# Supervised Learning

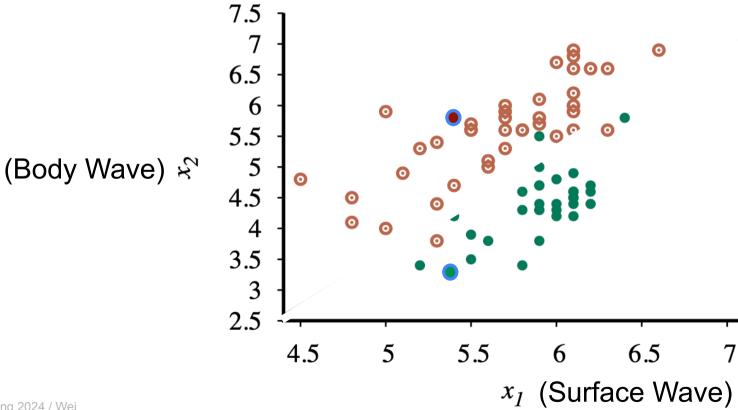
- Regression
- Classification

#### Classification

- Learning a predictor that has **discrete** outputs (labels)
  - Binary classification
  - Multi-class classification

#### **Example: Binary Classification**

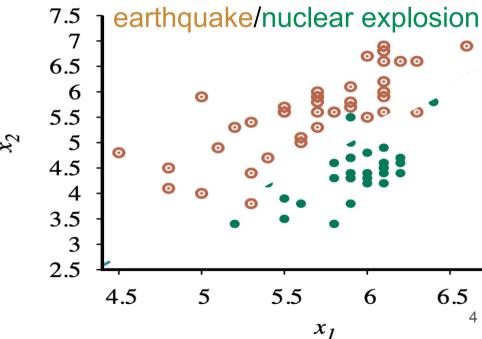
Two classes: earthquake/nuclear explosion



#### **Decision Boundary**

- A decision boundary is a line (or a surface, in higher dimensions) that separates the two classes
- A linear decision boundary is called a linear separator and data that admit such a separator are
   7.5 1 earthquake/nuclea

called linearly separable



### **Decision Boundary**

• Linear separator:  $x_2 = w_1 x_1 + w_0$ 

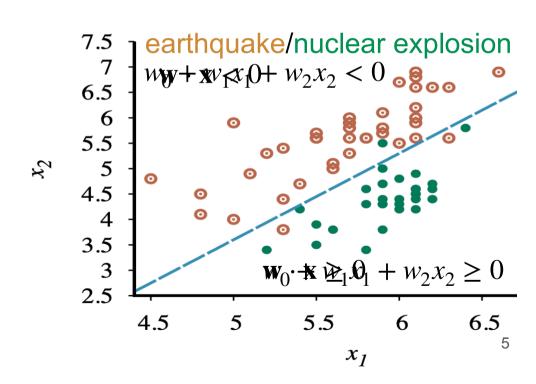
$$\Rightarrow w_0 + w_1 x_1 - x_2 = 0$$

$$\Rightarrow w_0 + w_1 x_1 + w_2 x_2 = 0$$

$$\Rightarrow \mathbf{w} \cdot \mathbf{x} = 0$$

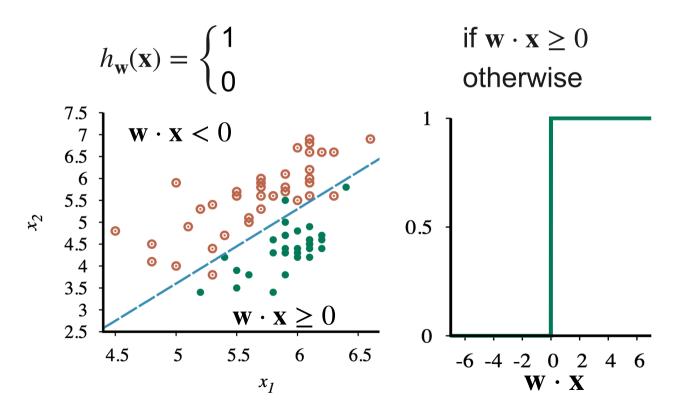
Weight vector:  $\mathbf{w} = \langle w_0, w_1, w_2 \rangle$ 

Input vector:  $\mathbf{x} = \langle 1, x1, x2 \rangle$ 



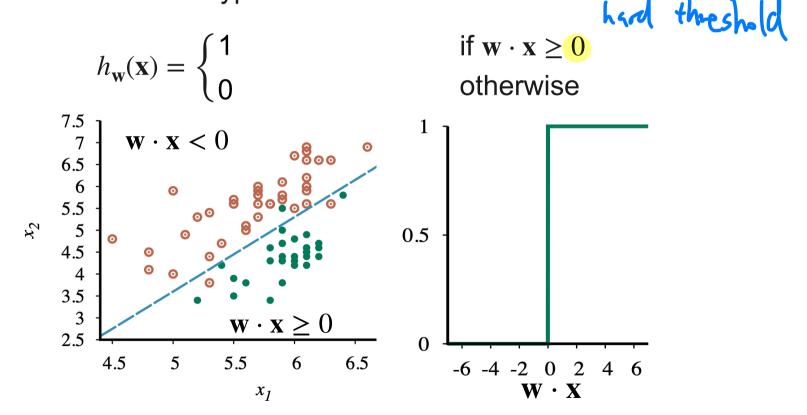
#### **Linear Classifiers**

ullet Given data points of two classes: earthquake/nuclear explosion learn a classification hypothesis h



#### Linear Classifiers with a Hard Threshold

 Given data points of two classes: earthquake/nuclear explosion learn a classification hypothesis h



### **Perceptron Learning Rule**

• Given data point  $(\mathbf{x}, y)$ , update each weight according to

$$w_i \leftarrow w_i + \alpha(y - h_{\mathbf{w}}(\mathbf{x})) \times x_i$$

У	$h_{\mathbf{w}}(\mathbf{x})$	$\mathcal{X}_i$	$w_i$
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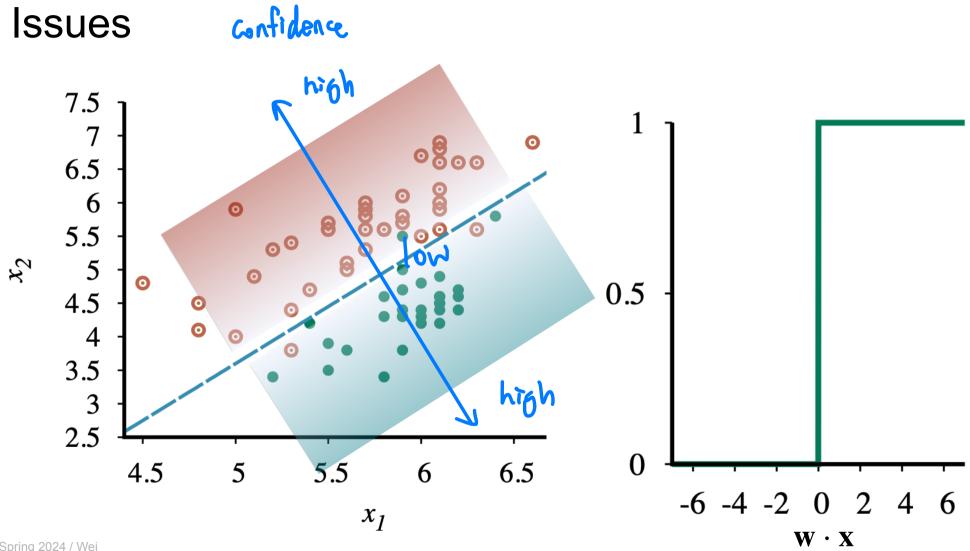
### Perceptron Learning Rule

• Given data point  $(\mathbf{x}, y)$ , update each weight according to

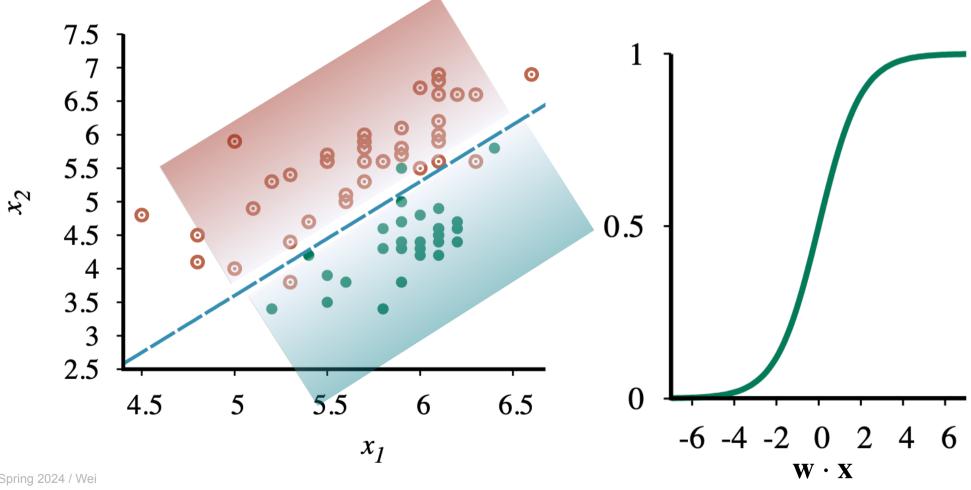
$$w_i \leftarrow w_i + \alpha(y - h_{\mathbf{w}}(\mathbf{x})) \times x_i$$

	У	$h_{\mathbf{w}}(\mathbf{x})$	$\mathcal{X}_{i}$	$w_i$	$\begin{bmatrix} 7.5 \\ 7 \\ 6.5 \end{bmatrix}  \mathbf{w} \cdot \mathbf{x} < 0$
w.v^	1	0	+	<b>↑</b>	_ 6 - 0 9 9
$\mathbf{w} \cdot \mathbf{x} \uparrow$	1	0	-	$\downarrow$	5.5
*** **	0	1	+	$\downarrow$	4.5
$\mathbf{w} \cdot \mathbf{x} \downarrow$	0	1	-	<b>↑</b>	3.5
<b>K</b>					$ \begin{array}{c} 3 \\ 2.5 \end{array} \qquad \mathbf{w} \cdot \mathbf{x} \ge 0 $
		,			4.5 5 5.5 6 6.5
					$x_1$

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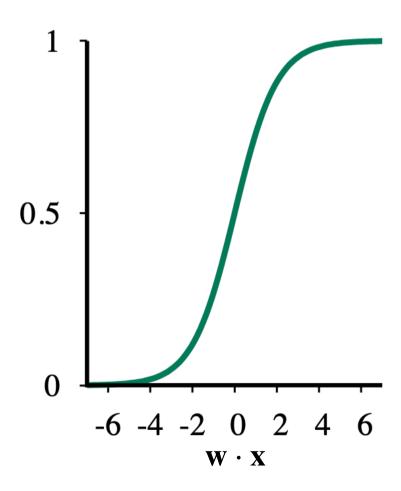
### Issues



#### Linear Classifies with a Soft Threshold

Logistic function (sigmoid function):

$$Logistic(z) = rac{1}{1+e^{-z}}$$



#### Linear Classifies with a Soft Threshold

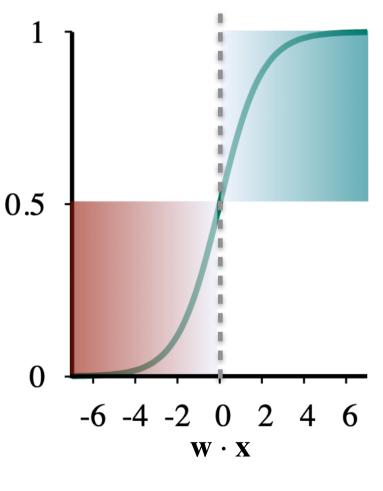
Logistic function (sigmoid function):

$$Logistic(z) = rac{1}{1 + e^{-z}}$$

Let a hypothesis be

$$h_{\mathbf{w}}(\mathbf{x}) = Logistic(\mathbf{w} \cdot \mathbf{x}) = \frac{1}{1 + e^{-\mathbf{w} \cdot \mathbf{x}}}$$

- ullet w (weights or coefficients):
  - A vector of learned parameters or weights that are optimized during training. Each element of this vector represents the importance of a particular feature in the dataset.
- The weight values are adjusted during the training process to best fit the training data, minimizing the prediction error (typically via cross-entropy loss).
- x (features):
  - A vector representing the features of a data point. Each element of this vector corresponds to a specific feature or characteristic used to predict the target variable.
- For example, if you're predicting whether an email is spam or not based on words used, each feature could represent the frequency of a specific word in the email.



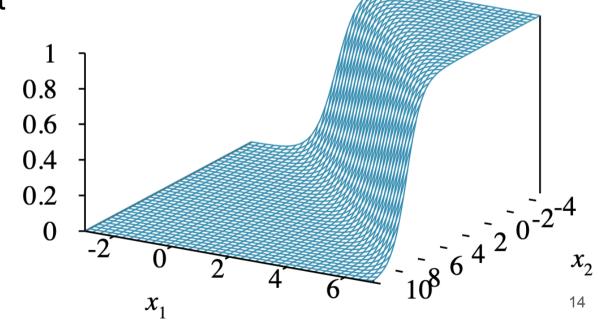
### **Logistic Regression**

The process to fit the weights of the model

$$h_{\mathbf{w}}(\mathbf{x}) = Logistic(\mathbf{w} \cdot \mathbf{x}) = \frac{1}{1 + e^{-\mathbf{w} \cdot \mathbf{x}}}$$

to minimize loss on a data set

•  $L_2$  loss



### Logistic Regression

- Find the optimal value of w with this model
  - Gradient descent computation

 $\mathbf{w} \leftarrow \text{any point in the parameter space}$   $\mathbf{while\ not\ converged\ do}$   $\mathbf{for\ each\ } w_i \mathbf{\ in\ w\ do}$ 

$$w_i \leftarrow w_i - lpha rac{\partial}{\partial w_i} Loss\left(\mathbf{w}
ight)$$

$$h_{\mathbf{w}}(\mathbf{x}) = g(\mathbf{w} \cdot \mathbf{x}) = \frac{1}{1 + e^{-\mathbf{w} \cdot \mathbf{x}}}$$

$$egin{aligned} rac{\partial}{\partial w_i} Loss(\mathbf{w}) &= rac{\partial}{\partial w_i} (y - h_\mathbf{w}(\mathbf{x}))^2 & \text{(L2 Loss)} \ &= 2(y - h_\mathbf{w}(\mathbf{x})) imes rac{\partial}{\partial w_i} (y - h_\mathbf{w}(\mathbf{x})) & \text{(Churn Pule)} \end{aligned}$$

$$h_{\mathbf{w}}(\mathbf{x}) = g(\mathbf{w} \cdot \mathbf{x}) = \frac{1}{1 + e^{-\mathbf{w} \cdot \mathbf{x}}}$$

$$\frac{\partial}{\partial w_i} Loss(\mathbf{w}) = \frac{\partial}{\partial w_i} (y - h_{\mathbf{w}}(\mathbf{x}))^2$$

$$= 2(y - h_{\mathbf{w}}(\mathbf{x})) \times \frac{\partial}{\partial w_i} (y - g(\mathbf{w} \cdot \mathbf{x})) \qquad (h_{\mathbf{w}}(\mathbf{x}) = g(\mathbf{w} \cdot \mathbf{x}))$$

$$h_{\mathbf{w}}(\mathbf{x}) = g(\mathbf{w} \cdot \mathbf{x}) = \frac{1}{1 + e^{-\mathbf{w} \cdot \mathbf{x}}}$$

$$egin{aligned} rac{\partial}{\partial w_i} Loss(\mathbf{w}) &= rac{\partial}{\partial w_i} (y - h_\mathbf{w}(\mathbf{x}))^2 \ &= 2(y - h_\mathbf{w}(\mathbf{x})) imes rac{\partial}{\partial w_i} (y - g(\mathbf{w} \cdot \mathbf{x})) \ &= -2(y - h_\mathbf{w}(\mathbf{x})) imes g'(\mathbf{w} \cdot \mathbf{x}) imes rac{\partial}{\partial w_i} \mathbf{w} \cdot \mathbf{x} \end{aligned}$$
 (Chain Pule)

$$h_{\mathbf{w}}(\mathbf{x}) = g(\mathbf{w} \cdot \mathbf{x}) = \frac{1}{1 + e^{-\mathbf{w} \cdot \mathbf{x}}}$$

Statient Descent Computation 
$$g(z) = \frac{1}{1 + e^{-z}} = \frac{e^{z}}{1 + e^{z}}$$

$$\frac{\partial}{\partial w_{i}} Loss(\mathbf{w}) = \frac{\partial}{\partial w_{i}} (y - h_{\mathbf{w}}(\mathbf{x}))^{2}$$

$$= 2(y - h_{\mathbf{w}}(\mathbf{x})) \times \frac{\partial}{\partial w_{i}} (y - g(\mathbf{w} \cdot \mathbf{x}))$$

$$= -2(y - h_{\mathbf{w}}(\mathbf{x})) \times g'(\mathbf{w} \cdot \mathbf{x}) \times \frac{\partial}{\partial w_{i}} \mathbf{w} \cdot \mathbf{x}$$

$$= -2(y - h_{\mathbf{w}}(\mathbf{x})) \times g'(\mathbf{w} \cdot \mathbf{x}) \times x_{i}.$$

$$g(z) = \frac{1}{1 + e^{-z}} = \frac{e^{z}}{1 + e^{z}}$$

$$= \frac{e^{z}}{(1 + e^{z})^{2}}$$

$$= g(z)(1 - g(z))$$

$$g'(\mathbf{w} \cdot \mathbf{x}) = g(\mathbf{w} \cdot \mathbf{x})(1 - g(\mathbf{w} \cdot \mathbf{x}))$$

$$h_{\mathbf{w}}(\mathbf{x}) = g(\mathbf{w} \cdot \mathbf{x}) = \frac{1}{1 + e^{-\mathbf{w} \cdot \mathbf{x}}}$$

$$\frac{\partial}{\partial w_i} Loss(\mathbf{w}) = \frac{\partial}{\partial w_i} (y - h_{\mathbf{w}}(\mathbf{x}))^2$$

$$= 2(y - h_{\mathbf{w}}(\mathbf{x})) \times \frac{\partial}{\partial w_i} (y - \mathbf{g}(\mathbf{w} \cdot \mathbf{x}))$$

$$= -2(y - h_{\mathbf{w}}(\mathbf{x})) \times g'(\mathbf{w} \cdot \mathbf{x}) \times \frac{\partial}{\partial w_i} \mathbf{w} \cdot \mathbf{x}$$

$$= -2(y - h_{\mathbf{w}}(\mathbf{x})) \times g'(\mathbf{w} \cdot \mathbf{x}) \times x_i.$$

$$g(z) = \frac{1}{1 + e^{-z}} = \frac{e^z}{1 + e^z}$$

$$g'(z) = \frac{e^z \cdot (1 + e^z) - e^z \cdot e^z}{(1 + e^z)^2}$$

$$= \frac{e^z}{(1 + e^z)^2}$$

$$= g(z)(1 - g(z))$$

$$g'(\mathbf{w} \cdot \mathbf{x}) = g(\mathbf{w} \cdot \mathbf{x})(1 - g(\mathbf{w} \cdot \mathbf{x})) = h_{\mathbf{w}}(\mathbf{x})(1 - h_{\mathbf{w}}(\mathbf{x}))$$

### Logistic Regression

- Find the optimal value of w with this model
  - Gradient descent computation

 $\mathbf{w} \leftarrow \text{any point in the parameter space}$ 

while not converged do

for each  $w_i$  in w do

$$w_i \leftarrow w_i - lpha rac{\partial}{\partial w_i} Loss\left(\mathbf{w}
ight)$$

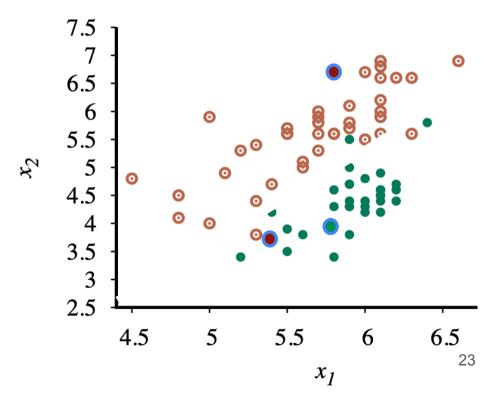
$$lpha\left(y-h_{\mathbf{w}}(\mathbf{x})
ight)\, imes\,h_{\mathbf{w}}(\mathbf{x})(1-h_{\mathbf{w}}(\mathbf{x}))\, imes\,x_i$$

#### Nearest-Neighbor Models for Binary Classification

Nearest-neighbor algorithm

• Given a query  $x_q$ , the algorithm chooses the class of the nearest

example to  $x_q$ 



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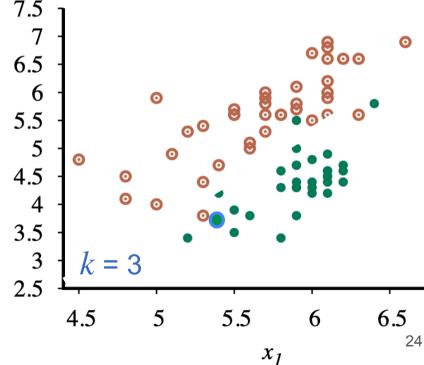
#### Nearest-Neighbor Models for Binary Classification

#### • k-nearest-neighbors algorithm

• Given a query  $x_q$ , the algorithm chooses the most common class

out of the k nearest examples to  $x_q$ 

• To avoid ties on binary classification, k is usually chosen to be an odd number



#### Distance Measurement

• Minkowski distance ( $L^p$  norm)

$$L^p(\mathbf{x}_j,\mathbf{x}_q) = \left(\sum_i \left|x_{j,i} - x_{q,i}
ight|^p
ight)^{1/p}$$

- Examples
  - p = 2: Euclidean distance
  - p = 1: Manhattan distance

#### Issues for Distance Measurement

- The total distance will be affected by a change in units in any dimension
- Different scales
- Scaling approach
  - Normalization

#### Normalization

Z-score normalization (Standardization)

$$x'_{j,i} = \frac{x_{j,i} - \mu_i}{\sigma_i}$$

- $\mu_i$  is the mean of the values in each dimension
- $\sigma_i$  is the standard deviation of the values in each dimension

#### **Normalization**

#### Min-max normalization

$$x'_{j,i} = \frac{x_{j,i} - min_i}{max_i - min_i}$$

- $max_i$  is the maximum of the values in each dimension
- $min_i$  is the minimum of the values in each dimension
- The new value  $x'_{j,i}$  is in [0,1]

# Example: Weather Data

Input Output

Outlook	Temperature	Humidity	Windy	Play
Sunny	Hot	High	False	No
Sunny	Hot	High	True	No
Overcast	Hot	High	False	Yes
Rainy	Mild	High	False	Yes
Rainy	Cool	Normal	False	Yes
Rainy	Cool	Normal	True	No
Overcast	Cool	Normal	True	Yes
Sunny	Mild	High	False	No
Sunny	Cool	Normal	False	Yes
Rainy	Mild	Normal	False	Yes
Sunny	Mild	Normal	True	Yes
Overcast	Mild	High	True	Yes
Overcast	Hot	Normal	False	Yes
Rainy	Mild	High	True	No

### **Example: Weather Data**

• The new data E:

Outlook	Temperature	Humidity	Windy	Play
Sunny	Cool	High	True	?

Q: Play is Yes or No?

### Recap: Probabilities

- Bayes' Rule
  - For any two propositions a and b,

$$P(b \,|\, a) = rac{P(a \,|\, b)P(b)}{P(a)}$$

 Conditional independence of two variables X and Y, given a third variable Z, is

$$P(X,Y \mid Z) = P(X \mid Z)P(Y \mid Z)$$

#### **Probabilistic Model**

#### • The new data E:

Outlook	Temperature	Humidity	Windy	Play
Sunny	Cool	High	True	?

#### Q: Play is Yes or No?

$$P(Play = yes | E) = ?$$

$$P(Play = no \mid E) = ?$$

#### Naïve Bayes Models

- Naïve Assumptions
  - Features/Attributes are equally important
  - Features/Attributes are conditionally independent

### Naïve Bayes Models

- Naïve Assumptions
  - Features/Attributes are equally important
  - Features/Attributes are conditionally independent

$$\Rightarrow P(E | Play = yes) = P(E_1 | Play = yes)P(E_2 | Play = yes) \cdots P(E_n | Play = yes)$$

$$= \prod_i (E_i | Play = yes)$$

$$P(Play = yes | E) = \frac{P(E | Play = yes)P(Play = yes)}{P(E)}$$

 $= \frac{\prod_{i} P(E_{i} | Play = yes) P(Play = yes)}{P(E)}$ 

#### Example: Naïve Bayes Models

#### The new data E:

Outlook	Temperature	Humidity	Windy	Play
Sunny	Cool	High	True	?

$$P(O = sunny | Play = yes)P(T = cool | Play = yes)P(H = high | Play = yes)P(W = true | Play = yes)$$

$$P(Play = yes | E) = \frac{\prod_{i} P(E_{i} | Play = yes) P(Play = yes)}{P(E)}$$

Outlook		Temperature		Humidity		Windy			Play				
	Yes	No		Yes	No		Yes	No		Yes	No	Yes	No
Sunny	2	3	Hot	2	2	High	3	4	False	6	2	9	5
Overcast	4	0	Mild	4	2	Normal	6	1	True	3	3		
Rainy	3	2	Cool	3	1								

Outlook	Temperature	Humidity	Windy	Play
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Outlook		Temperature		Humidity		Windy			Play				
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Outlook		Tem	perature	•	Hu	midity		Windy		Play			
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Outlook	Temperature	Humidity	Windy	Play
Sunny	Cool	High	True	?

P(O = sunny | Play = yes)P(T = cool | Play = yes)P(H = high | Play = yes)P(W = true | Play = yes)P(W

$$P(Play = yes | E) = \frac{\prod_{i} P(E_{i} | Play = yes)}{P(E)} P(Play = yes)$$
$$= \frac{\frac{2}{9} \times \frac{3}{9} \times \frac{3}{9} \times \frac{3}{9} \times \frac{9}{14}}{P(E)} = \frac{0.0053}{P(E)}$$

Outlook		Tem	perature		Hu	midity		Windy		Play			
	Yes	No		Yes	No		Yes	No		Yes	No	Yes	No
Sunny	2/9	3/5	Hot	2/9	2/5	High	3/9	4/5	False	6/9	2/5	9/14	5/14
Overcast	4/9	0/5	Mild	4/9	2/5	Normal	6/9	1/5	True	3/9	3/5		
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Outlook	Temperature	Humidity	Windy	Play
Sunny	Cool	High	True	?

P(O = sunny | Play = no)P(T = cool | Play = no)P(H = high | Play = no)P(W = true | Play = no)P(M = true | Play =

$$P(Play = no | E) = \frac{\prod_{i} P(E_{i} | Play = no) P(Play = no)}{P(E)}$$
$$= \frac{\frac{3}{5} \times \frac{1}{5} \times \frac{4}{5} \times \frac{3}{5} \times \frac{5}{14}}{P(E)} = \frac{0.0206}{P(E)}$$

## Example: Naïve Bayes Models

#### • The new data E:

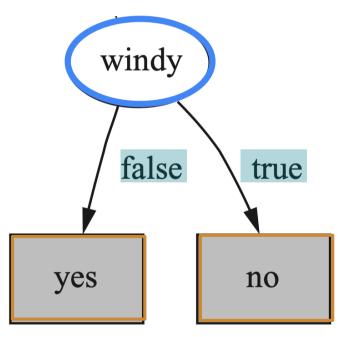
Outlook	Temperature	Humidity	Windy	Play
Sunny	Cool	High	True	?

$$P(Play = yes | E) = \frac{0.0053}{0.0053 + 0.0206} = 20.5\%,$$

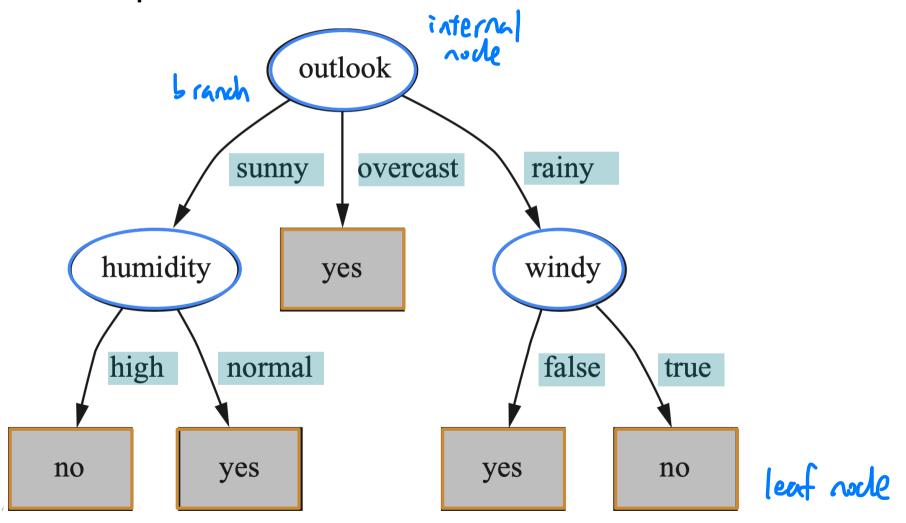
$$P(Play = no | E) = \frac{0.0206}{0.0053 + 0.0206} = 79.5\%.$$

#### **Decision Trees**

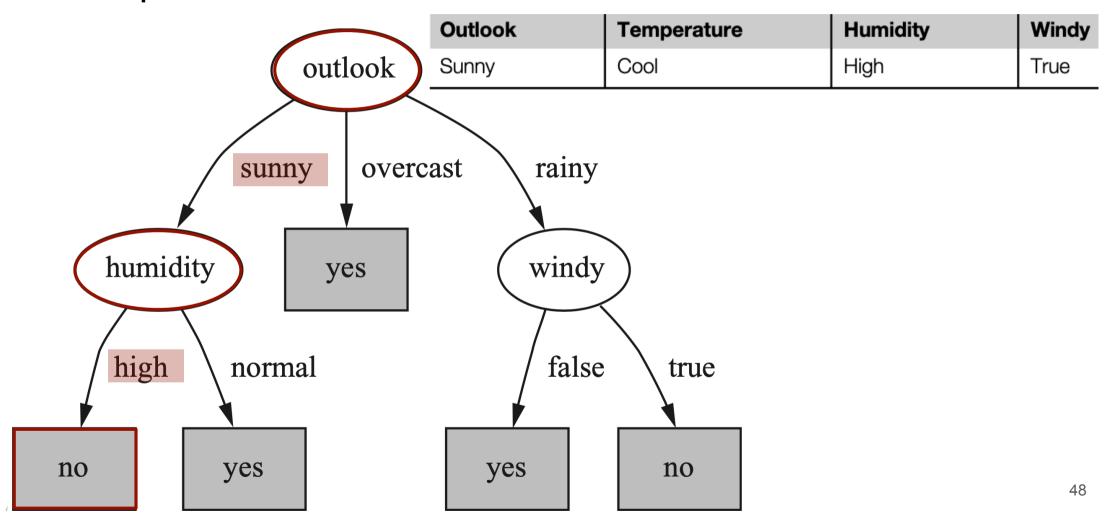
- A decision tree is a representation of a function that maps a vector of attribute values to a single output value, a "decision"
  - Each **internal node** in the tree corresponds to a test of the value of one of the input attributes
  - The branches from the node are labeled with the possible values of the attribute
  - The leaf nodes specify what value is to be returned by the function



### **Example: Decision Trees**



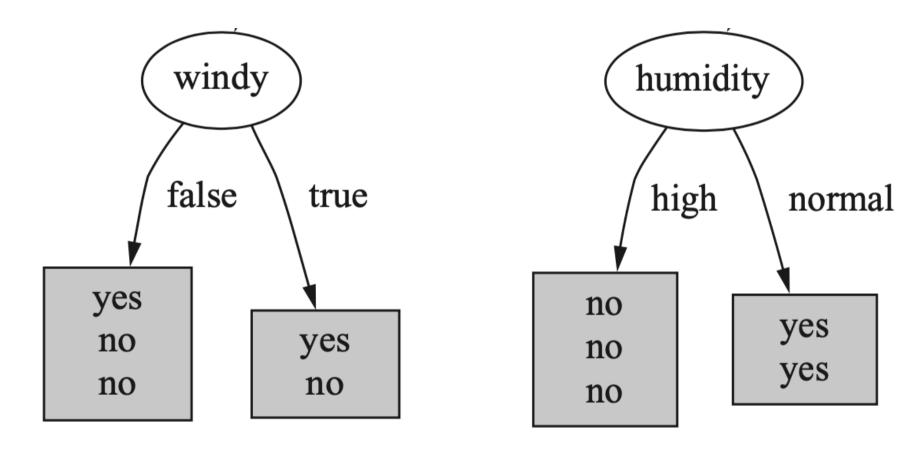
## **Example: Decision Trees**



## Learning Decision Trees from Examples

- Idea
  - Get to the correct classification with a small number of tests
  - Find a tree that is consistent with the examples and the tree is as small as possible
- A greedy divide-and-conquer strategy
  - Always test the most important attribute first
    - Makes the most difference to the classification of an example
  - Recursively solve the smaller subproblems that are defined by the possible results of the test

## Example: Attribute Importance



## Learning Decision Trees from Examples

- Four cases to consider for these recursive subproblems
  - The remaining examples are all positive (or all negative):
     Done! We can answer Yes or No
  - Some positive and some negative examples: Choose the best attribute to split them
  - No examples left:
    - (i.e., no example has been observed for this combination of attribute values), Return the most common output value from the set of examples that were used in constructing the node's parent
  - No attributes left, but both positive and negative examples: (This can happen because there is an error or noise in the data.) Return the *most common output value of the remaining examples*

## Decision Tree Learning Algorithm

**function** LEARN-DECISION-TREE(examples, attributes, parent\_examples) **returns** a tree

**if** examples is empty **then return** PLURALITY-VALUE(parent\_examples) else if all examples have the same classification then return the classification **else if** attributes is empty **then return** PLURALITY-VALUE(examples) else

```
A \leftarrow \operatorname{argmax}_{a \in attributes} \operatorname{IMPORTANCE}(a, examples)
tree \leftarrow a new decision tree with root test A
for each value v of A do
    exs \leftarrow \{e : e \in examples \text{ and } e.A = v\} \text{ # examples for the subset}
    subtree \leftarrow LEARN-DECISION-TREE(exs, attributes - A, examples)
    add a branch to tree with label (A = v) and subtree
return tree
```

Plurality-Value Select the most common output value among a set of examples, breaking ties randomly Spring 2024 / Wei

- Entropy (Information Theory)
  - The average amount of information contained in each message received (that is measured in bits)
  - A measure of the uncertainty of a random variable
    - e.g., a coin that always comes up heads has no uncertainty and its entropy is defined as zero
- The entropy of a random variable V with values  $v_k$  having probability  $P(v_k)$  is defined as

$$ext{Entropy:} \quad H(V) = \sum_k P(v_k) \log_2 rac{1}{P(v_k)} = -\sum_k P(v_k) \log_2 P(v_k)$$

### Fair Coin Flip

#### Four-sided Die





1 2 3 4

$$H(V) = \sum_k P(v_k) \log_2 rac{1}{P(v_k)} = -\sum_k P(v_k) \log_2 P(v_k)$$
Examples: Entropy

The entropy of a fair coin flip is 1 bit:

$$H(Fair) = -(0.5\log_2 0.5 + 0.5\log_2 0.5) = 1$$

• The entropy of a four-sided die is 2bit:

$$H(Die4) = -(0.25\log_2 0.25 + 0.25\log_2 0.25 + 0.25\log_2 0.25 + 0.25\log_2 0.25) = 2$$

The entropy of a Boolean random variable that is true with probability q:

$$B(q) = -(q \log_2 q + (1-q) \log_2 (1-q))$$

If a training set contains p positive examples and n negative examples,
 then the entropy of the output variable on the whole set is

$$H(Output) = Bigg(rac{p}{p+n}igg)$$

# **Examples: Entropy**

$$egin{aligned} H(Output) &= Bigg(rac{p}{p+n}igg) \ B(q) &= -(q\log_2q + (1-q)\log_2(1-q)) \end{aligned}$$

Outlook		Tem	nperature		Hu	midity		١	Windy		Play		
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• H(Play) = 
$$B(\frac{9}{9+5}) = -(\frac{9}{14}log_2\frac{9}{14} + \frac{5}{14}log_2\frac{5}{14}) = 0.940$$
 bits

- An attribute A with d distinct values divides the training set E into subsets  $E_1, \dots, E_d$
- ullet Each subset  $E_k$  has  $p_k$  positive examples and  $n_k$  negative examples
- A randomly chosen example from the training set has the kth value for the attribute (i.e., is in  $E_k$  with probability  $\frac{p_k + n_k}{p + n}$ ), so **the expected**

#### entropy remaining after testing attribute A is

$$Remainder(A) = \sum_{k=1}^d rac{p_k + n_k}{p+n} Bigg(rac{p_k}{p_k + n_k}igg)$$

# **Examples: Entropy**

$$Remainder(A) = \sum_{k=1}^d rac{p_k + n_k}{p+n} Bigg(rac{p_k}{p_k + n_k}igg)$$

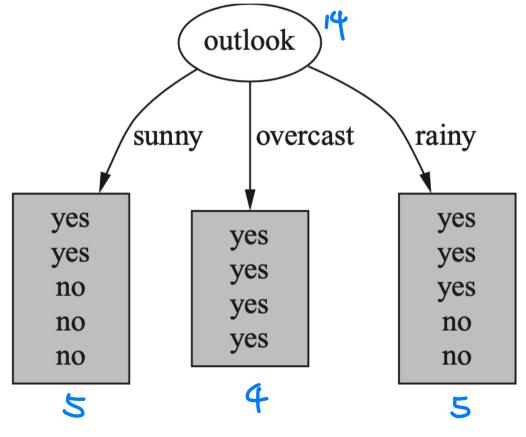
$$B(q) = -(q \log_2 q + (1-q) \log_2 (1-q))$$

Remainder(outlook)

$$= \frac{5}{14}\mathbf{B}(\frac{2}{5}) + \frac{4}{14}\mathbf{B}(\frac{4}{4}) + \frac{5}{14}\mathbf{B}(\frac{3}{5})$$

$$= (5/14) \times 0.971 + (4/14) \times 0 + (5/14) \times 0.971$$

= 0.693 bits



- Importance function
  - The information gain from the attribute test on A is the expected reduction in entropy:

$$Gain(A) = Bigg(rac{p}{p+n}igg) - Remainder(A).$$

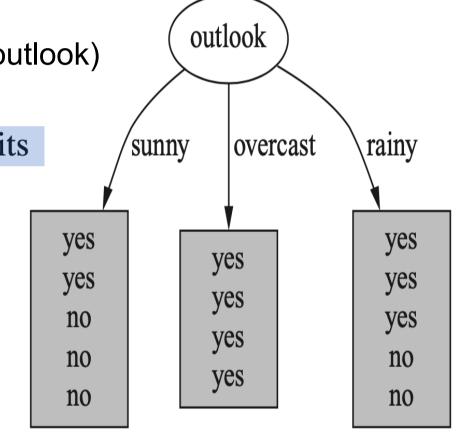
$$Gain(A) = Bigg(rac{p}{p+n}igg) - Remainder(A).$$

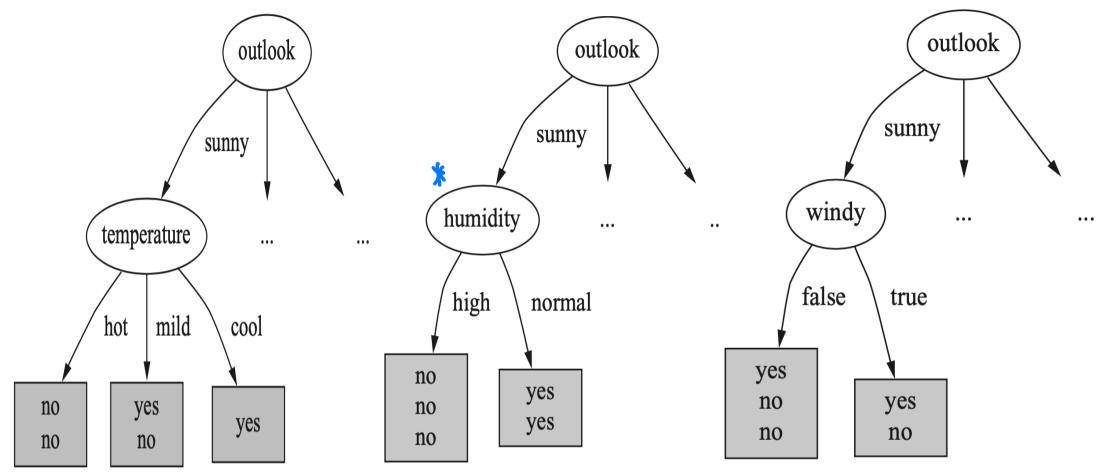
## **Example: Information Gain**

Gain(outlook) = B( $\frac{9}{9+5}$ ) - Remainder(outlook)

= 0.940 - 0.693 = 0.247 bits

- Gain(temperature) = 0.029 bits
- Gain(humidity) = 0.152 bits
- Gain(windy) = 0.048 bits





gain(temperature) = 0.571 bits gain(humidity) = 0.971 bits gain(windy) = 0.020 bits

### Performance Metrics for Classification Models

#### Confusion matrix

Example: two-class prediction

		Predict	ed Class
		yes	no
Actual Class	yes	true positive (TP)	false negative(FN)
	no	false positive (FP)	true negative (TN)

$$Accuracy = \frac{TP + TN}{TP + TN + FP + FN} \qquad F1 - score = \frac{2}{\frac{1}{Precision} + \frac{1}{Recall}} = \frac{2 \times Precision \times Recall}{Precision + Recall}$$

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