

10-301/10-601 Introduction to Machine Learning

Machine Learning Department School of Computer Science Carnegie Mellon University

Machine Learning as Function Approximation

Matt Gormley & Geoff Gordon Lecture 2 Aug. 27, 2025

Reminders

- Homework 1: Background
 - Out: Mon, Aug 25
 - Due: Wed, Sep 3 at 11:59pm
 - Two parts:
 - 1. written part to Gradescope
 - 2. programming part to Gradescope
 - unique policies for this assignment:
 - 1. unlimited submissions for programming (i.e. keep submitting until you get 100%)
 - 2. we will grant (essentially) any and all extension requests

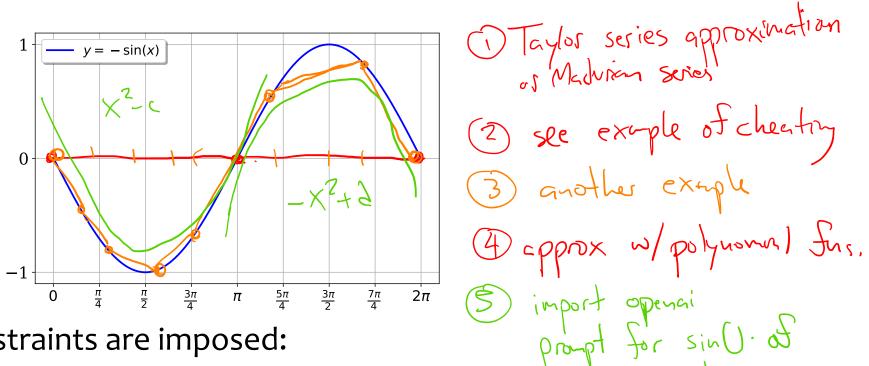
Big Ideas

- 1. How to formalize a learning problem
- 2. How to learn an expert system (i.e. Decision Tree)
- 3. Importance of inductive bias for generalization
- 4. Overfitting

FUNCTION APPROXIMATION

Function Approximation

Quiz: Implement a simple function which returns $-\sin(x)$.



A few constraints are imposed:

- You can't call any other trigonometric functions
- You can call an existing implementation of sin(x) a few times (e.g. 100) to test your solution
- You only need to evaluate it for x in [0, 2*pi]

SUPERVISED MACHINE LEARNING

Medical Diagnosis

- Setting:
 - Doctor must decide whether or not patient is sick
 - Looks at attributes of a patient to make a medical diagnosis
 - (Prescribes treatment if diagnosis is positive)
- Key problem area for Machine Learning
- Potential to reshape health care

Medical Diagnosis

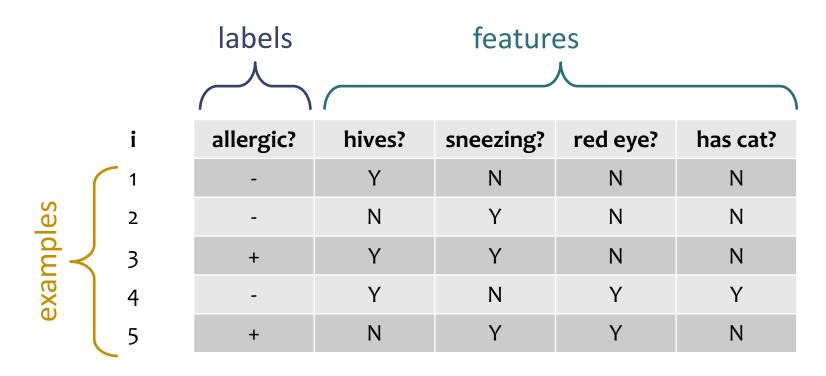
Interview Transcript

Date: Jan. 15, 2023

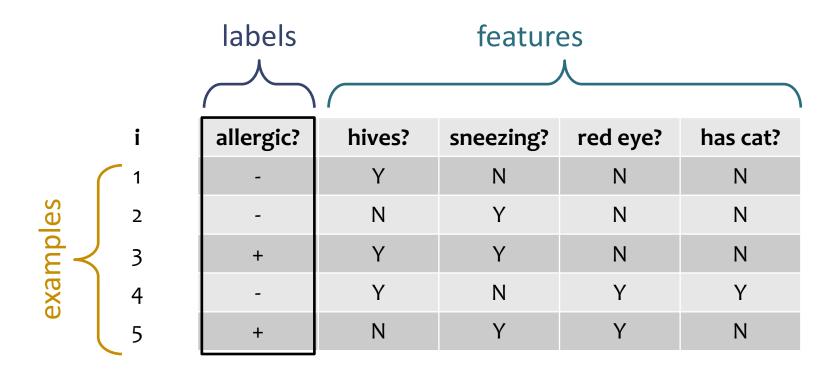
Parties: Matt Gormley and Doctor S.

Topic: Medical decision making

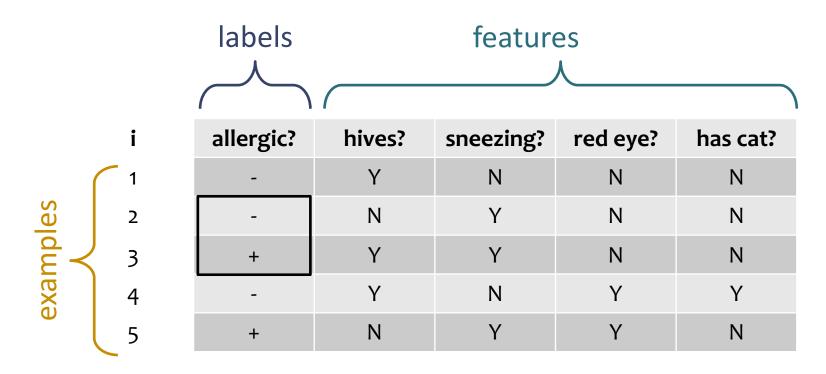
As a (supervised) binary classification task



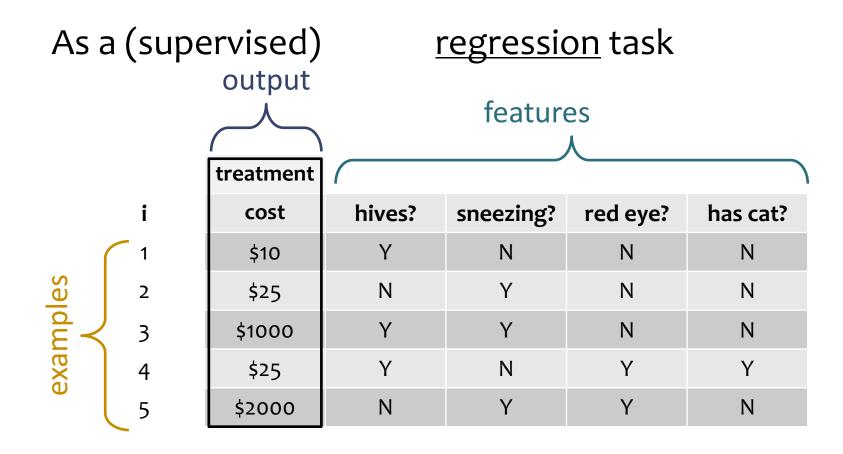
As a (<u>supervised</u>) binary classification task



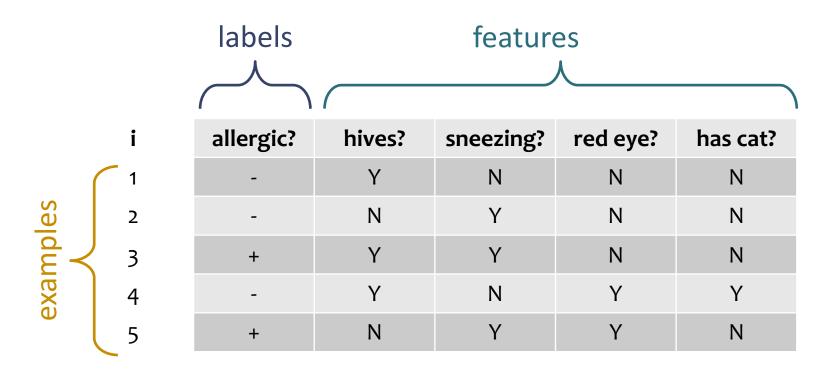
As a (supervised) binary classification task



As a (supervised) classification task labels features allergy sneezing? red eye? hives? has cat? Υ Ν Ν Ν none examples 2 Ν Ν Ν none Ν 3 Υ Ν dust Ν Υ 4 Υ Y none mold Ν Υ Υ Ν



As a (supervised) binary classification task



Doctor diagnoses the patient as sick or not $y \in \{+, -\}$ based on attributes of the patient $x_1, x_2, ..., x_M$

	у	X_1	X ₂	X_3	X ₄
i	allergic?	hives?	sneezing?	red eye?	has cat?
1	-	Υ	N	N	N

Doctor diagnoses the patient as sick or not $y \in \{+, -\}$ based on attributes of the patient $x_1, x_2, ..., x_M$

	у	X_1	X_2	X_3	X ₄
i	allergic?	hives?	sneezing?	red eye?	has cat?
1	-	Y	N	N	N
2	-	N	Υ	N	N
3	+	Υ	Υ	N	N
4	-	Υ	N	Υ	Υ
5	+	N	Y	Y	N

Doctor diagnoses the patient as sick or not $y \in \{+, -\}$ based on attributes of the patient $x_1, x_2, ..., x_M$

	у	X_1	X_2	X_3	X_4
i	allergic?	hives?	sneezing?	red eye?	has cat?
1	y ⁽¹⁾ -	X ₁ ⁽¹⁾ Y	$x_2^{(1)} N$	x ₃ ⁽¹⁾ N	x ₄ ⁽¹⁾ N
2	y ⁽²⁾ -	$X_1^{(2)} N$	$X_2^{(2)} Y$	$X_3^{(2)} N$	$X_4^{(2)} N$
3	y ⁽³⁾ +	X ₁ ⁽³⁾ Y	X ₂ ⁽³⁾ Y	x ₃ ⁽³⁾ N	x ₄ ⁽³⁾ N
4	y ⁽⁴⁾ -	X ₁ ⁽⁴⁾ Y	$X_2^{(4)} N$	x ₃ ⁽⁴⁾ Y	x ₄ ⁽⁴⁾ Y
5	y ⁽⁵⁾ +	X ₁ ⁽⁵⁾ N	X ₂ ⁽⁵⁾ Y	x ₃ ⁽⁵⁾ Y	x ₄ ⁽⁵⁾ N

Doctor diagnoses the patient as sick or not $y \in \{+, -\}$ based on attributes of the patient $x_1, x_2, ..., x_M$

	У	X ₁	X_2	X_3	X ₄	
i	allergic?	hives?	sneezing?	red eye?	has cat?	
1	y ⁽¹⁾ -	X ₁ ⁽¹⁾ Y	$X_2^{(1)} N$	x ₃ ⁽¹⁾ N	x ₄ ⁽¹⁾ N	X ⁽¹⁾
2	y ⁽²⁾ -	$X_1^{(2)} N$	$X_2^{(2)} Y$	$x_3^{(2)} N$	x ₄ ⁽²⁾ N	X ⁽²⁾
3	y ⁽³⁾ +	Χ ₁ ⁽³⁾ Υ	X ₂ ⁽³⁾ Y	x ₃ ⁽³⁾ N	x ₄ ⁽³⁾ N	X (3)
4	y ⁽⁴⁾ -	X ₁ ⁽⁴⁾ Y	x ₂ ⁽⁴⁾ N	x ₃ ⁽⁴⁾ Y	x ₄ ⁽⁴⁾ Y	X ⁽⁴⁾
5	y ⁽⁵⁾ +	X ₁ ⁽⁵⁾ N	X ₂ ⁽⁵⁾ Y	x ₃ ⁽⁵⁾ Y	x ₄ ⁽⁵⁾ N	X (5)

N = 5 training examples

M = 4 attributes

ML as Function Approximation

Problem Setting

- Set of possible imputs & (all possible treature vectors)
- Set of possible outputs y (all possible labels)
- Unknown farget function C* : 2 -> y
- Set of condidate hypotheses

Learner is given

- Training examples $D = \{(\vec{x}^{(1)}, y^{(1)}), (\vec{x}^{(2)}, y^{(2)}), ..., (\vec{x}^{(N)}, y^{(N)})\}$ of unknown target function $y^{(i)} = c*(x^{(i)}) \ \forall i \in \{1,...,N\}$
- N = # training examples M = # of features = $|\vec{X}^{(i)}|$

Learner produces

- Hypothasis he H that "best approximates" c* according to D

To Evaluate

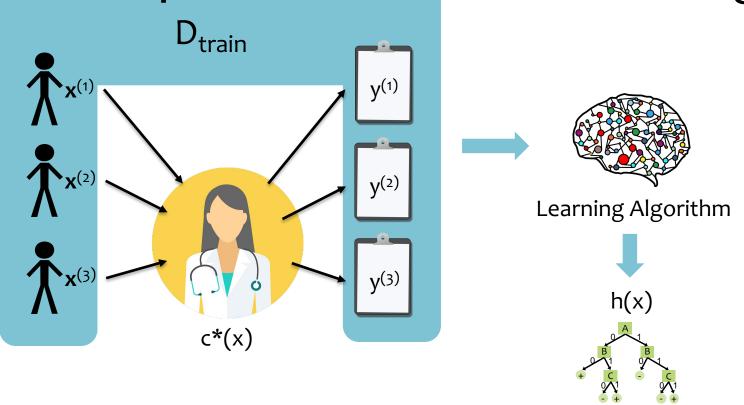
- Loss function l: yxy, -> R measures how "bad" predictions $\hat{y} = h(\vec{x})$ are compared to $c^*(\hat{x})$
- Another dataset $D_{test} = \{(\dot{x}^{(i)}, y^{(i)}), \dots, (\dot{x}^{(N')}, y^{(N')})\}$
- Evaluate the average loss on Dtest

Aside: Fur thum Types

$$f(x_1, x_2, x_3) = (x_1 x_2)^2 + x_3$$

$$f: \mathbb{R}^3 \longrightarrow \mathbb{R}$$

Supervised Machine Learning



Doctor diagnoses the patient as sick or not $y \in \{+, -\}$ based on attributes of the patient $x_1, x_2, ..., x_M$

Y = N	(i)	y	X ₁	, X ₂	x ₃	X_4	
(i	allergic? _{c*}	hives?	sneezing?	red eye?	has cat?	
	1	y ⁽¹⁾ - **	X ₁ ⁽¹⁾ Y	$X_2^{(1)}$ N	x ₃ ⁽¹⁾ N	x ₄ ⁽¹⁾ N	X ⁽¹⁾
+	2	y ⁽²⁾ - **	X ₁ ⁽²⁾ N	X ₂ (2) Y	x ₃ ⁽²⁾ N	x ₄ ⁽²⁾ N	X ⁽²⁾
+	3	y(3) #	Χ ₁ ⁽³⁾ Υ	X ₂ (3) Y	x ₃ ⁽³⁾ N	x ₄ ⁽³⁾ N	X ⁽³⁾
_	4	y(4) - **	X ₁ ⁽⁴⁾ Y	X ₂ (4) N	x ₃ ⁽⁴⁾ Y	x ₄ ⁽⁴⁾ Y	X ⁽⁴⁾
+	5	y(5)	X ₁ ⁽⁵⁾ N	X2(5) Y	х ₃ ⁽⁵⁾ Ү	x ₄ ⁽⁵⁾ N	X ⁽⁵⁾

N = 5 training examples M = 4 attributes

Example hypothesis function: $h(\mathbf{x}) = \begin{cases} + \text{ if sneezing} = Y \\ - \text{ otherwise} \end{cases}$

Supervised Machine Learning

Problem Setting

- Set of possible inputs, $\mathbf{x} \in \mathcal{X}$ (all possible patients)
- Set of possible outputs, $y \in \mathcal{Y}$ (all possible diagnoses)
- Exists an unknown target function, $c^* : \mathcal{X} \rightarrow \mathcal{Y}$ (the doctor's brain)
- Set, \mathcal{H} , of candidate hypothesis functions, $h: \mathcal{X} \rightarrow \mathcal{Y}$ (all possible decision trees)
- Learner is given N training examples $D = \{(\mathbf{x}^{(1)}, \mathbf{y}^{(1)}), (\mathbf{x}^{(2)}, \mathbf{y}^{(2)}), ..., (\mathbf{x}^{(N)}, \mathbf{y}^{(N)})\}$ where $\mathbf{y}^{(i)} = \mathbf{c}^*(\mathbf{x}^{(i)})$ (history of patients and their diagnoses)
- Learner produces a hypothesis function, $\hat{y} = h(x)$, that best approximates unknown target function $y = c^*(x)$ on the training data

Supervised Machine Learning

Problem Setting

- Set of possible inputs, $x \in \mathcal{X}$ (all possible patients)
- Set of possible outputs, $y \in \mathcal{Y}$ (all possible diagnoses)
- Exists an unknown tar function, $c^*: \mathcal{X} \rightarrow \mathcal{Y}$ (the doctor's brain)
- Set, \mathcal{H} , of candidate hypoth (all possible decision trees) consider:
- Learner is given N training
 D = {(x⁽¹⁾, y⁽¹⁾), (x⁽²⁾, y⁽²⁾), ...,
 where y⁽ⁱ⁾ = c*(x⁽ⁱ⁾)
 (history of patients and the
- Learner produces a hypoth approximates unknown tar

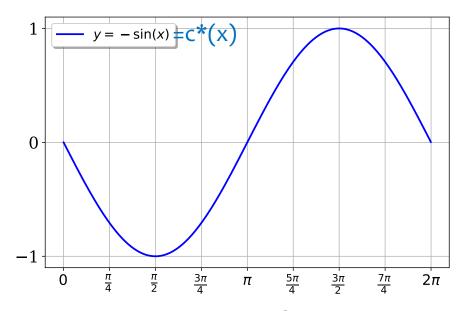
Two important settings we'll consider:

- Classification: the possible outputs are discrete
- 2. Regression: the possible outputs are real-valued

data

Function Approximation

Quiz: Implement a simple function which returns $-\sin(x)$.



A few constraints are imposed:

- 1. You can't call any other trigonometric functions
- You can call an existing implementation of sin(x) a few times (e.g. 100) to test your solution
- You only need to evaluate it for x in [0, 2*pi]

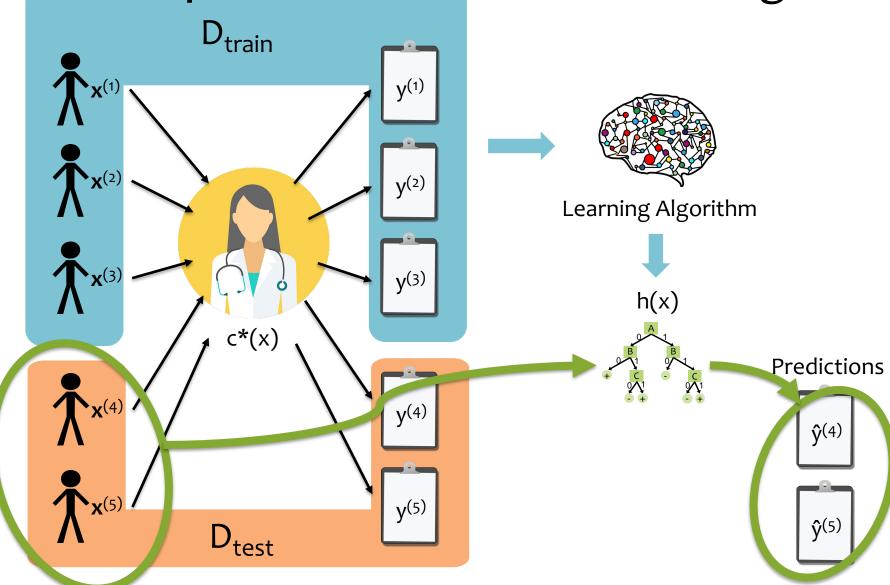
Supervised Machine Learning

Problem Setting

- Set of possible inputs, $x \in \mathcal{X}$ (all values in [0, 2*pi])
- Set of possible outputs, $y \in \mathcal{Y}$ (all values in [-1,1])
- Exists an unknown target function, $c^*: \mathcal{X} \rightarrow \mathcal{Y}$ $(c^*(x) = \sin(x))$
- Set, \mathcal{H} , of candidate hypothesis functions, $h: \mathcal{X} \rightarrow \mathcal{Y}$ (all possible piecewise linear functions)
- Learner is given N training examples $D = \{(\mathbf{x}^{(1)}, \mathbf{y}^{(1)}), (\mathbf{x}^{(2)}, \mathbf{y}^{(2)}), ..., (\mathbf{x}^{(N)}, \mathbf{y}^{(N)})\}$ where $\mathbf{y}^{(i)} = \mathbf{c}^*(\mathbf{x}^{(i)})$ (true values of sin(x) for a few random x's)
- Learner produces a hypothesis function, $\hat{y} = h(x)$, that best approximates unknown target function $y = c^*(x)$ on the training data

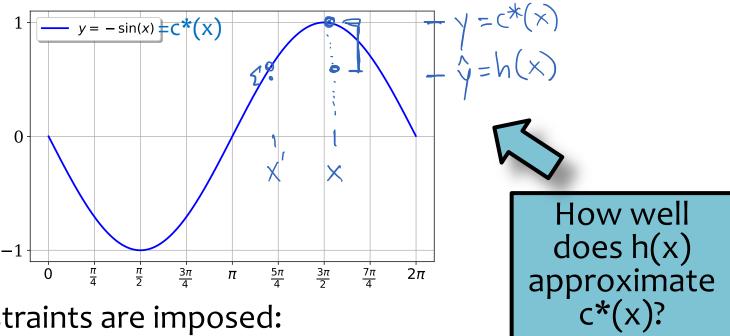
EVALUATION OF MACHINE LEARNING ALGORITHM

Supervised Machine Learning



Function Approximation

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Evaluation of ML Algorithms

- **Definition:** loss function, $\ell: \mathcal{Y} \times \mathcal{Y} \to \mathbb{R}$

 - o Defines how "bad" predictions, $\hat{y} = h(x)$, are compared to the true labels, $y = c^*(x)$ o Common choices:

 1. Squared loss (for regression): $\ell(y,\hat{y}) = (y-\hat{y})^2$ 2. Binary or 0-1 loss (for classification): $\ell(y,\hat{y}) = \mathbb{1}(y \neq \hat{y}) = 0$

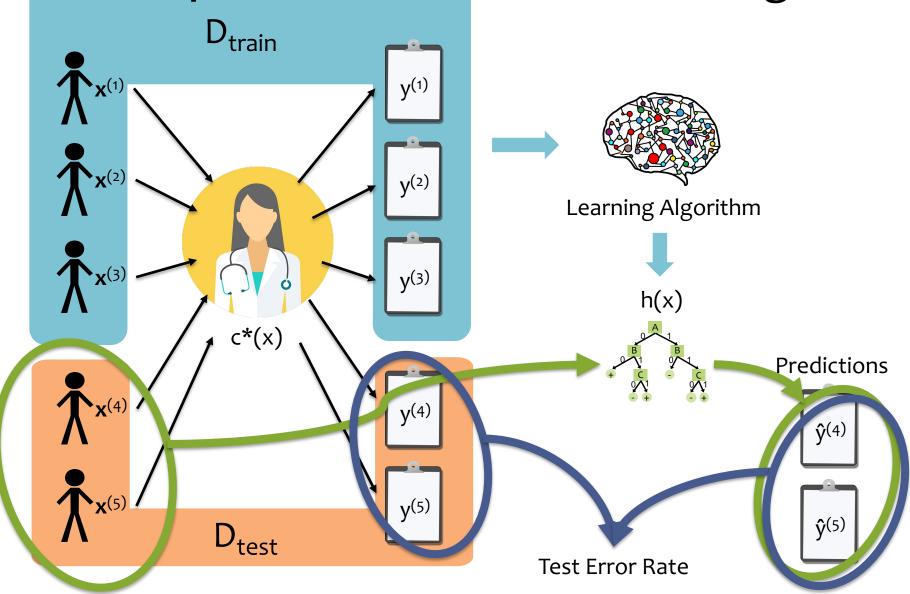
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 - 2. Binary or 0-1 loss (for classification): $\ell(y, \hat{y}) = \mathbb{1}(y \neq \hat{y})$
- **Definition:** the error rate of a hypothesis h on a dataset \mathcal{D} is the average 0-1 loss:

$$\operatorname{error}(h,\mathcal{D}) = \frac{1}{N} \sum_{n=1}^{N} \mathbb{1}(y^{(n)} \neq \hat{y}^{(n)})$$

- **Definition:** the mean squared error is the average squared loss (more on this later)
- Q: How do we evaluate a machine learning algorithm? A: Check its average loss on a separate test dataset, $\mathcal{D}_{\text{test}}$.

Supervised Machine Learning



Error Rate

Consider a hypothesis h its...

... error rate over all training data:

... error rate over all test data:

... true error over all data:

error(h, D_{train}) error(h, D_{test}) So we'll use error(h, D_{test})
as a surrogate for error_{true}(h) in practice



error_{true}(h)

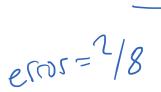
This is the quantity we care most about! But, in practice, error_{true}(h) is **unknown**.

Majority Vote Classifier Example

Majority=+

Dataset: Features

Output Y, Attributes A and B



	Υ	Α	В
+	-	1	О
+	-	1	0
+	+	1	0
+	+	1	0
+	+	1	1
+	+	1	1
+	+	1	1
+	+	1	1

In-Class Exercise

What is the **training** error (i.e. error rate on the training data) of the majority vote classifier on this dataset?

Choose one of: $\{0/8, 1/8, 2/8, ..., 8/8\}$

Majority Vote Classifier Example

Dataset:

Output Y, Attributes A and B

Υ	Α	В	
-	1	0	7
-	1	0	V
+	1	0	
+	1	0	
+	1	1	
+	1	1	
+	1	1	
+	1	1	

In-Class Exercise

"problem setting" defined earlier?

Why or why not?

LEARNING ALGORITHMS FOR SUPERVISED CLASSIFICATION

Algorithms for Classification

Algorithm 1 majority vote: predict the most common label in the training dataset

	у	X_1	X_2	X_3	x_4
predictions	allergic?	hives?	sneezing?	red eye?	has cat?
-	-	Y	N	N	N
-	-	N	Υ	N	N
-	+	Υ	Υ	N	N
-	-	Υ	N	Υ	Υ
-	+	N	Y	Y	N

Algorithms for Classification

<u>Algorithm 2</u> memorizer: if a set of features exists in the training dataset, predict its corresponding label; otherwise, predict a random label

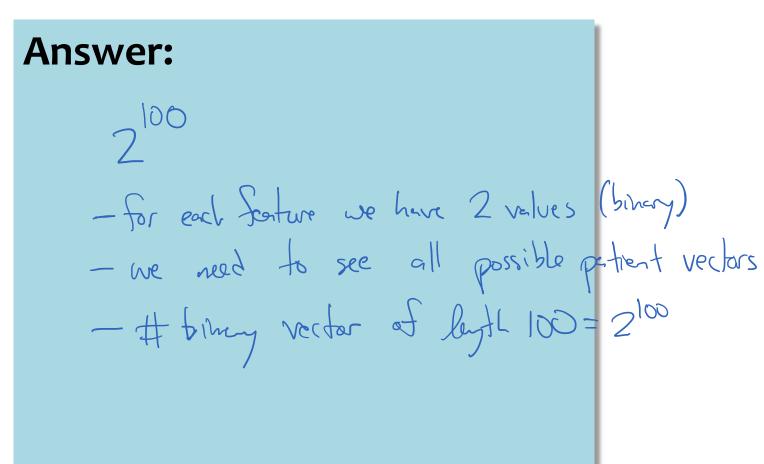
	у	X_1	X_2	X_3	X_4
predictions	allergic?	hives?	sneezing?	red eye?	has cat?
-	-	Y	N	N	N
-	-	N	Υ	N	N
+	+	Υ	Υ	N	N
-	-	Υ	N	Υ	Υ
+	+	N	Υ	Y	N

The memorizer always gets zero training error!

Assum ()= *() Algorithms for Classification

Question:

If we have 100 binary features, how many patients does the memorizer need to see to ensure zero test error?



Algorithm 1: Majority Vote

Pseudocode

def train (D):

store
$$v = majority_vote(D)$$

= most common label $y \in Y$ in our destret D

def $h(x)$:

return v

def predict (D test)

For $(\dot{x}^{(i)}, y^{(i)}) \in D_{test}$
 $y \in Y$

any classifier

 $y = h(\dot{x}^{(i)})$

Algorithm 2: Memorizer

Pseudocode

def train (D):

store detaset D

def h(x):

if
$$\exists x^{(i)} \in D$$
 s.t. $x^{(i)} = x$:

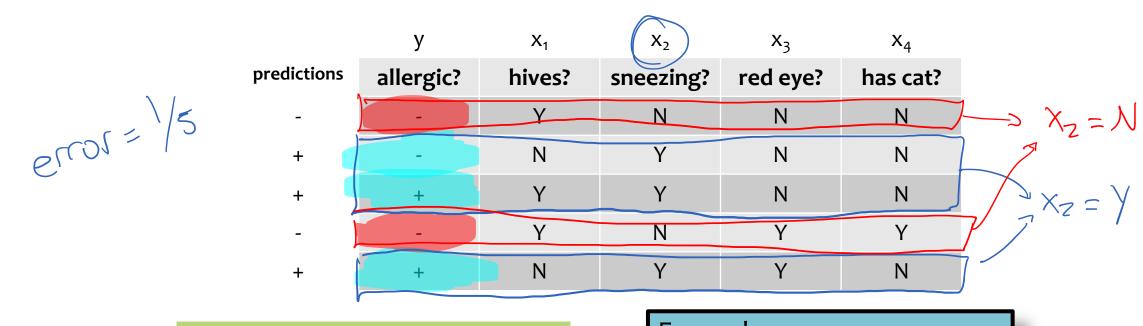
return $y^{(i)}$

else:

return $y \in \mathcal{Y}$ randomly

Algorithms for Classification

<u>Algorithm 3</u> decision stump: based on a single feature, x_d , predict the most common label in the training dataset among all data points that have the same value for x_d



Nonzero training error, but perhaps still better than the memorizer

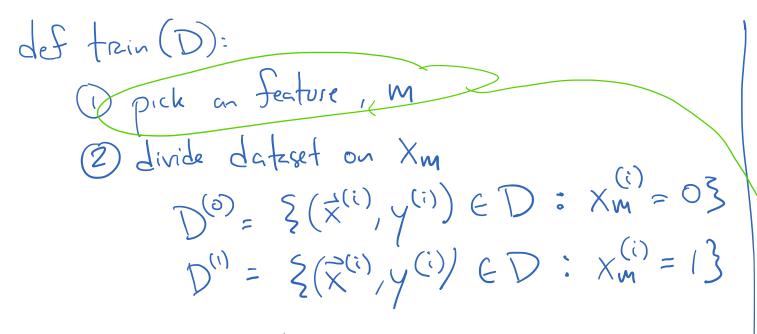
Example decision stump:

$$h(x) = \int + if \text{ sneezing} = Y$$

- otherwise

Algorithm 3: Decision Stump

Pseudocode



3) two votes
$$v^{(0)} = \text{majority-vote}(D^{(0)})$$

$$v^{(1)} = \text{majority-vote}(D^{(1)})$$

$$\frac{1}{1} = \frac{1}{1} \cdot \frac{1$$



Algorithms for Classification

Algorithm 3 decision stump: based on a single feature, x_d , predict the most common label in the training dataset among all data points that have the same value for x_d

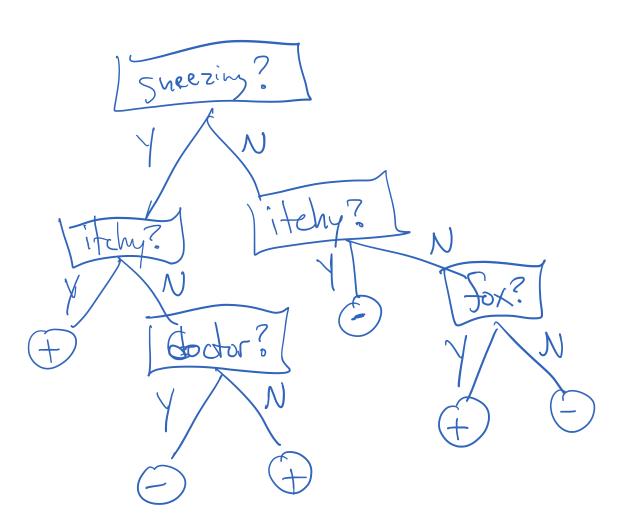
Questions:

1. How do we pick which feature to split on?

2. Why stop at one feature?

Algorithm 4: Decision Tree (preview)

Example



Tree to Predict C-Section Risk

Learned from medical records of 1000 women (Sims et al., 2000) Negative examples are C-sections [833+,167-] .83+ .17-Fetal_Presentation = 1: [822+,116-] .88+ .12-Previous_Csection = 0: [767+,81-] .90+ .10-Primiparous = 0: [399+,13-] .97+ .03-Primiparous = 1: [368+,68-] .84+ .16- $| \text{Fetal_Distress} = 0: [334+,47-] .88+ .12-$ | Birth_Weight < 3349: [201+,10.6-] .95+ . $| | Birth_Weight >= 3349: [133+,36.4-] .78+$ Fetal_Distress = 1: [34+,21-] .62+ .38-Previous_Csection = 1: [55+,35-] .61+ .39-Fetal_Presentation = 2: [3+,29-] .11+ .89-Fetal_Presentation = 3: [8+,22-] .27+ .73-