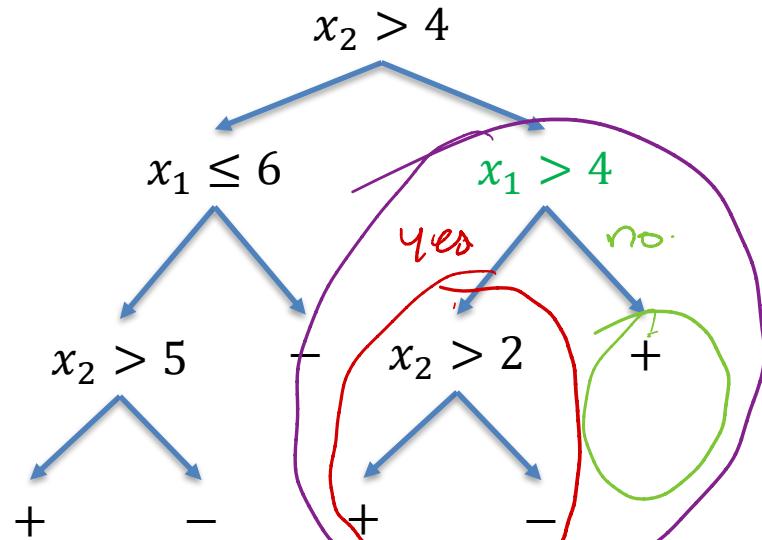
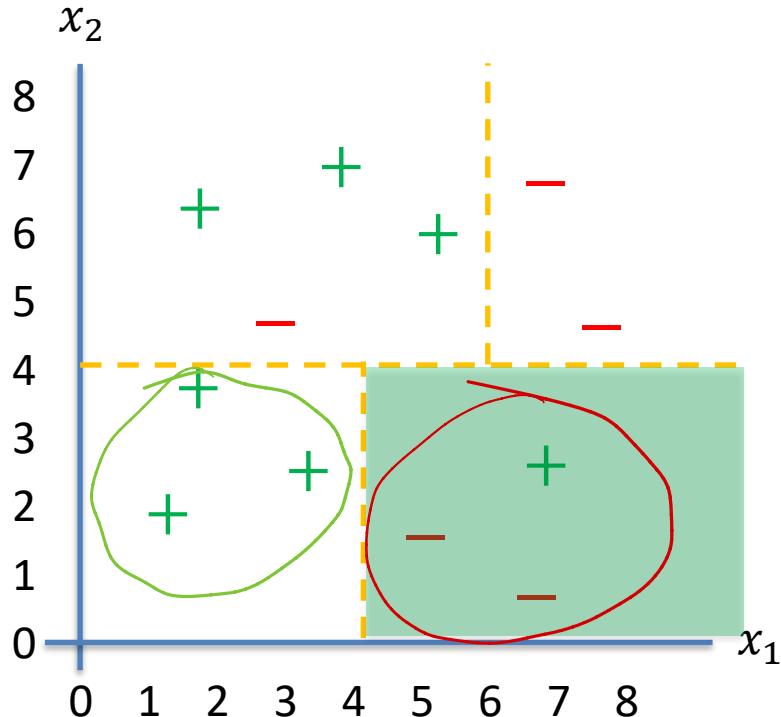
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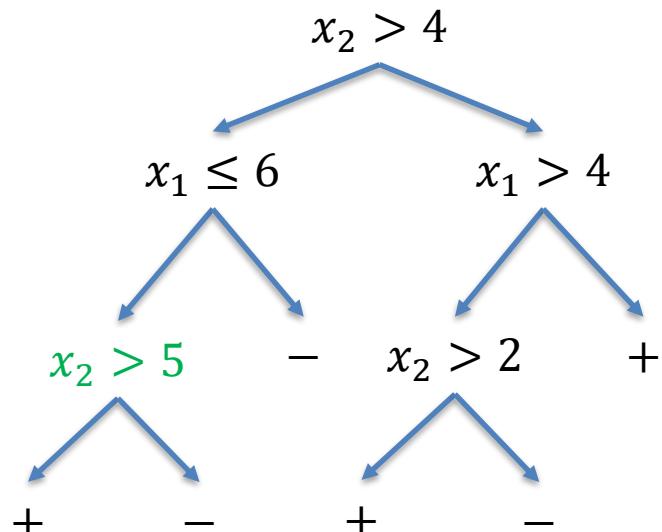
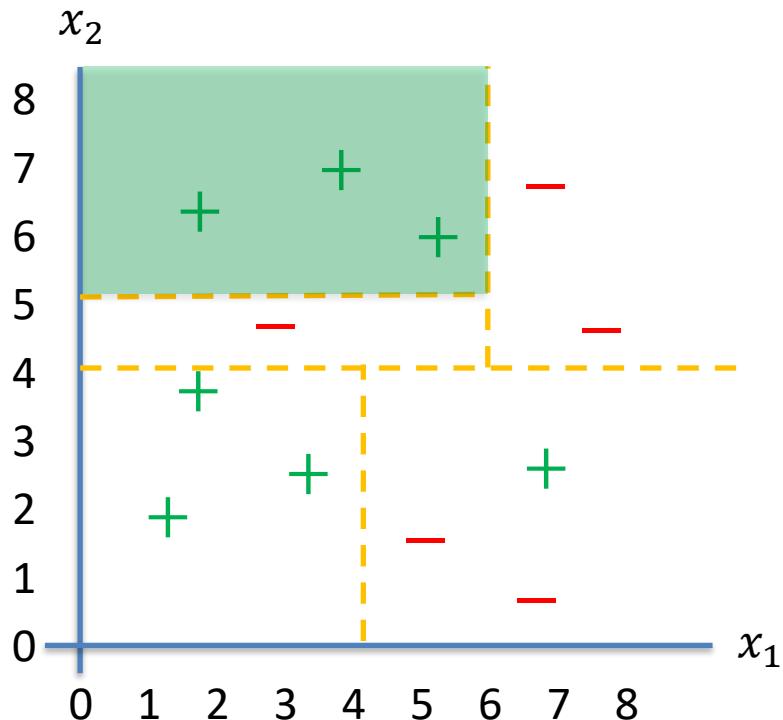
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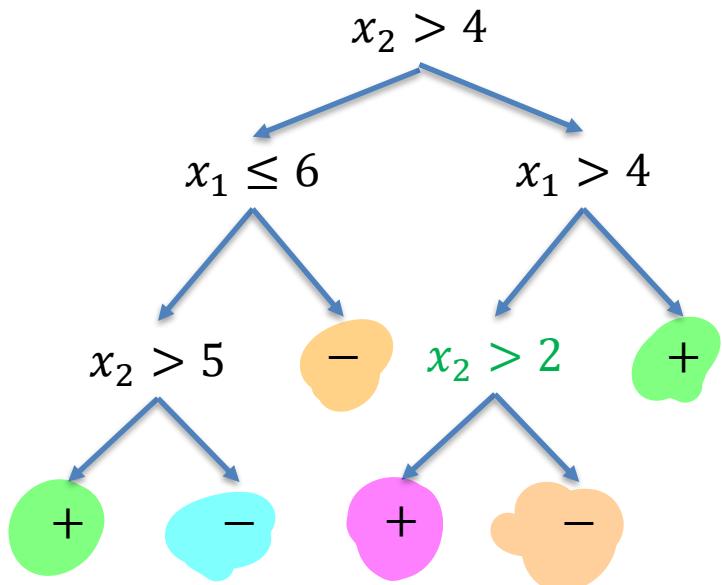
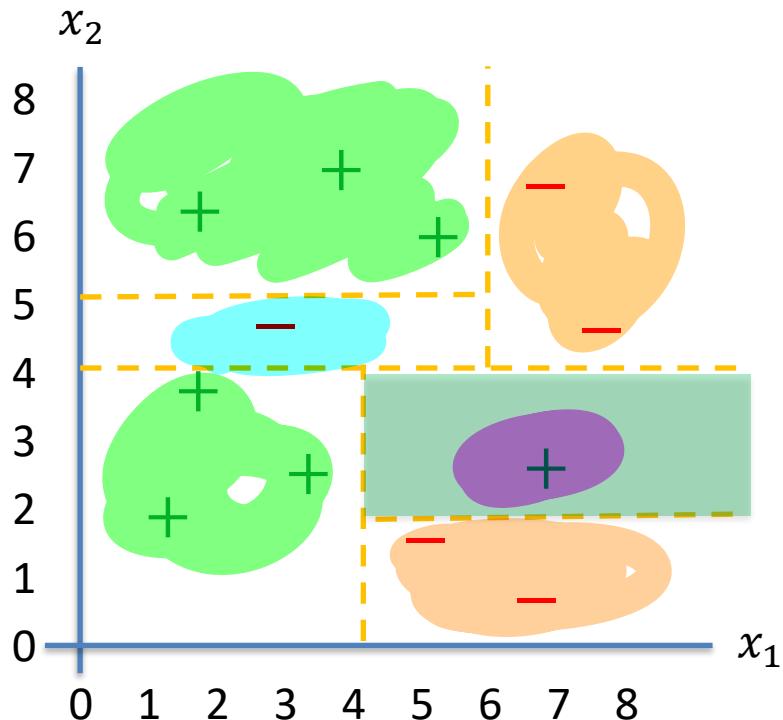
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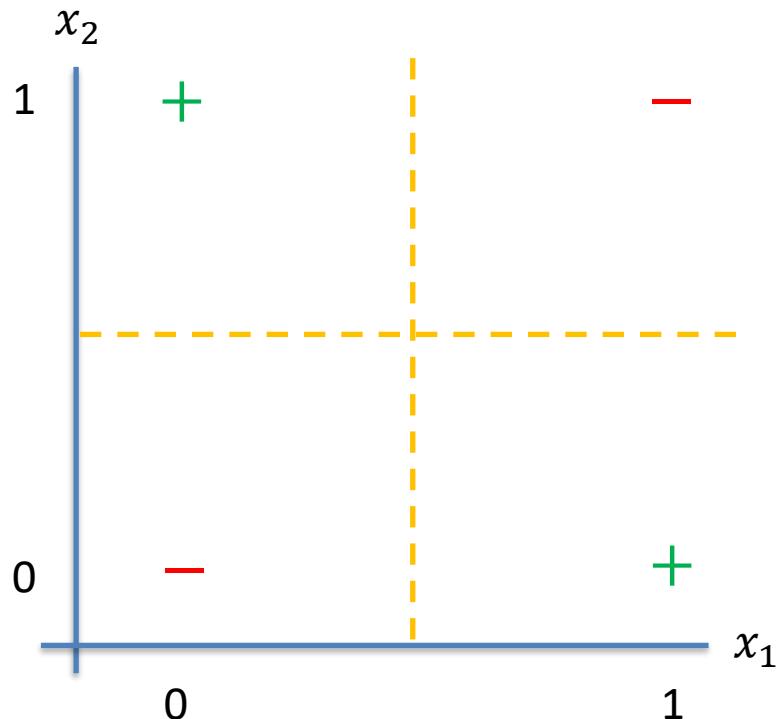
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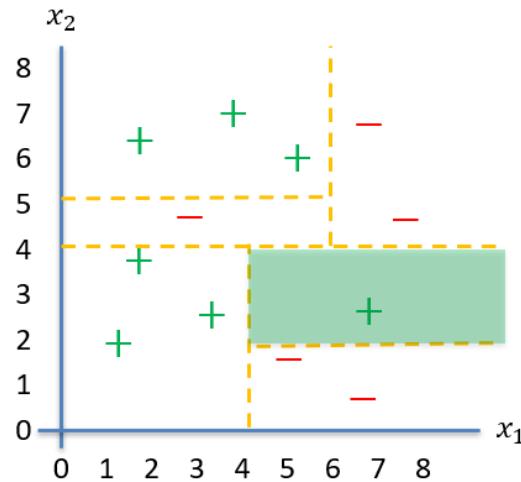
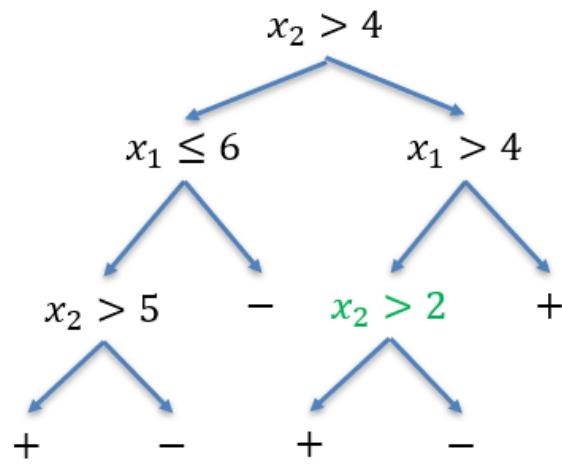


# Decision Trees

- Worst case decision tree may require exponentially many nodes



# Decision Tree Learning

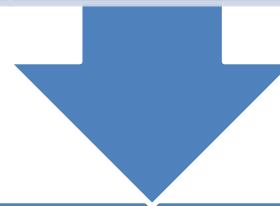


Basic decision tree building algorithm:

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)

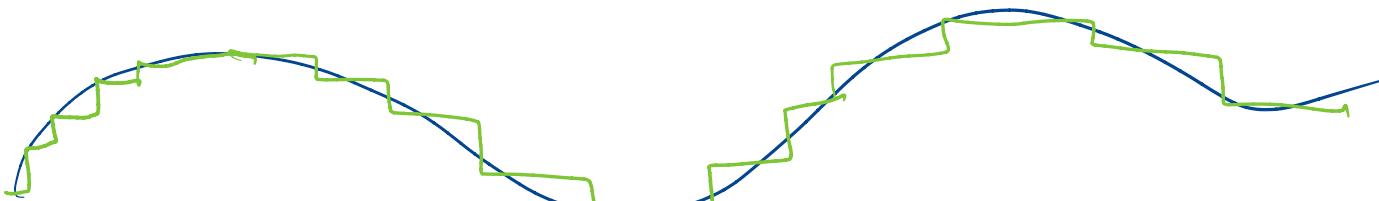
# Decision Trees



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

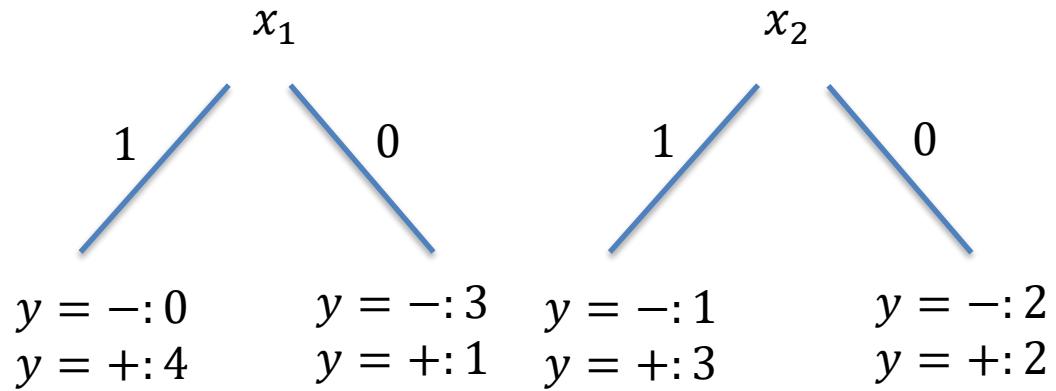
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- Because the complexity of storage and classification increases with the size of the tree, should prefer smaller trees
  - Simplest models that explain the data are usually preferred over more complicated ones
  - Finding the smallest tree is an NP-hard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

# Choosing the Best Attribute

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

Which attribute should you split on?

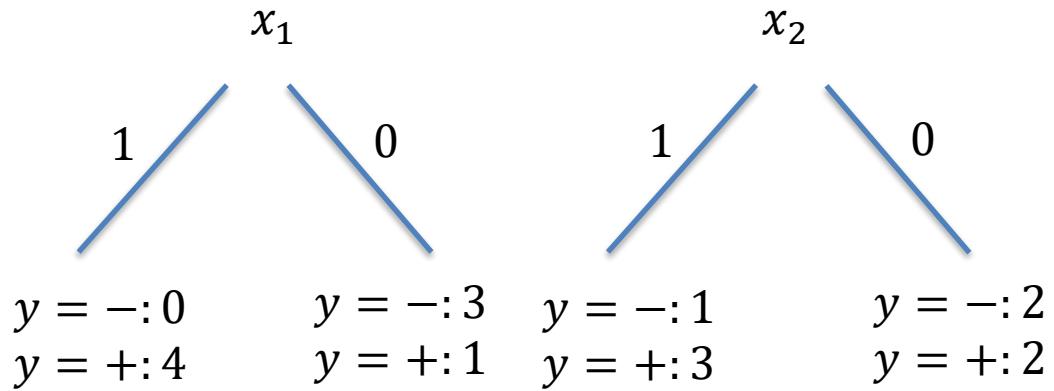


$x_1$	$x_2$	$y$
1	1	+
1	0	+
1	1	+
1	0	+
0	1	+
0	0	-
0	1	-
0	0	-

# 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

# 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?

# Recap: Information Gain

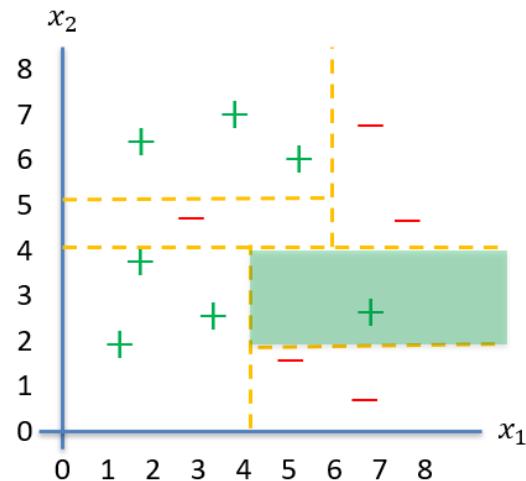
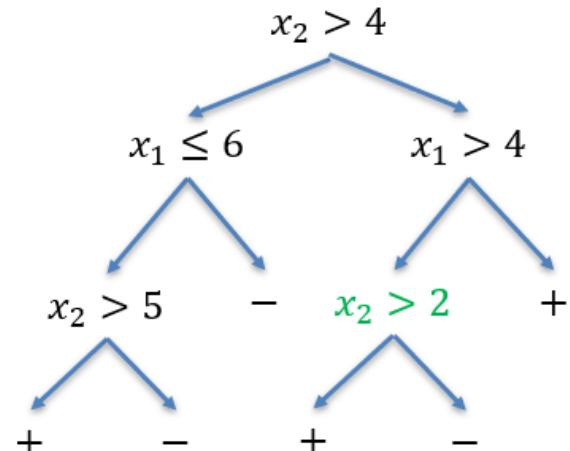
- Using entropy to measure uncertainty, we can greedily select an attribute that guarantees the largest expected decrease in entropy (with respect to the empirical partitions)

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

- 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

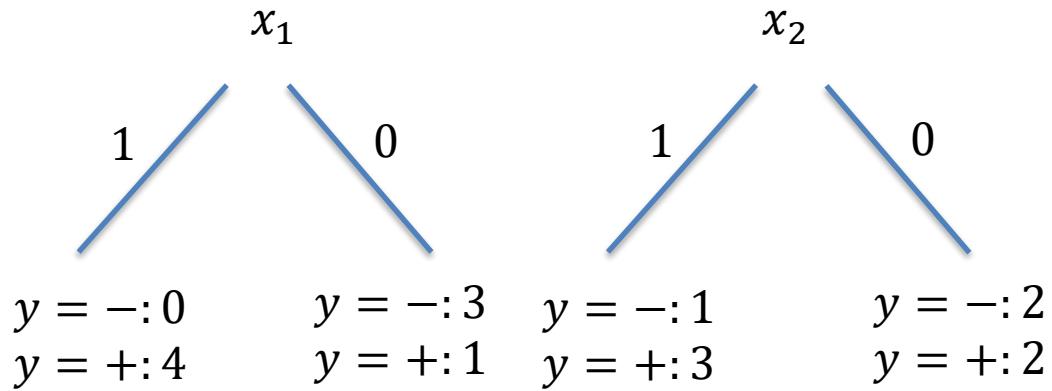
- Basic decision tree building algorithm:
  - Pick the feature/attribute with the highest information gain
  - Partition the data based on the value of this attribute
  - Recurse over each new partition



# Choosing the Best Attribute

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

Which attribute should you split on?



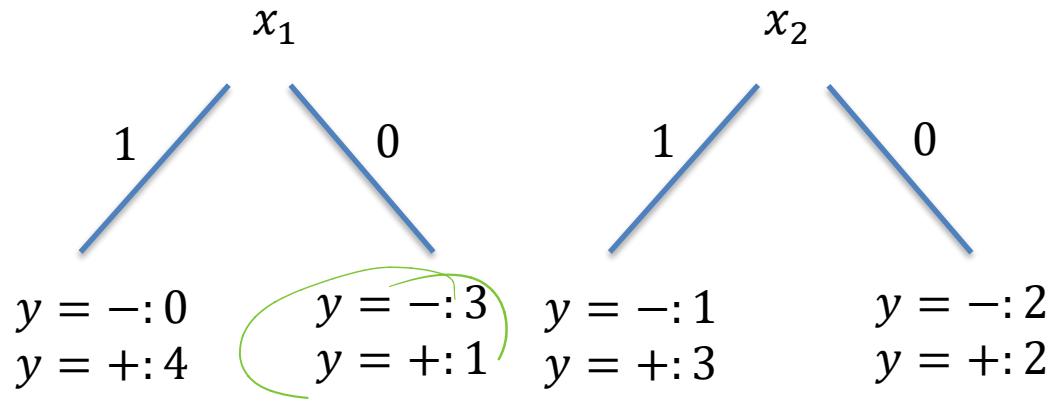
$x_1$	$x_2$	$y$
1 /	1 /	+
1	0	+
1	1	+
1	0	+
0	1	+
0	0	-
0	1	-
0	0	-

What is the information gain in each case?

# Choosing the Best Attribute

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

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	-

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

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

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

$$\underbrace{H(Y) - H(Y|X_1)}_{\text{IG}(X_1)} \geq \underbrace{H(Y) - H(Y|X_2)}_{\text{IG}(X_2)} \quad \text{Should split on } x_1$$

$$H(Y|X)$$

$$X = (x_1, x_2)$$

$$\boxed{I(Y|X)} = H(Y) - H(Y|X)$$

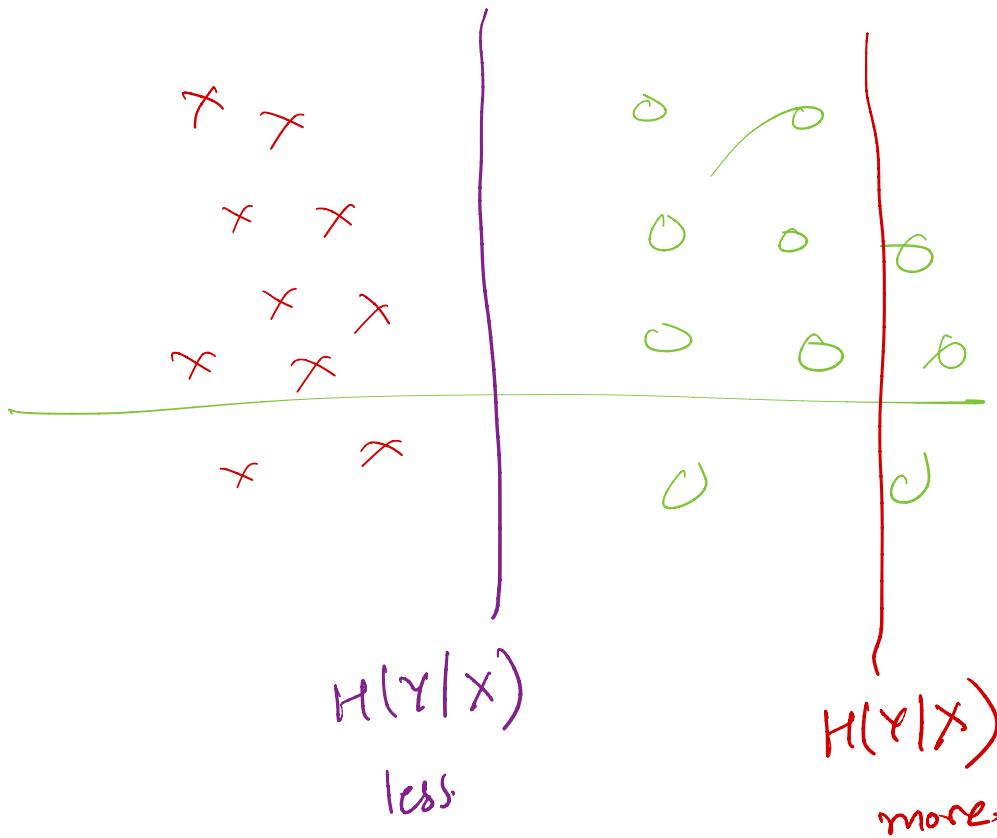
$$H(Y|x_1)$$
$$H(Y|x_2)$$

Split

$$\max_{\text{"split"}} [I(Y|X_{\text{split}})] \approx \min_{\text{split}} H(Y|X_{\text{split}})$$

$$X_{\text{split}} = \underbrace{\text{Splitting Condition on } X}_{\text{Splitting Condition on } X}$$

$$x_1 = \underline{1/0} \quad x_2 = \underline{1/0}$$



# 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



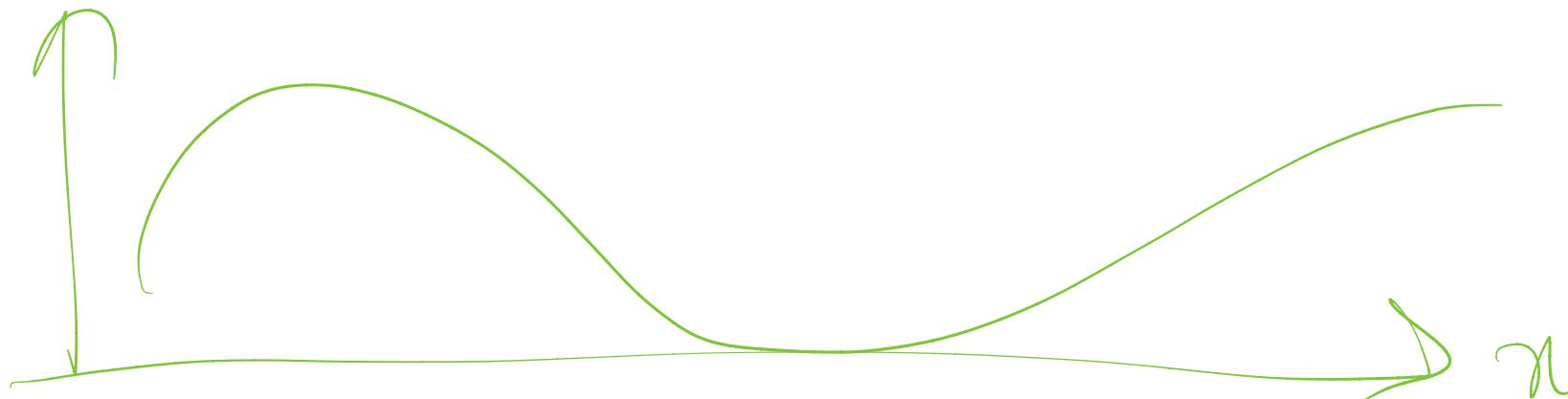
If a partition contains no data items, nothing to recurse on



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

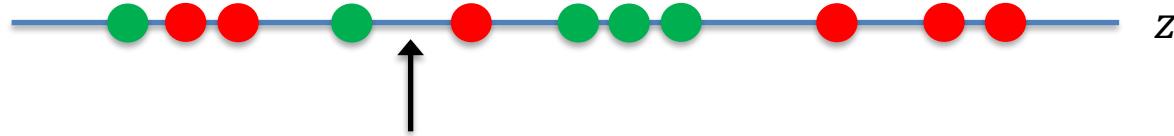
- For continuous attributes, use threshold splits
  - Split the tree into  $x_k < t$  and  $x_k \geq t$
  - Can split on the same attribute multiple times on the same path down the tree
- How to pick the threshold  $t$ ?
  - Try every possible  $t$

[0, 1]

How many possible  $t$  are there?

# Handling Real-Valued Attributes

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

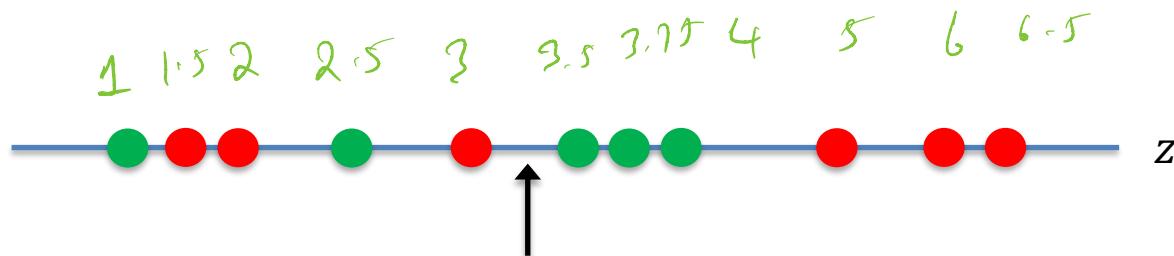


- Only a finite number of thresholds make sense

$$t_i = \frac{z_i + z_{i+1}}{2}$$

# Handling Real-Valued Attributes

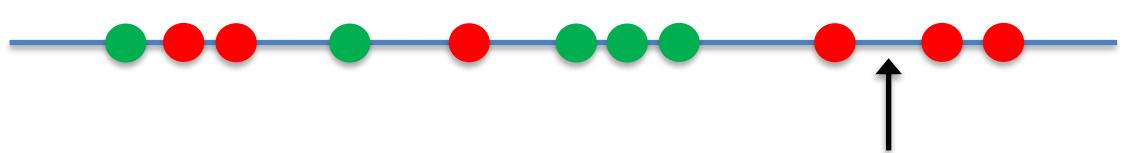
- Sort the data according to the  $k^{th}$  attribute:  $z_1 > z_2 > \dots > z_n$



- 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:  $z_1 > z_2 > \dots > z_n$



- Only a finite number of thresholds make sense

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

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

# Handling Real-Valued Attributes

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

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

$\nabla$

$$-p(X \geq t) \sum_y p(Y = y|X \geq t) \log p(Y = y|X \geq t)$$

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

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

[Every feature & threshold]

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

[Every feature]

# Decision Trees



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

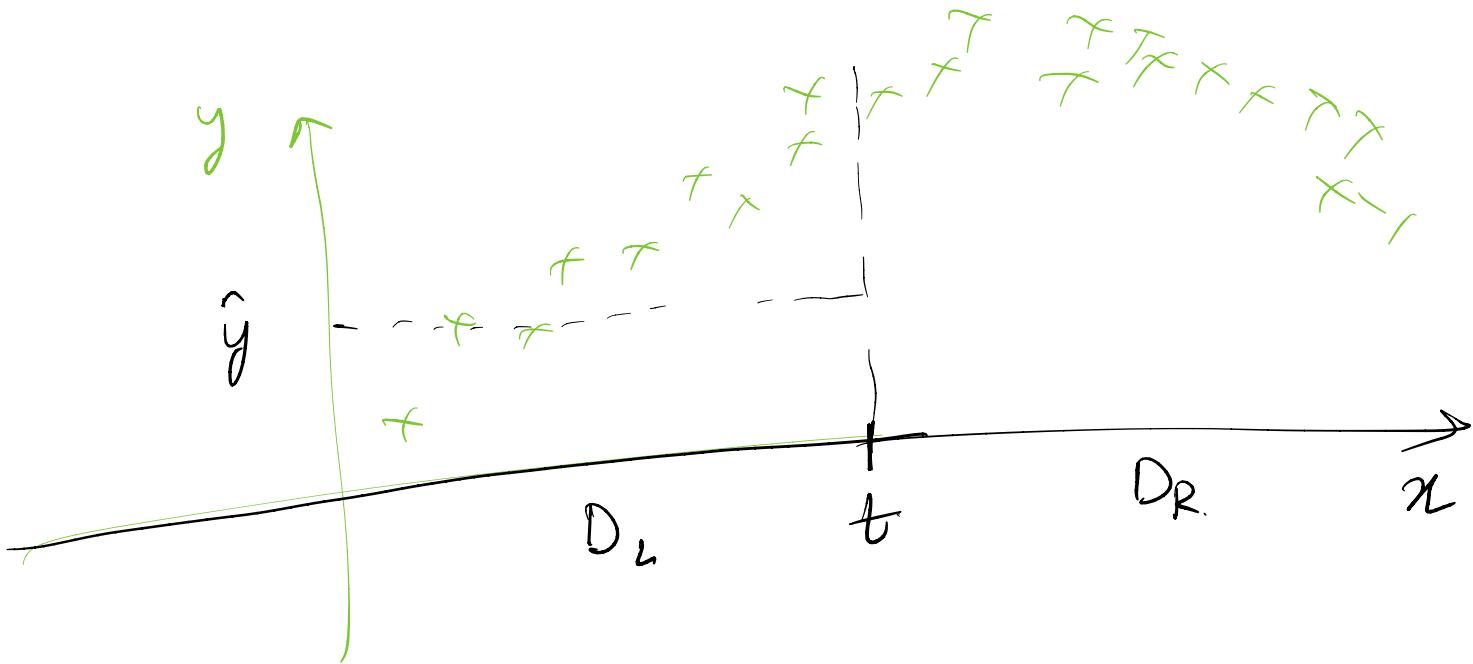
Can be used for regression too



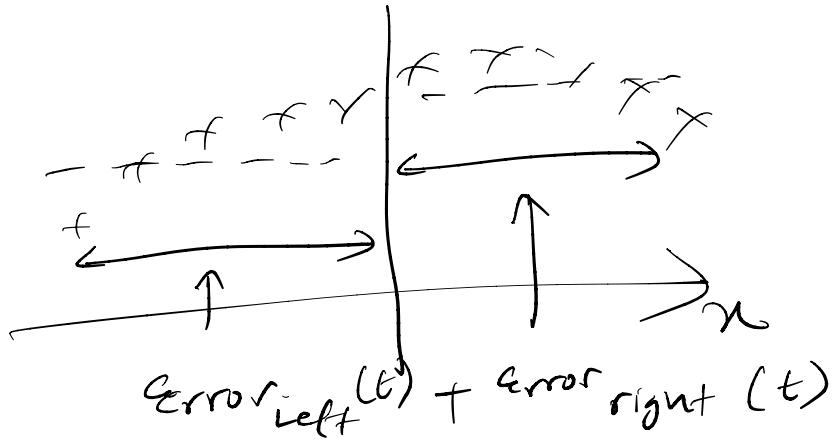
Decision trees will **always** overfit!

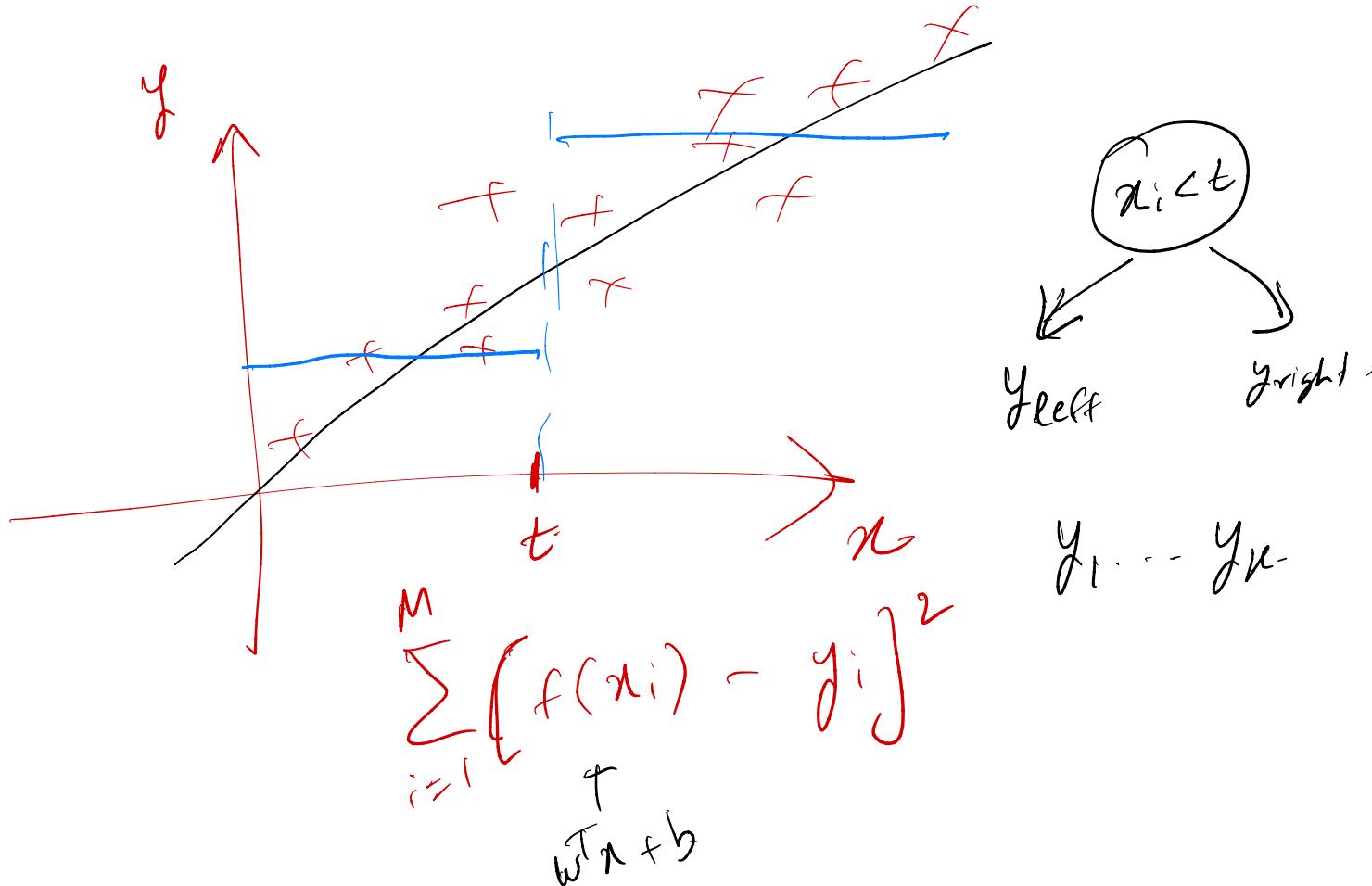
It is always possible to obtain zero training error on the input data with a deep enough tree (if there is no noise in the labels)

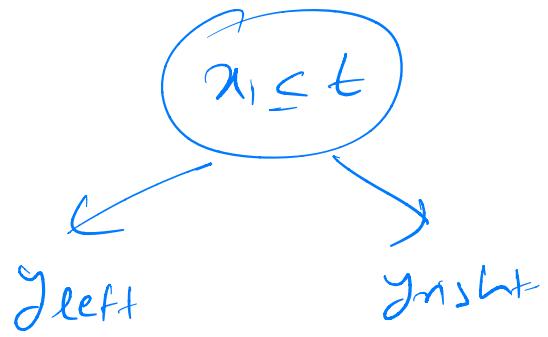
Solution?



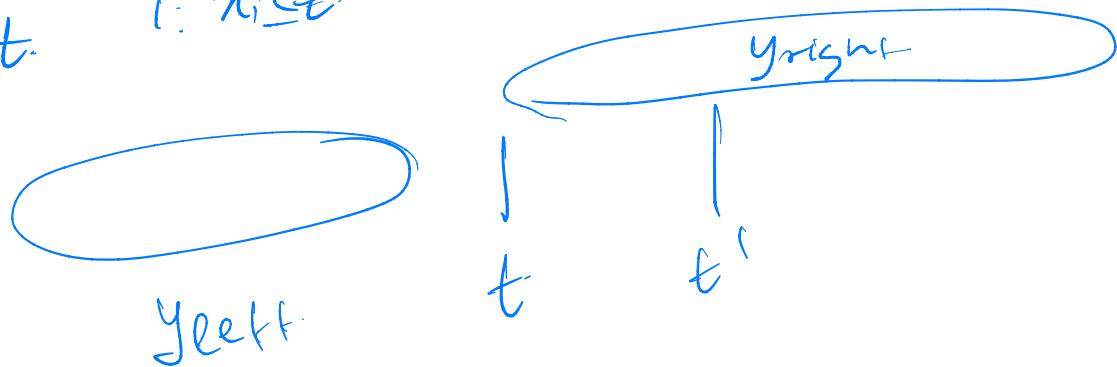
$$\min_{\hat{y}} \sum_{i \in D_L} [y_i - \hat{y}]^2, \quad \hat{y} = \frac{\sum_{i \in D_L} y_i}{|D_L|}$$

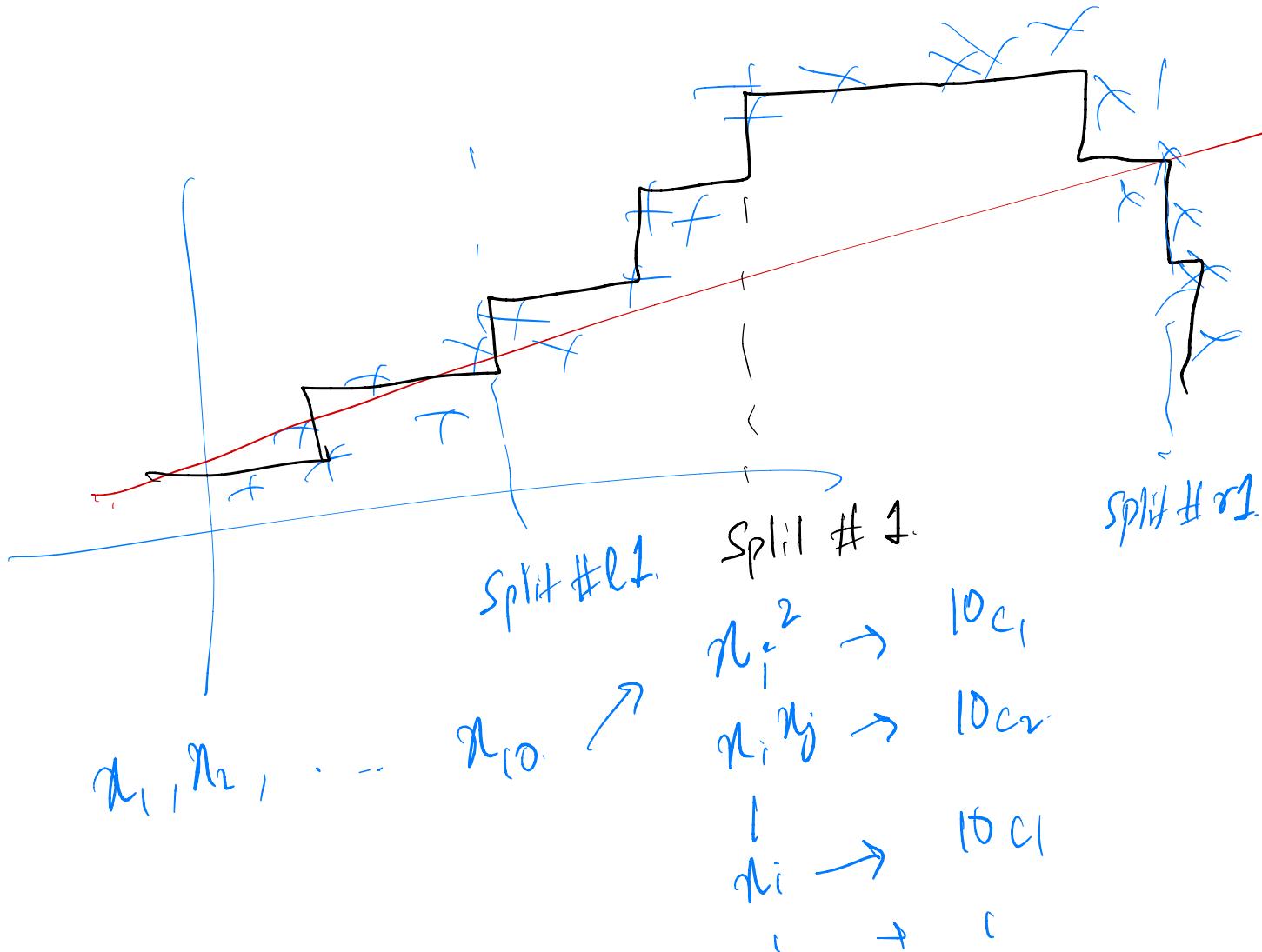






$$\min_t \sum_{i: x_i \leq t} [y_{left}^t - y_i]^2 + \sum_{i: x_i > t} [y_{right}^t - y_i]^2$$





$$f = \{ 'y', 'n', '?' \} \rightarrow K$$

$$\begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \quad \left. \right\} 3K$$