# Supervised Learning: The Setup

Machine Learning



#### Last lecture

We saw

- What is learning?

Learning as generalization

The badges game

## This lecture

- More badges
- Formalizing supervised learning
  - Instance space and features
    - What are inputs to the learning problem?
  - Label space
    - What is the output of the learned function
  - Hypothesis space
    - What is being learned?

#### The badges game

Name	Label
Claire Cardie	-
Jude Shavlik	+
Eric Baum	-
Haym Hirsh	_
Leslie Pack Kaelbling	+
Philip Chan	+

(Full data on the class website, you can stare at it longer if you want)

Name	Label
Claire Cardie	-
Jude Shavlik	+
Eric Baum	-
Haym Hirsh	_
Leslie Pack Kaelbling	+
Philip Chan	+

What is the label for Indiana Jones?

(Full data on the class website, you can stare at it longer if you want)

Name	Label
Claire Cardie	_
Jude Shavlik	+
Eric Baum	-
Haym Hirsh	_
Leslie Pack Kaelbling	+
Philip Chan	+

How were the labels generated?

Name	Label
Claire Cardie	-
Jude Shavlik	+
Eric Baum	-
Haym Hirsh	-
Leslie Pack Kaelbling	+
Philip Chan	+

How were the labels generated?

```
If third letter of last name is in first half of the alphabet:
    label = +
else
    label = -
```

(Full data on the class website, you can stare at it longer if you want)

# Questions to think about

How could you be certain that you got the right function?

• How did you arrive at it?

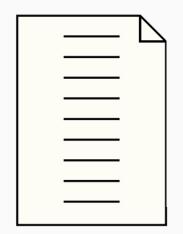
#### Learning issues:

- Is this prediction or just modeling data? Is there a difference?
- How did you know that you should look at the letters?
- What background knowledge about letters did you use? How did you know that it is relevant?
- What "learning algorithm" did you use?

#### What is supervised learning?

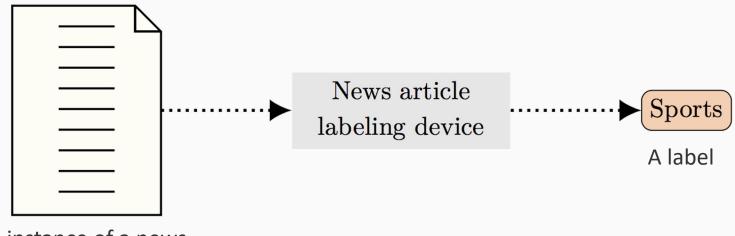
Running example: Automatically tag news articles

Running example: Automatically tag news articles



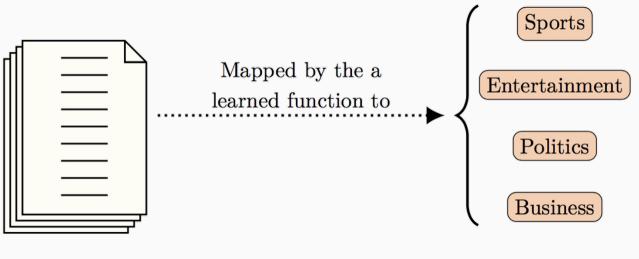
An instance of a news article that needs to be classified

Running example: Automatically tag news articles



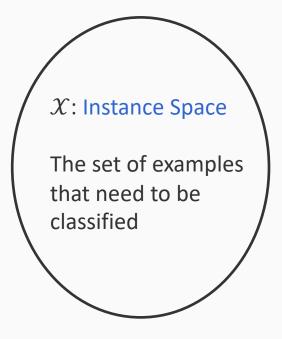
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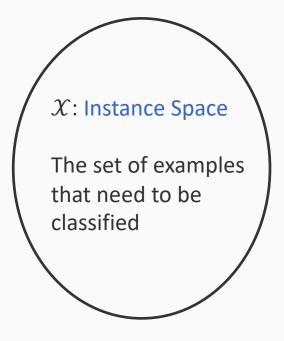


Instance Space: All possible news articles

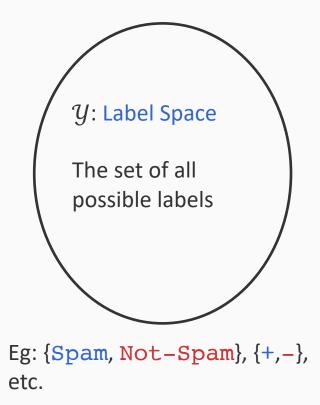
Label Space: All possible labels

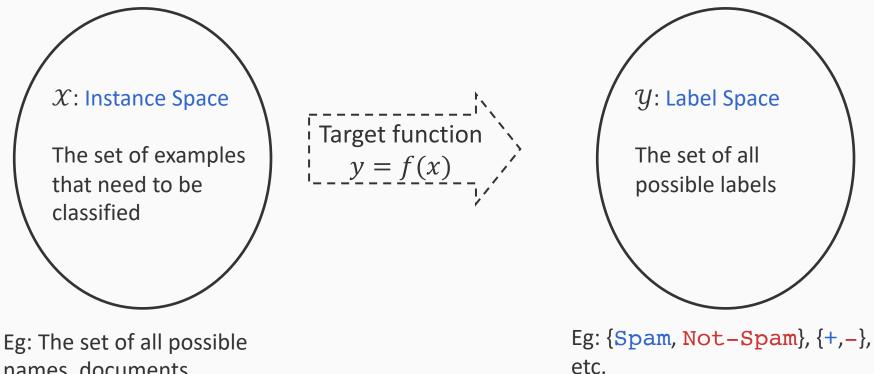


Eg: The set of all possible names, documents, sentences, images, emails, etc

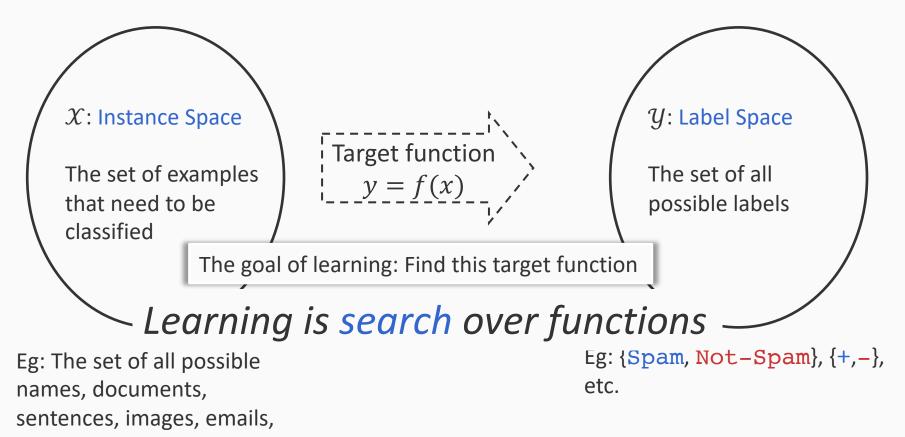


Eg: The set of all possible names, documents, sentences, images, emails, etc

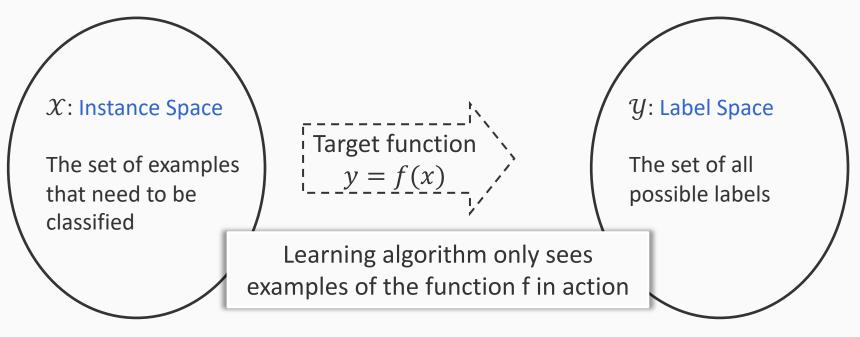


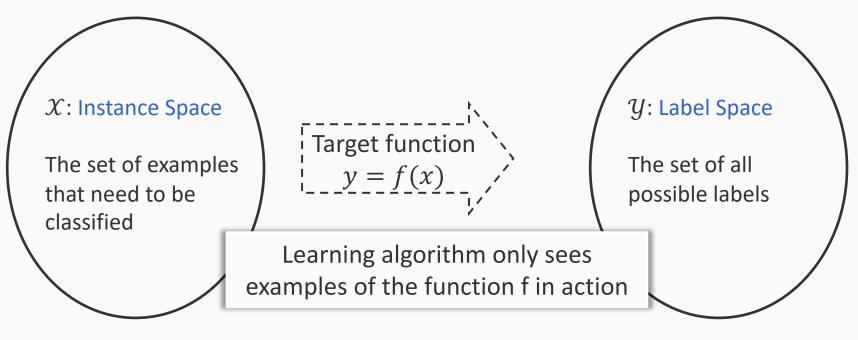


names, documents, sentences, images, emails, etc



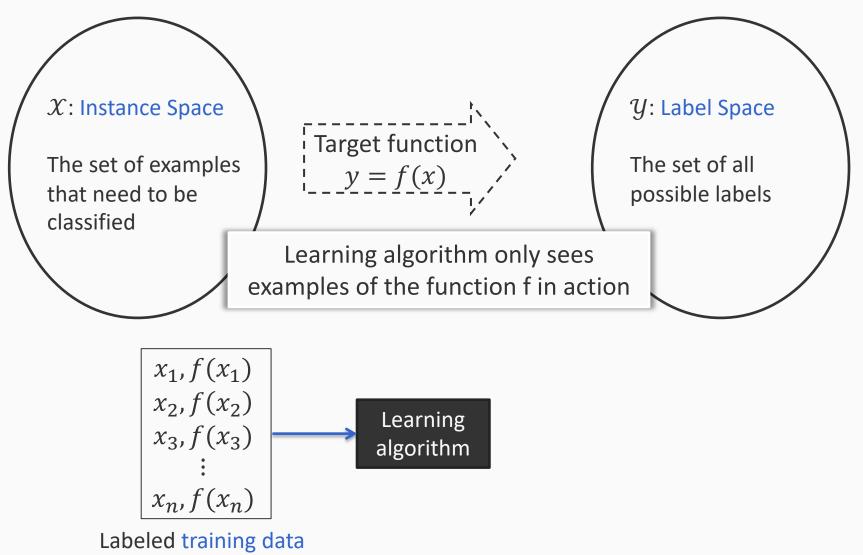
etc

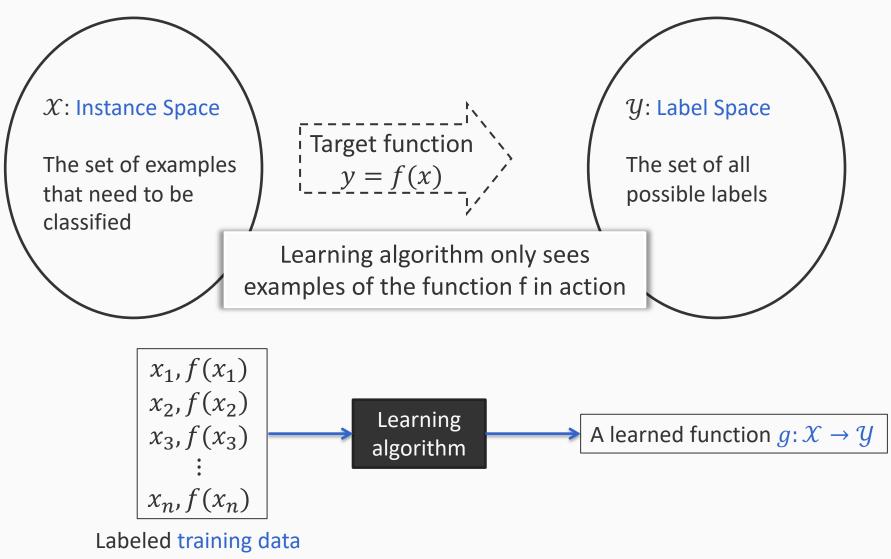


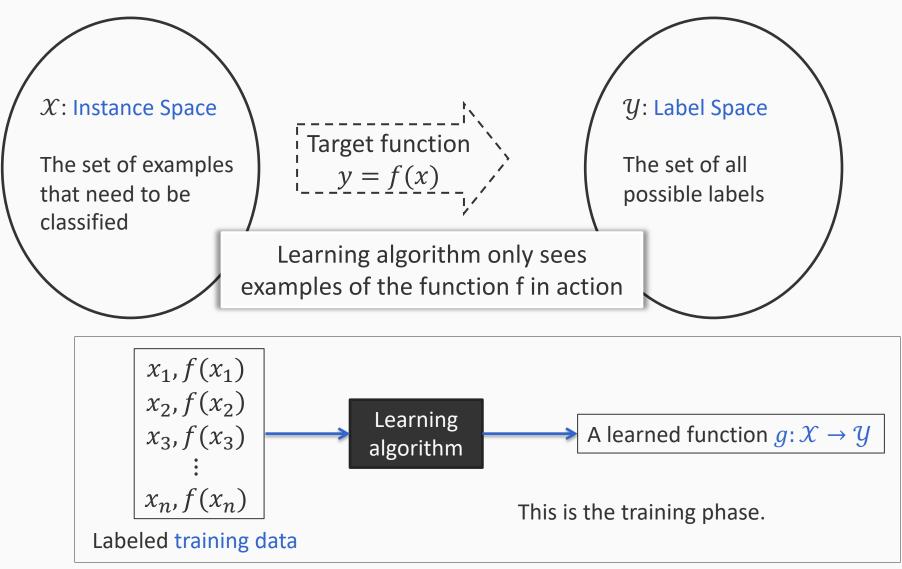


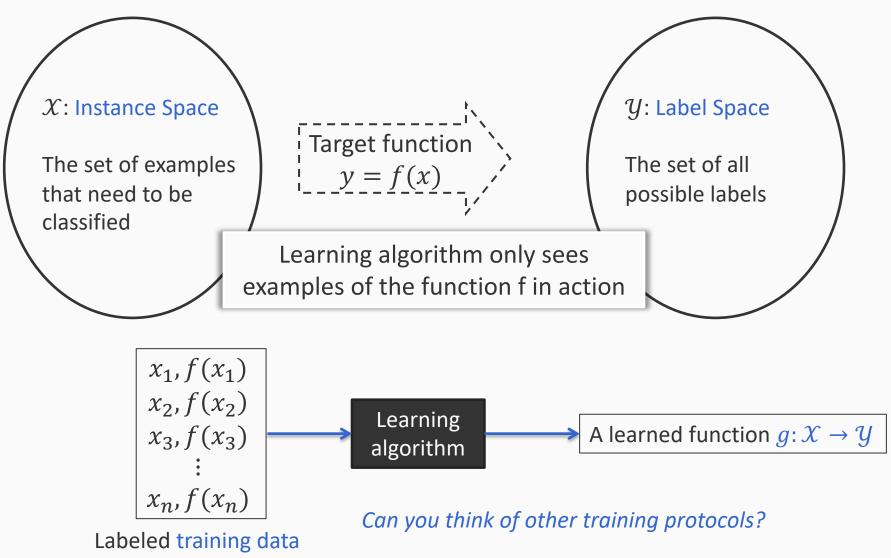
$$\begin{array}{c}
x_{1}, f(x_{1}) \\
x_{2}, f(x_{2}) \\
x_{3}, f(x_{3}) \\
\vdots \\
x_{n}, f(x_{n})
\end{array}$$

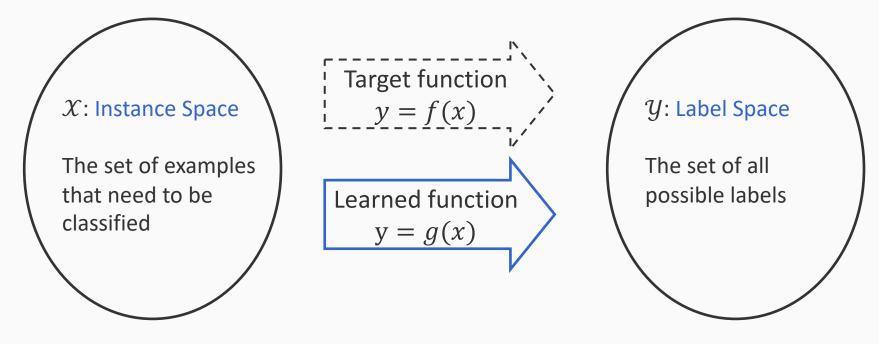
Labeled training data

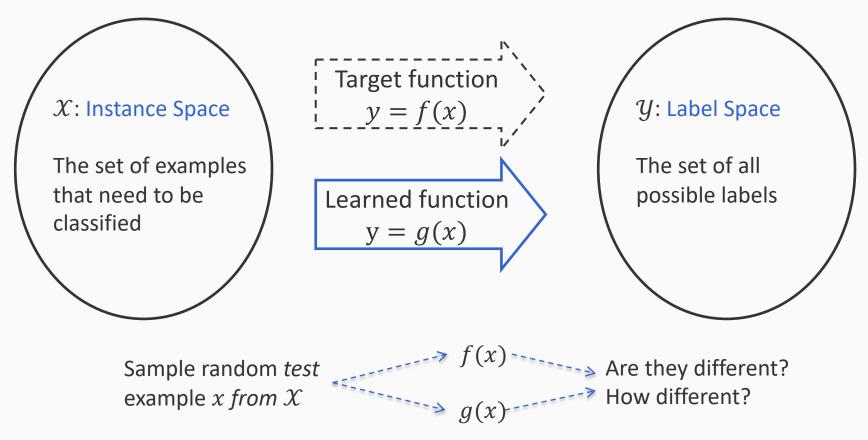


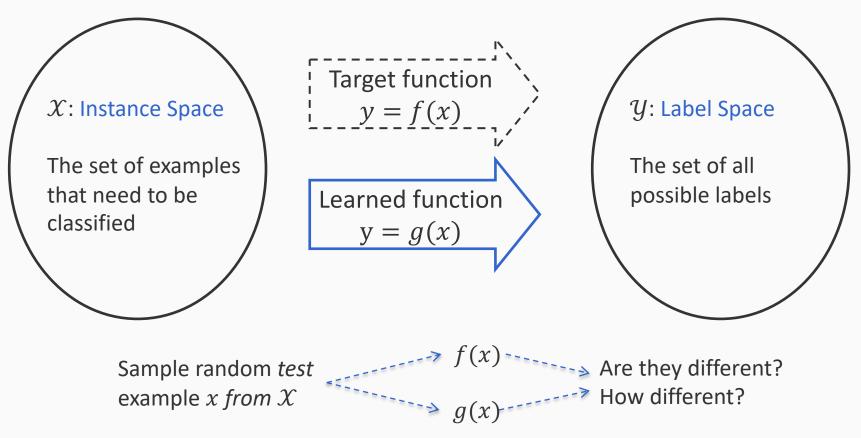






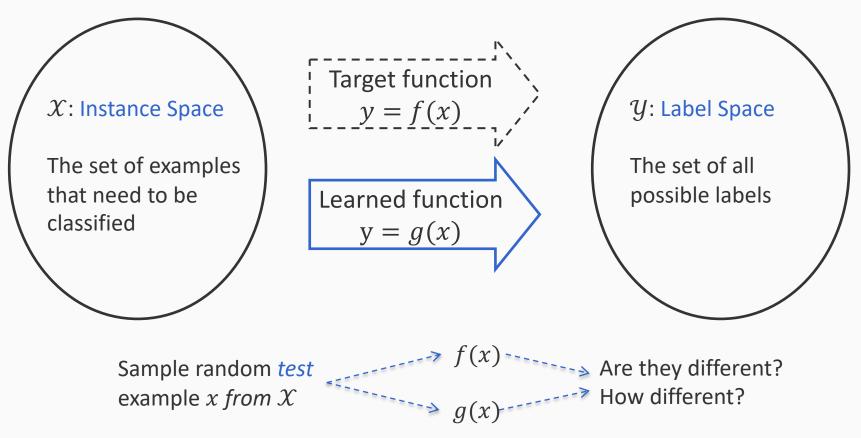






Apply the model to many test examples and compare to the target's prediction

Aggregate these results to get a quality measure

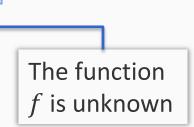


Apply the model to many test examples and compare to the target's prediction

Can we use these test examples during the training phase?

Given: Training examples that are pairs of the form (x, f(x))

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Typically the input *x* is represented as *feature vectors* 

- Example:  $x \in \{0,1\}^d$  or  $x \in \Re^d$  (d-dimensional vectors)
- A deterministic mapping from instances in your problem (e.g., news articles) to features

The function *f* is unknown

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For a training example (x, f(x)), the value of f(x) is called its *label* 

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The label determines the kind of problem we have

- Binary classification: label space = {-1,1}
- Multiclass classification: label space = {1, 2, 3, …, K}
- Regression: label space =  $\Re$

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#### Questions?

# Examples of binary classification

(the label space consists of two elements)

- Spam filtering
  - Is an email spam or not?
- Recommendation systems
  - Given user's movie preferences, will she like a new movie?
- Anomaly detection
  - Is a smartphone app malicious?
  - Is a Twitter user a bot?
- Authorship identification
  - Were these two documents written by the same person?
- Time series prediction
  - Will the future value of a stock increase or decrease with respect to its current value?

## On supervised learning

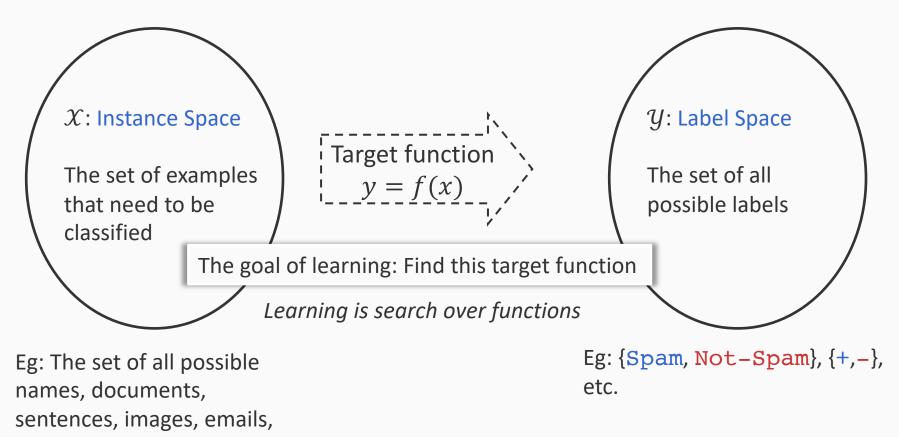
We should be able to decide:

1. What is our instance space?

What are the inputs to the problem? What are the features?

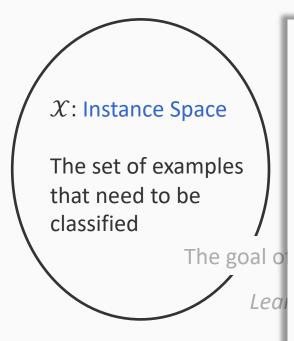
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#### 1. The Instance Space ${\mathcal X}$



etc

## 1. The Instance Space ${\mathcal X}$



Eg: The set of all possible names, documents, sentences, images, emails, etc Designing an appropriate *feature representation* of the instance space is crucial

Instances  $x \in \mathcal{X}$  are defined by features/attributes

Features could be Boolean

• Example: Does the email contain the word "free"?

#### Features could be real valued

- Example: What is the height of the person?
- Example: What was the stock price yesterday?

Features could be hand-crafted or themselves learned

An input to the problem (Eg: emails, names, images) Feature function

A feature vector

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A feature vector

Feature functions, also known as feature extractors

- Often deterministic, but could also be learned
- Convert the examples a collection of attributes Typically thought of as high-dimensional vectors

Important part of the design of a learning based solution

### 1. The Instance Space ${\mathcal X}$

Features are supposed to capture all the information needed for a learned system to make its prediction

- Think of them as the sensory inputs for the learned system

Not all information about the instances is necessary or relevant

Bad features could even confuse a learner

What might be good features for the badges game?

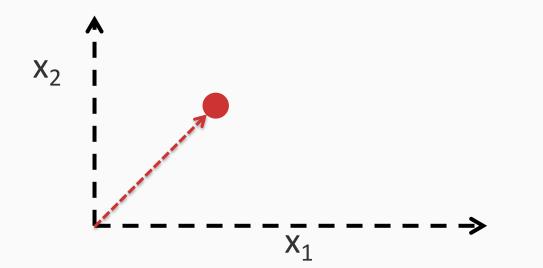
- Features functions convert inputs to vectors
- The instance space  $\mathcal{X}$  is a d-dimensional vector space (e.g.  $\Re^d$  or  $\{0,1\}^d$ )
  - Each dimension is one feature, we have d features in all
- Each  $x \in \mathcal{X}$  is a feature vector
  - Each  $\mathbf{x} = [\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_d]$  is a point in the vector space with d dimensions

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 $X_{2}$ 

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When designing feature functions, think of them as templates

- Feature: "The second letter of the name"

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  - Naoki  $a \rightarrow [1 \ 0 \ 0 \ ...]$
  - Abe  $b \rightarrow [0 \ 1 \ 0 \ 0 \ ...]$
  - Manning  $a \rightarrow [1 \ 0 \ 0 \ \dots]$
  - Scrooge  $c \rightarrow [0 \ 0 \ 1 \ 0 \ ...]$

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What is the dimensionality of these feature vectors?

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26 (One dimension per letter)

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What is the dimensionality of these feature vectors?

26 (One dimension per letter)

Such vectors where exactly one dimension is 1 and all others are zero are called one-hot vectors.

This is the one-hot representation of the feature "The second letter of the name"

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  - Naoki  $a \rightarrow [1 \ 0 \ 0 \ ...]$
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- Feature: "The length of the name"
  - Naoki  $\rightarrow 5$
  - Abe  $\rightarrow 3$
- "The second letter of the name, Length of the first name, length of the last name"
  - Naoki Abe  $\rightarrow [1 \ 0 \ 0 \ \dots \ 5 \ 3]$

Features can be accumulated by concatenating the vectors

#### Good features are essential

- Good features decide how well a task can be learned
  - Eg: A bad feature for the badges game
    - "Is there a day of the week that begins with the last letter of the first name?"

Something to think about: Why would we think that this is a bad feature?

- Much effort goes into designing features
  - Or learning them
- Will touch upon general principles for designing good features
  - But feature definition largely domain specific
  - Comes with experience

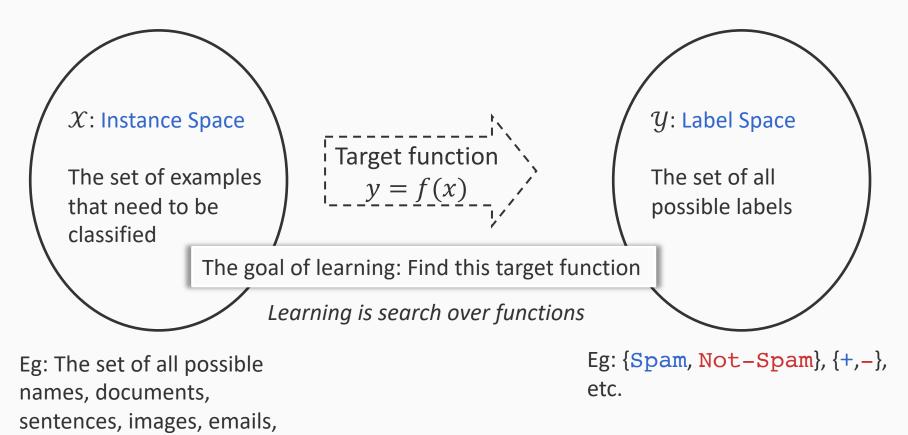
## On supervised learning

✓ What is our instance space?

What are the inputs to the problem? What are the features?

- 2. What is our label space? What is the learning task?
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## 2. The Label Space ${\mathcal Y}$

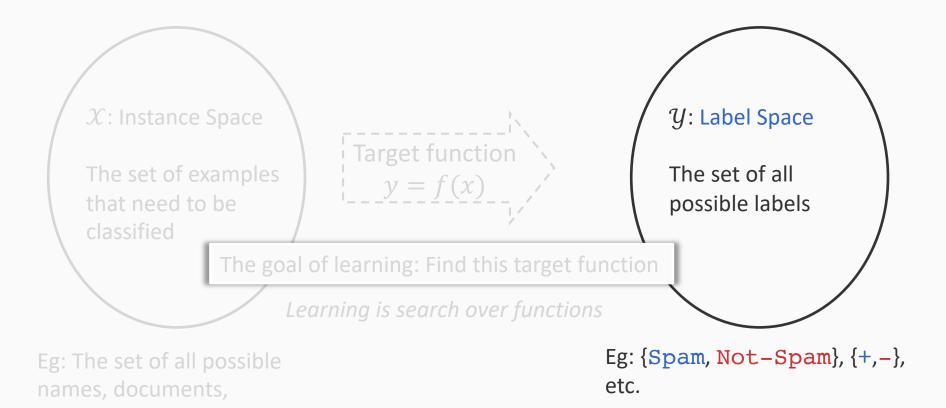


etc

# 2. The Label Space ${\mathcal Y}$

sentences, images, emails,

etc



# The label space depends on the nature of the problem

*Classification*: The outputs are categorical

- Binary classification: Two possible labels
  - We will see a lot of this

Multiclass classification: K possible labels

• We may see a bit of this if time permits

Structured classification: Graph valued outputs

• A different class

Classification is the primary focus of this class

# The label space depends on the nature of the problem

#### The output space can be numerical/ordinal

#### - Regression

• The label space  $\mathcal Y$  is the set (or a subset) of real numbers

#### - Ranking

- Labels are ordinal
- That is, there is an ordering over the labels
- Eg: A Yelp 5-star review is only slightly different from a 4-star review, but very different from a 1-star review

## On supervised learning

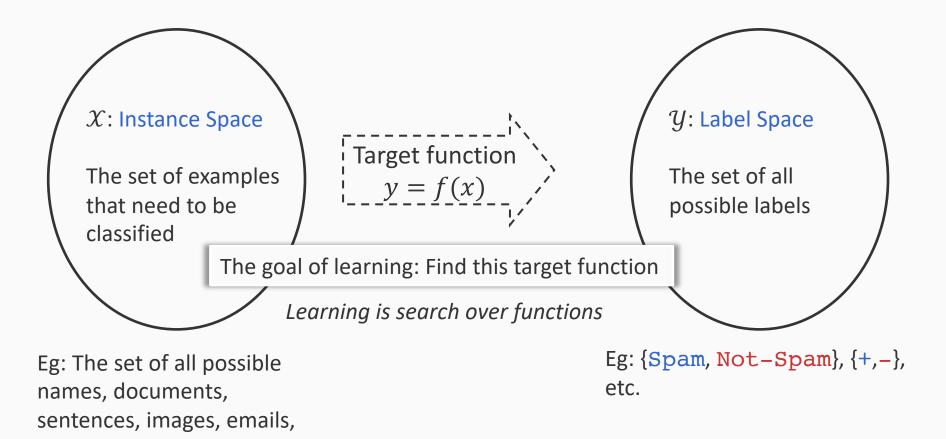
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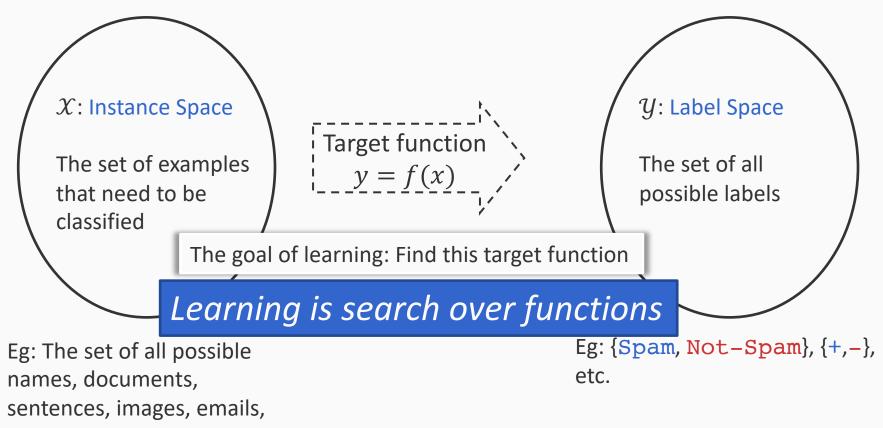
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etc



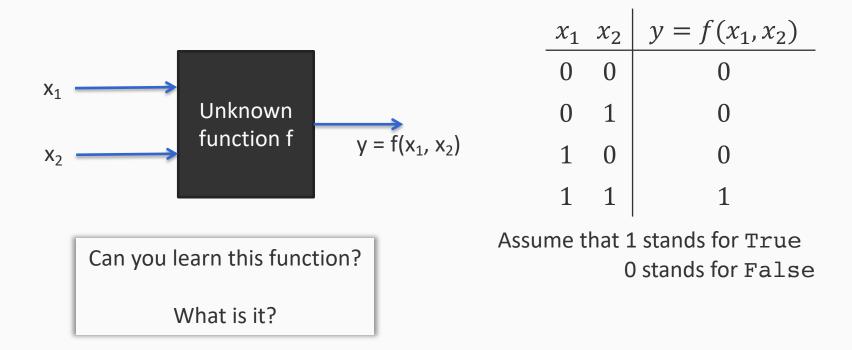
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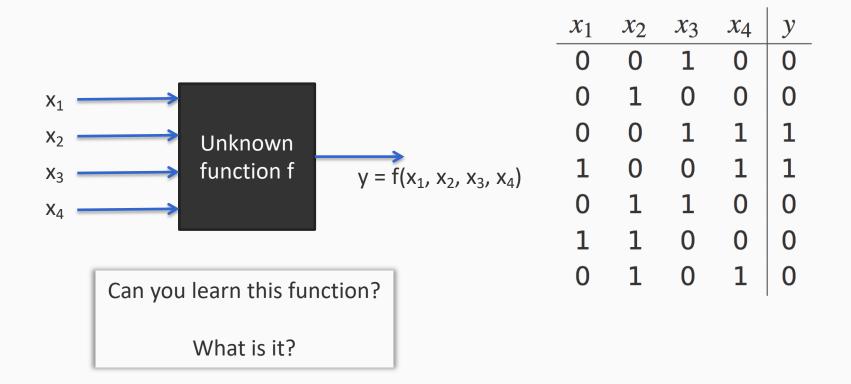


etc

#### Example of search over functions



### The fundamental problem Machine learning is ill-posed!



There are  $2^{16} = 65536$  possible Boolean functions over 4 inputs

Why? There are 16 possible outputs. Each way to fill these 16 slots is a different function, giving 2<sup>16</sup> functions.

$x_1$	$x_2$	$x_3$	$x_4$	y
0	0	0	0	
0	0	0	1	
0	0	1	0	
0	0	1	1	
0	1	0	0	
0	1	0	1	
0	1	1	0	
0	1	1	1	
1	0	0	0	
1	0	0	1	
1	0	1	0	
1	0	1	1	
1	1	0	0	
1	1	0	1	
1	1	1	0	
1	1	1	1	

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We have seen only 7 outputs

$x_1$	$x_2$	$x_3$	$x_4$	y
0	0	0	0	
0	0	0	$\overset{\circ}{1}$	? ?
0	0	1	0	$0 \leftarrow 0$
0	0	1	1	$1 \leftarrow$
0	1	0	0	$\rightarrow 0$
0	1	0	1	$\rightarrow 0$
0	1	1	0	$\rightarrow 0$
0	1	1	1	?
1	0	0	0	?
1	0	0	1	$1 \leftarrow$
1	0	1	0	?
1	0	1	1	?
1	1	0	0	$0 \leftarrow$
1	1	0	1	?
1	1	1	0	? ? ?
1	1	1	1	?

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- How could we possibly know the rest without seeing every label?
  - Think of an adversary filling in the labels every time you make a guess at the function

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0	0	0	0	?
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0	0	1	0	$\rightarrow 0$
0	0	1	1	$1 \leftarrow$
0	1	0	0	$\rightarrow 0$
0	1	0	1	$\rightarrow 0$
0	1	1	0	$0 \leftarrow$
0	1	1	1	?
1	0	0	0	?
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1	1	1	0	?
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$x_1$	$x_2$	$x_3$	$x_4$	y
0	0	0	0	?
0	0	0	1	?
0	0	1	0	0 <
0	0	1	1	$1 \leftarrow$
0	1	0	0	0 <
-		2	1	<b>0</b> +
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1 1 0

1 1

?

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 $\mathbf{0} \leftarrow$ 

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0

#### How could we possibly learn anything?

We have seen only / outputs

- How could we possibly know the rest without seeing every label?
  - Think of an adversary filling in the labels every time you make a guess at the function

## Solution: Restrict the search space

(The "When in doubt, make an assumption" school of thought!)

A *hypothesis space* is the set of possible functions we consider

- We were looking at the space of all Boolean functions
- Instead choose a hypothesis space that is not <u>all possible</u> functions
  - Only simple conjunctions (with four variables, there are only 16 conjunctions without negations)
  - m-of-n rules: Pick a set of n variables. At least m of them must be true
  - Linear functions
  - Deep neural networks
  - ...

#### Example Hypothesis space 1

#### Simple conjunctions

There are only 16 simple **conjunctive rules** of the form  $g(x) = x_i \wedge x_j \wedge x_k \cdots$ 

$x_1$	$x_2$	<i>x</i> <sub>3</sub>	<i>x</i> <sub>4</sub>	y
0	0	1	0	0
0	1	0	0	0
0	0	1	1	1
1	0	0	1	1
0	1	1	0	0
1	1	0	0	0
0	1	0	1	0

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0	0	1	0	0
0	1	0	0	0
0	0	1	1	1
1	0	0	1	1
0	1	1	0	0
1	1	0	0	0
0	1	0	1	0

Rule	Rule
Always False	$x_2 \wedge x_3$
$x_1$	$x_2 \wedge x_4$
<i>x</i> <sub>2</sub>	$x_3 \wedge x_4$
<i>x</i> <sub>3</sub>	$x_1 \wedge x_2 \wedge x_3$
$x_4$	$x_1 \wedge x_2 \wedge x_4$
$x_1 \wedge x_2$	$x_1 \wedge x_3 \wedge x_4$
$x_1 \wedge x_3$	$x_2 \wedge x_3 \wedge x_4$
$x_1 \wedge x_4$	$x_1 \wedge x_2 \wedge x_3 \wedge x_4$

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$x_1$	$x_2$	<i>x</i> <sub>3</sub>	<i>x</i> <sub>4</sub>	y
0	0	1	0	0
0	1	0	0	0
0	0	1	1	1
1	0	0	1	1
0	1	1	0	0
1	1	0	0	0
0	1	0	1	0

#### Rule

Always False

Rule

Y	
$x_1$	Exercise: How many simple conjunctions are
$x_2$	possible when there are n inputs instead of 4?
<i>x</i> <sub>3</sub>	$x_1 \wedge x_2 \wedge x_3$
$x_4$	$x_1 \wedge x_2 \wedge x_4$
$x_1 \wedge x_2$	$x_1 \wedge x_3 \wedge x_4$
$x_1 \wedge x_3$	$x_2 \wedge x_3 \wedge x_4$
$x_1 \wedge x_4$	$x_1 \wedge x_2 \wedge x_3 \wedge x_4$

#### $x_2 \wedge x_3$

Example	_			<i>x</i> <sub>1</sub>	<i>x</i> <sub>2</sub>	<i>x</i> <sub>3</sub>	<i>x</i> <sub>4</sub>	y
Hypothes	is space	ce 1		0	0	1	0	0
	-	Is there	e a <i>consistent</i>	0 0	1 0	0 1	0 1	01
Simple conjur	nctions		nesis in this space?	1	0	0	1	1
Ther	e are only 16	simple <b>c</b>	onjunctive rules	0	1	1	0	0
	e form $g(x)$	•	•	1	1	0	0	0
				0	1	0	1	0
Rule			Rule					
Always False			$x_2 \wedge x_3$	_				
$x_1$			$x_2 \wedge x_4$					
$x_2$			$x_3 \wedge x_4$					
$x_3$			$x_1 \wedge x_2 \wedge x_3$					
$x_4$			$x_1 \wedge x_2 \wedge x_4$					
$x_1 \wedge x_2$			$x_1 \wedge x_3 \wedge x_4$					
$x_1 \wedge x_3$			$x_2 \wedge x_3 \wedge x_4$					
$x_1 \wedge x_4$			$x_1 \wedge x_2 \wedge x_3 \wedge x_4$				72	

#### Example Hypothesis space 1

#### Simple conjunctions

There are only 16 simple **conjunctive rules** of the form  $g(x) = x_i \wedge x_j \wedge x_k \cdots$ 

$x_1$	$x_2$	<i>x</i> <sub>3</sub>	<i>x</i> <sub>4</sub>	y
0	0	1	0	0
0	1	0	0	0
0	0	1	1	1
1	0	0	1	1
0	1	1	0	0
1	1	0	0	0
0	1	0	1	0

Rule	Counter-example	Rule	Counter-example
Always False	1001	$x_2 \wedge x_3$	0011
$x_1$	1100	$x_2 \wedge x_4$	0011
<i>x</i> <sub>2</sub>	0100	$x_3 \wedge x_4$	1001
<i>x</i> <sub>3</sub>	0110	$x_1 \wedge x_2 \wedge x_3$	0011
$x_4$	0101	$x_1 \wedge x_2 \wedge x_4$	0011
$x_1 \wedge x_2$	1100	$x_1 \wedge x_3 \wedge x_4$	0011
$x_1 \wedge x_3$	0011	$x_2 \wedge x_3 \wedge x_4$	0011
$x_1 \wedge x_4$	0011	$x_1 \wedge x_2 \wedge x_3 \wedge x_4$	0011

Example			$x_1$	<i>x</i> <sub>2</sub>	<i>x</i> <sub>3</sub>	<i>x</i> <sub>4</sub>	<i>y</i>
	sis space 1		0	0 1 1 0 0 1 0 0 1 1 1 0 1 0 1 0	0	0	
i i j po en e			0		0	0	
			0	0	1	1	1
Simple conjunctions			1	0	0	1	1
Th	ere are only 16 simple <b>c</b>	onjunctive rules	0	1	1	0	0
	the form $g(x) = x_i \wedge x_j$		1 1 0		0	0	
			0	1	0	1	0
Rule	Counter-example	Rule	Counter-example				
Always False	1001	$\sim \wedge \sim$	0011				
AlwaysTalse	1001	$x_2 \wedge x_3$		0	UII		
(Confirm t	No simple conjunction each counterexample by	on explains the data! going through the list ace is too small and e looking for is not in it		wards	;)		
(Confirm t	No simple conjunction each counterexample by Our hypothesis spa he true function we were	on explains the data! going through the list ace is too small and e looking for is not in it		wards	5)		
(Confirm t	No simple conjunction each counterexample by Our hypothesis spat he true function we were 0101 1100	on explains the data! going through the list ace is too small and e looking for is not in it $x_1 \land x_2 \land x_4$ $x_1 \land x_3 \land x_4$		wards	5) 011 011		
(Confirm t	No simple conjunction each counterexample by Our hypothesis spa he true function we were	on explains the data! going through the list ace is too small and e looking for is not in it		wards	5)		

## Solution: Restrict the search space

A *hypothesis space* is the set of possible functions we consider

- We were looking at the space of all Boolean functions
- Instead choose a hypothesis space that is not <u>all possible</u> functions
  - Only simple conjunctions (with four variables, there are only 16 conjunctions without negations)
  - m-of-n rules: Pick a set of n variables. At least m of them must be true
  - Linear functions
  - Deep neural networks
  - ...
- How do we pick a hypothesis space?
  - Using some prior knowledge (or by guessing)

## Solution: Restrict the search space

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  - ...
- How do we pick a hypothesis space?
  - Using some prior knowledge (or by guessing)
- What if the hypothesis space is so small that nothing in it agrees with the data?
  - We need a hypothesis space that is flexible enough

#### Example Hypothesis space 2

#### m-of-n rules

Pick a subset with n variables. The label y = 1 if at least m of them are 1

Example: If at least 2 of {x<sub>1</sub>, x<sub>3</sub>, x<sub>4</sub>} are 1, then the output is 1. Otherwise, the output is 0.

Is there a consistent hypothesis in this space?

**Exercise**: Check if there is one First, how many m-of-n rules are there for four variables?

$x_1$	$x_2$	<i>x</i> <sub>3</sub>	<i>x</i> <sub>4</sub>	y
0	0	1	0	0
0	1	0	0	0
0	0	1	1	1
1	0	0	1	1
0	1	1	0	0
ן 1	1	0	0	0
0	1	0	1	0

## Restricting the hypothesis space

- Our guess of the hypothesis space may be incorrect
- General strategy
  - Pick an expressive hypothesis space expressing concepts
    - Concept = the target classifier that is hidden from us. Sometimes we
      may call it the oracle.
    - Example hypothesis spaces: m-of-n functions, decision trees, linear functions, grammars, multi-layer perceptron, transformer networks, convolutional neural networks, etc
  - Develop algorithms that find an element the hypothesis space that fits data well (or well enough)
  - Hope that it generalizes

### Perspectives on learning

- Learning is the removal of *remaining* uncertainty over a hypothesis space
  - If we knew that the unknown function is a simple conjunction, we could use the training data to figure out which one it is
- Requires guessing a *good, small* hypothesis class
  - And we could be wrong
  - We could find a consistent hypothesis and still be incorrect with a new example!

## On using supervised learning

✓ What is our instance space?

What are the inputs to the problem? What are the features?

- ✓ What is our label space? What is the learning task?
- ✓ What is our hypothesis space?
   What functions should the learning algorithm search over?
- 4. What is our learning algorithm? How do we learn from the labeled data?

Much of the rest of this semester

5. What is our loss function or evaluation metric? What is success?