

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

Let's play

| Name | Label |
|-----------------------|-------|
| Claire Cardie | - |
| Peter Bartlett | + |
| Eric Baum | + |
| Haym Hirsh | - |
| Leslie Pack Kaelbling | + |
| Yoav Freund | - |

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

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What is the label for *Indiana Jones*?

Let's play

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How were the labels generated?

Let's play

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How were the labels generated?

```
If last letter of first name is before last letter of last name:  
    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?

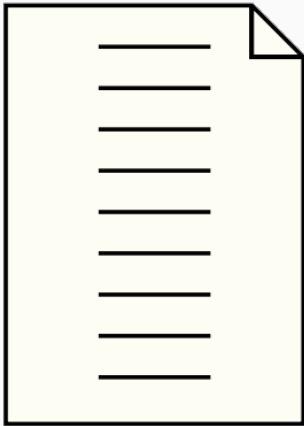
What is supervised learning?

Instances and Labels

Running example: Automatically tag news articles

Instances and Labels

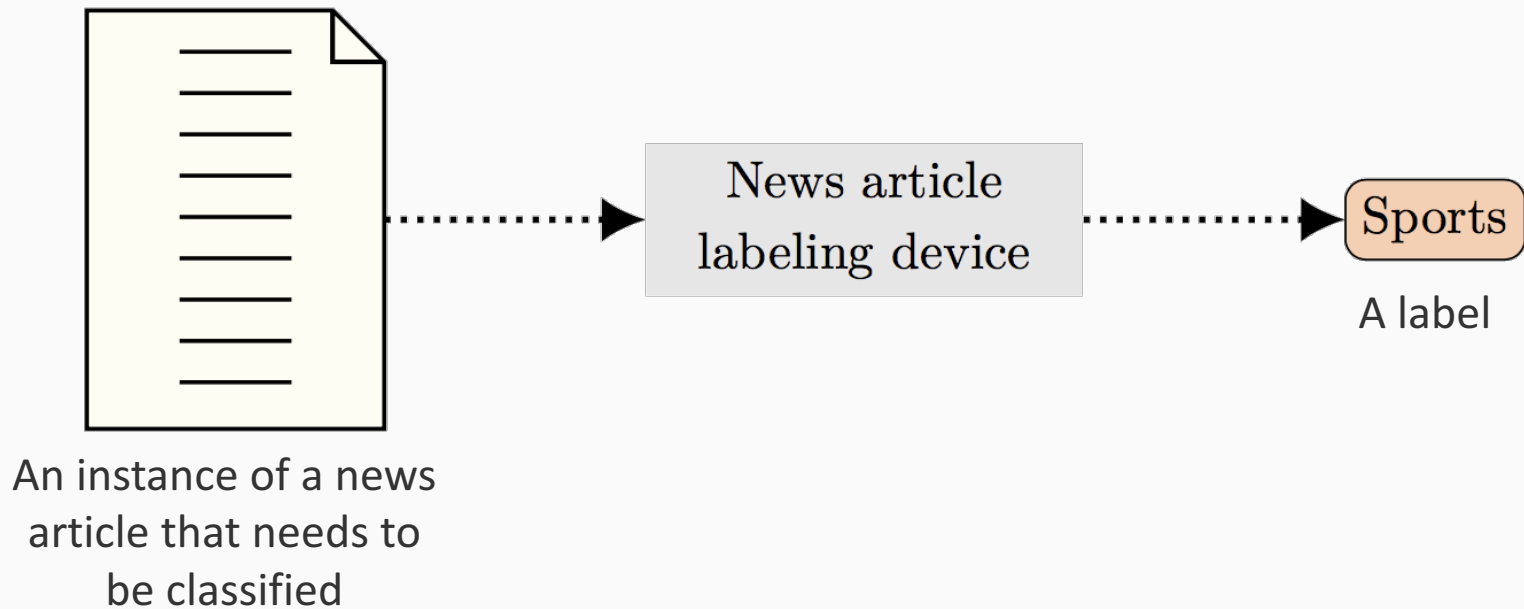
Running example: Automatically tag news articles



An instance of a news
article that needs to
be classified

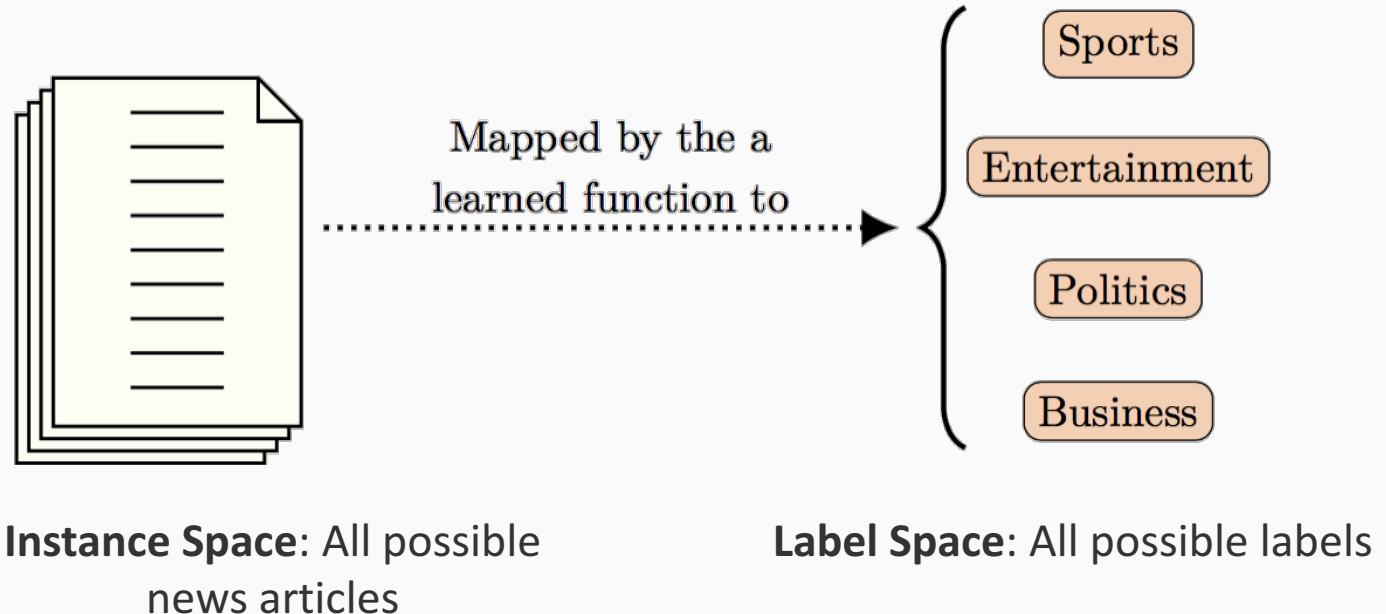
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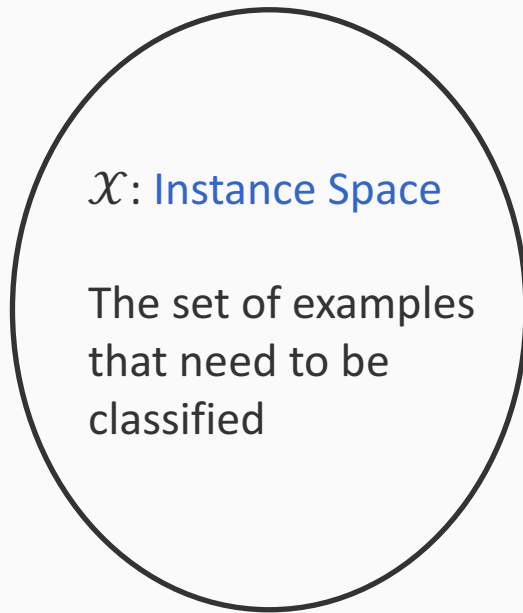


Instances and Labels

Running example: Automatically tag news articles



Instances and Labels



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

Instances and Labels

\mathcal{X} : Instance Space

The set of examples
that need to be
classified

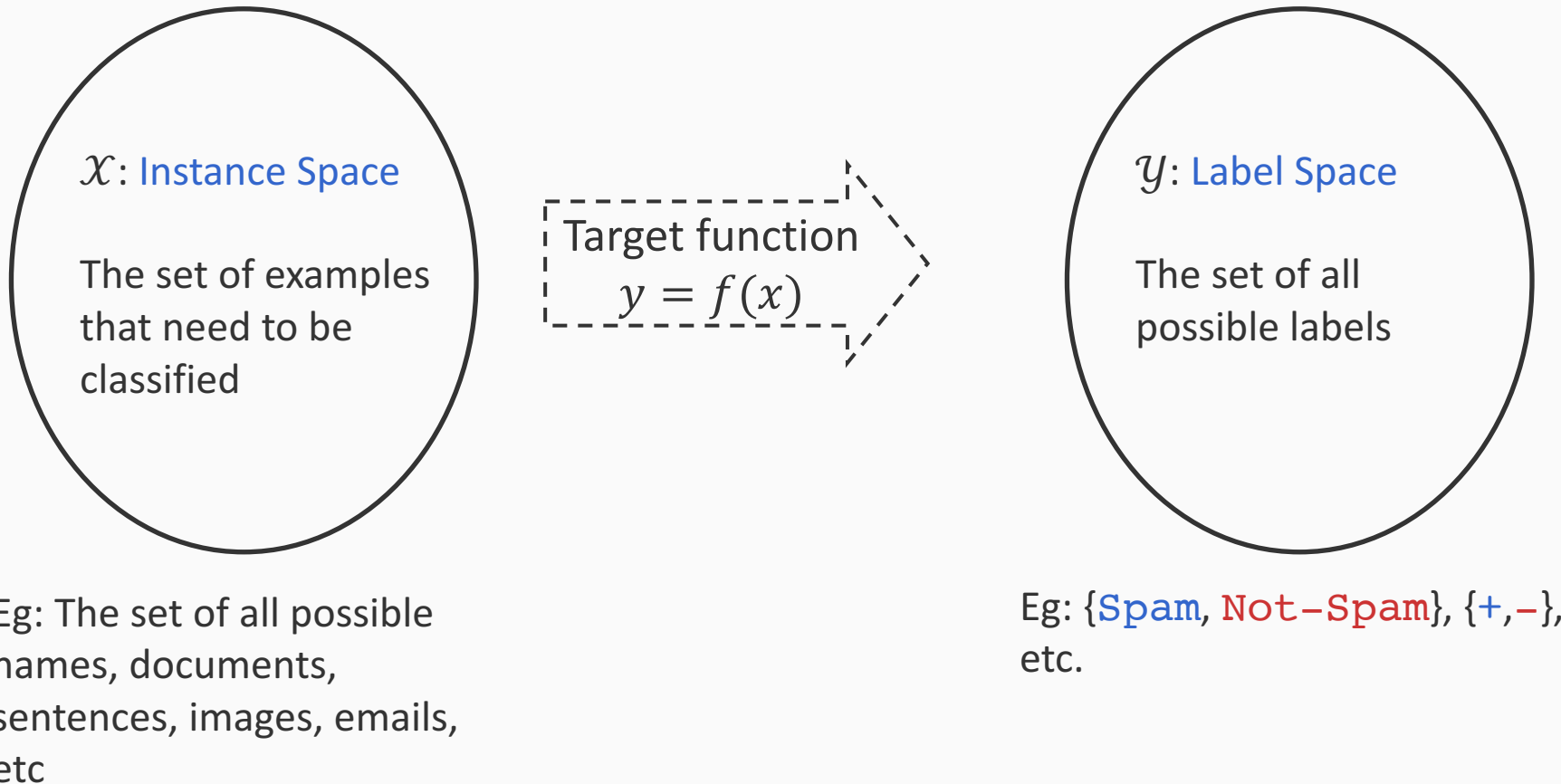
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\mathcal{Y} : Label Space

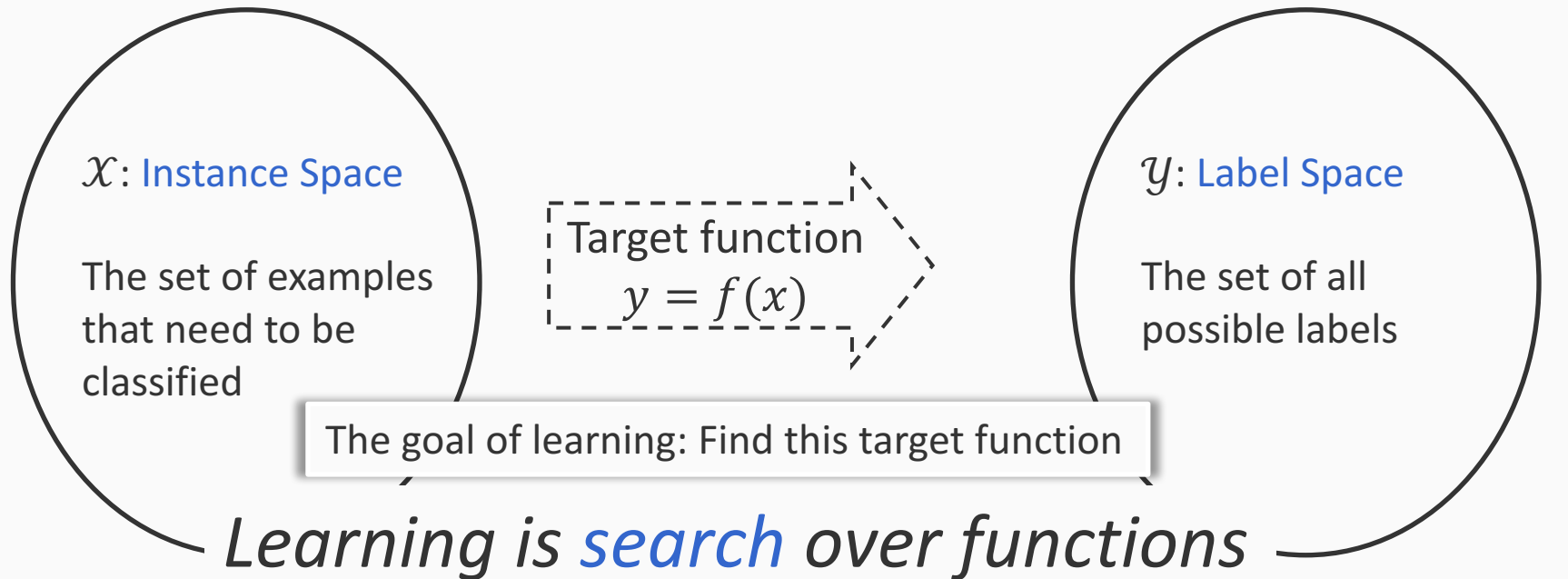
The set of all
possible labels

Eg: {Spam, Not-Spam}, {+, -},
etc.

Instances and Labels



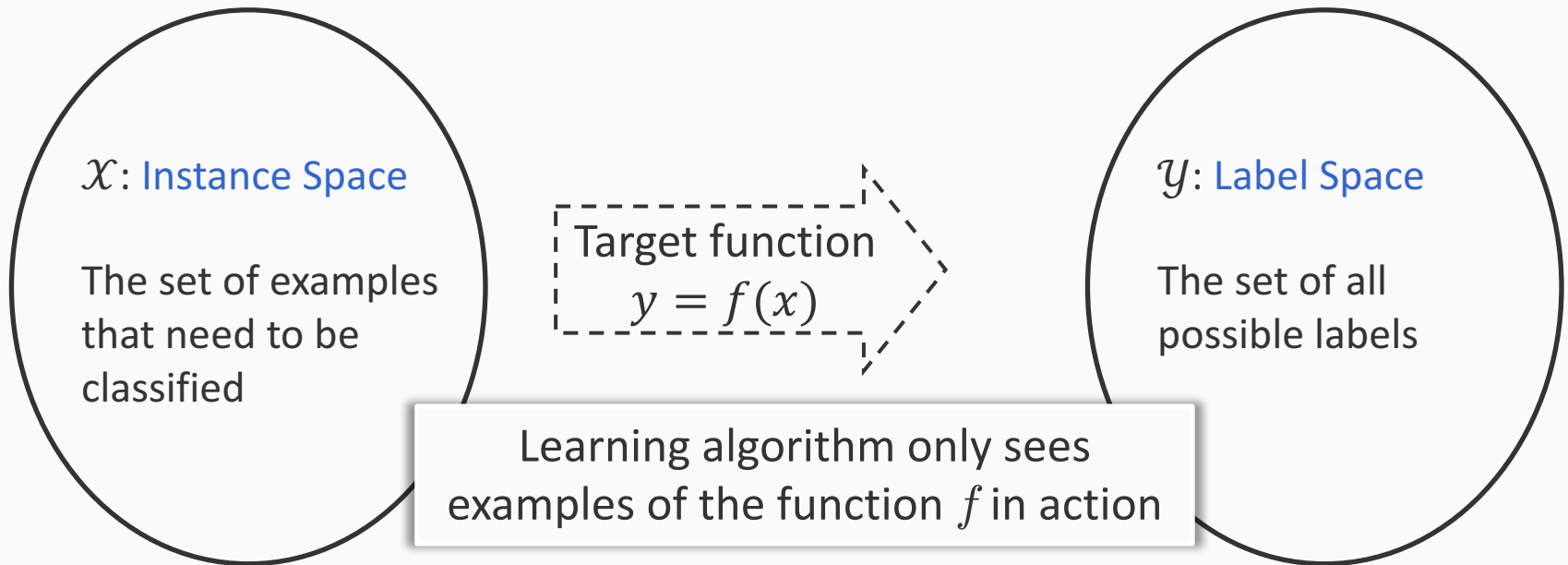
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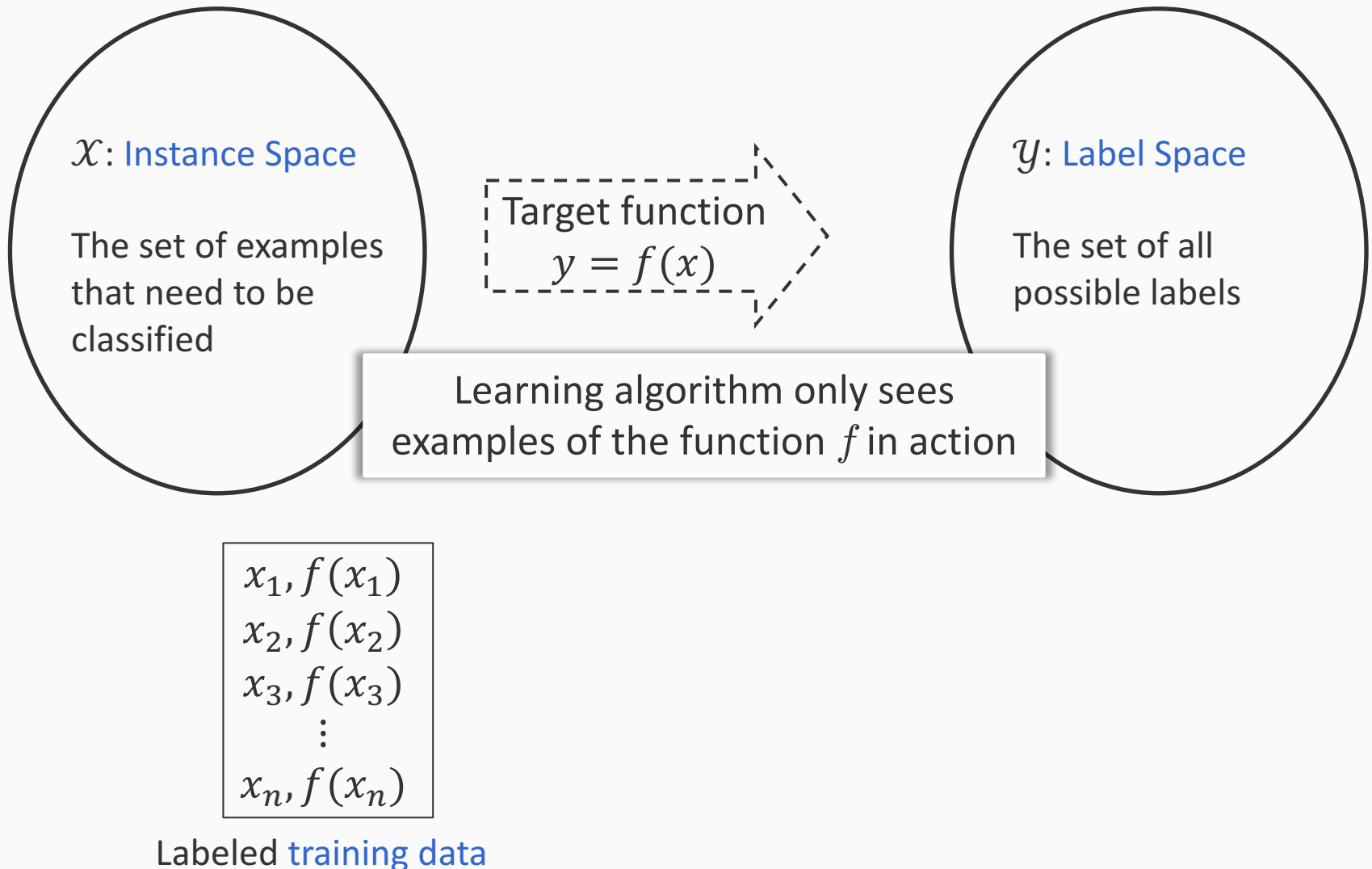
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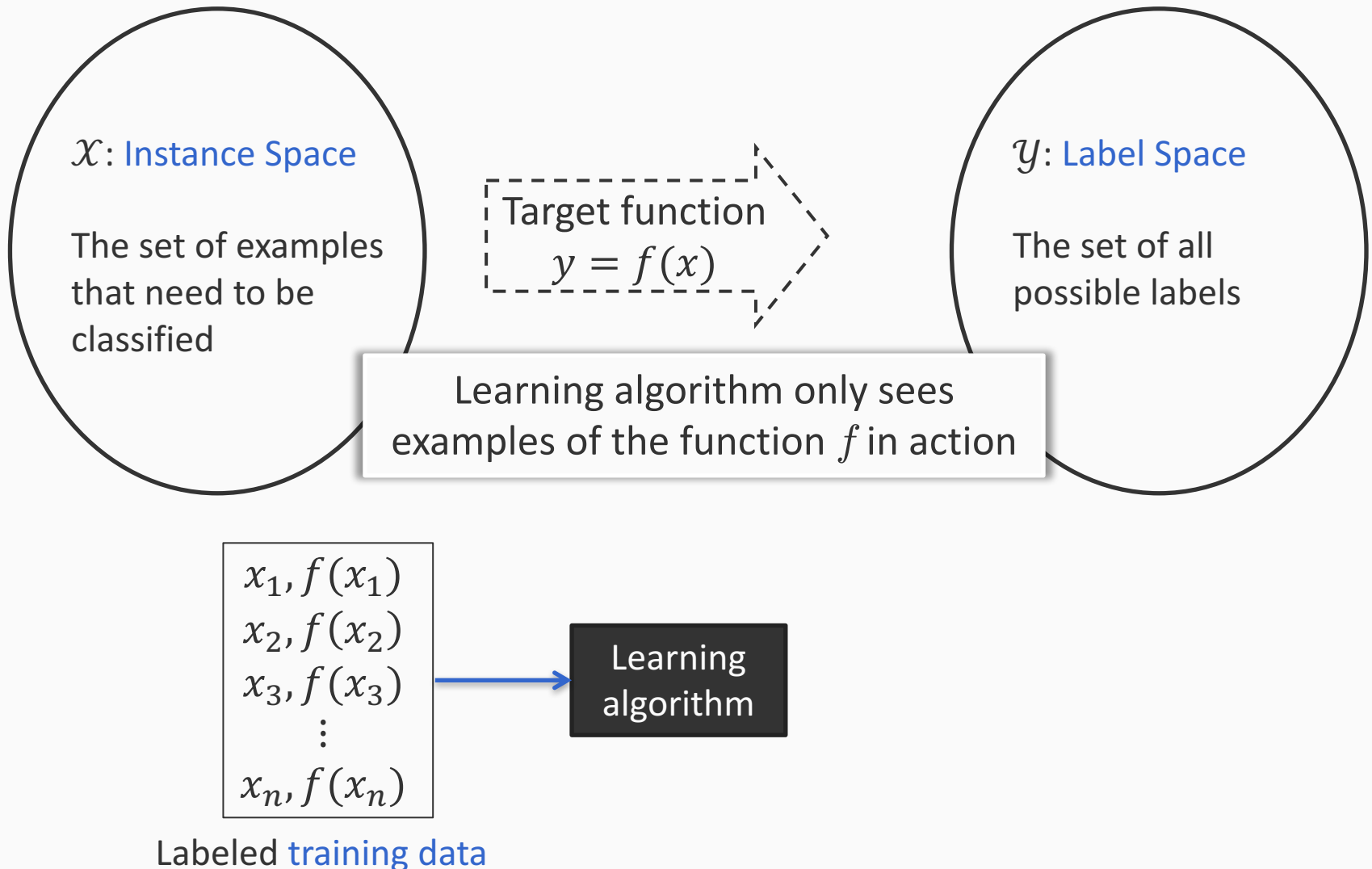
Supervised learning



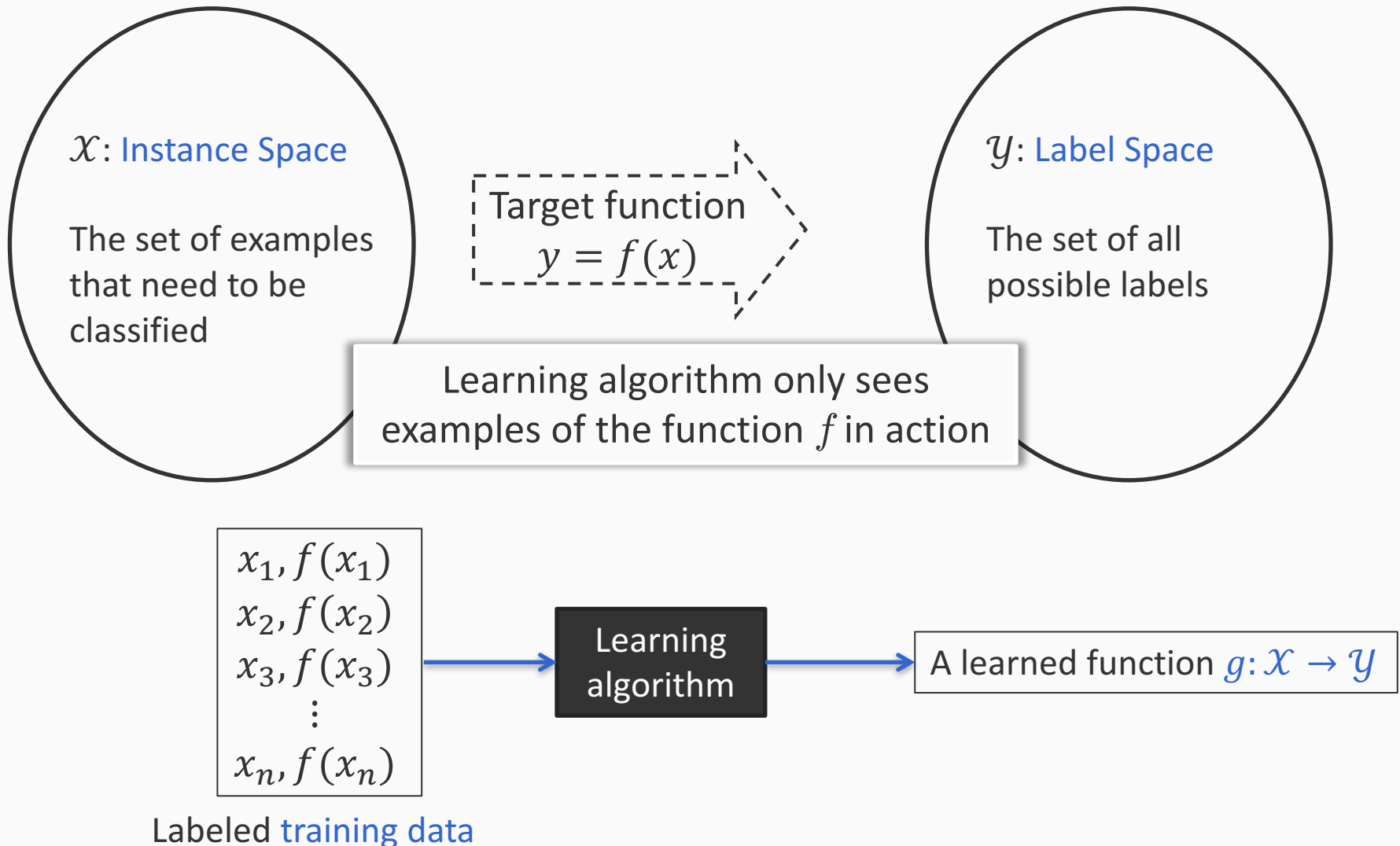
Supervised learning



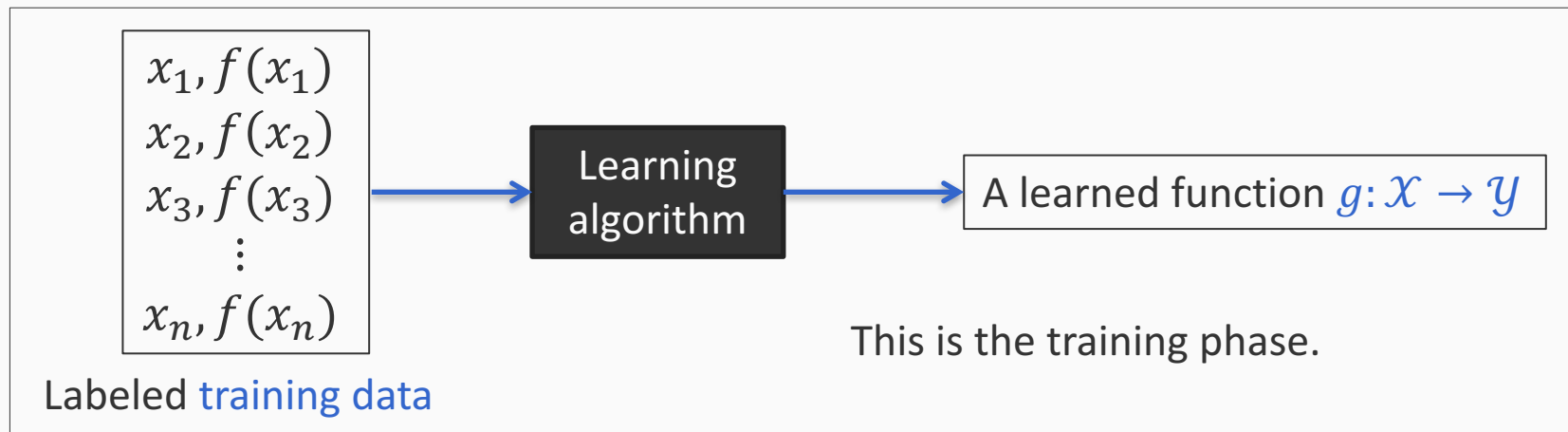
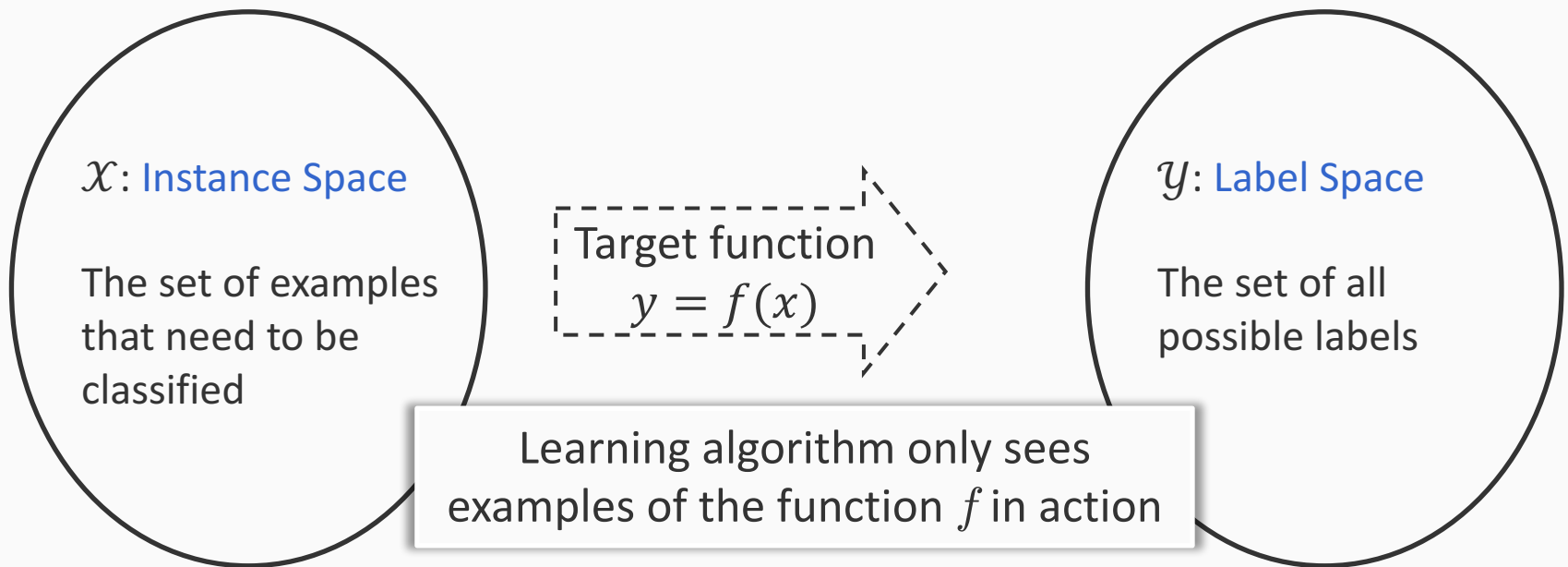
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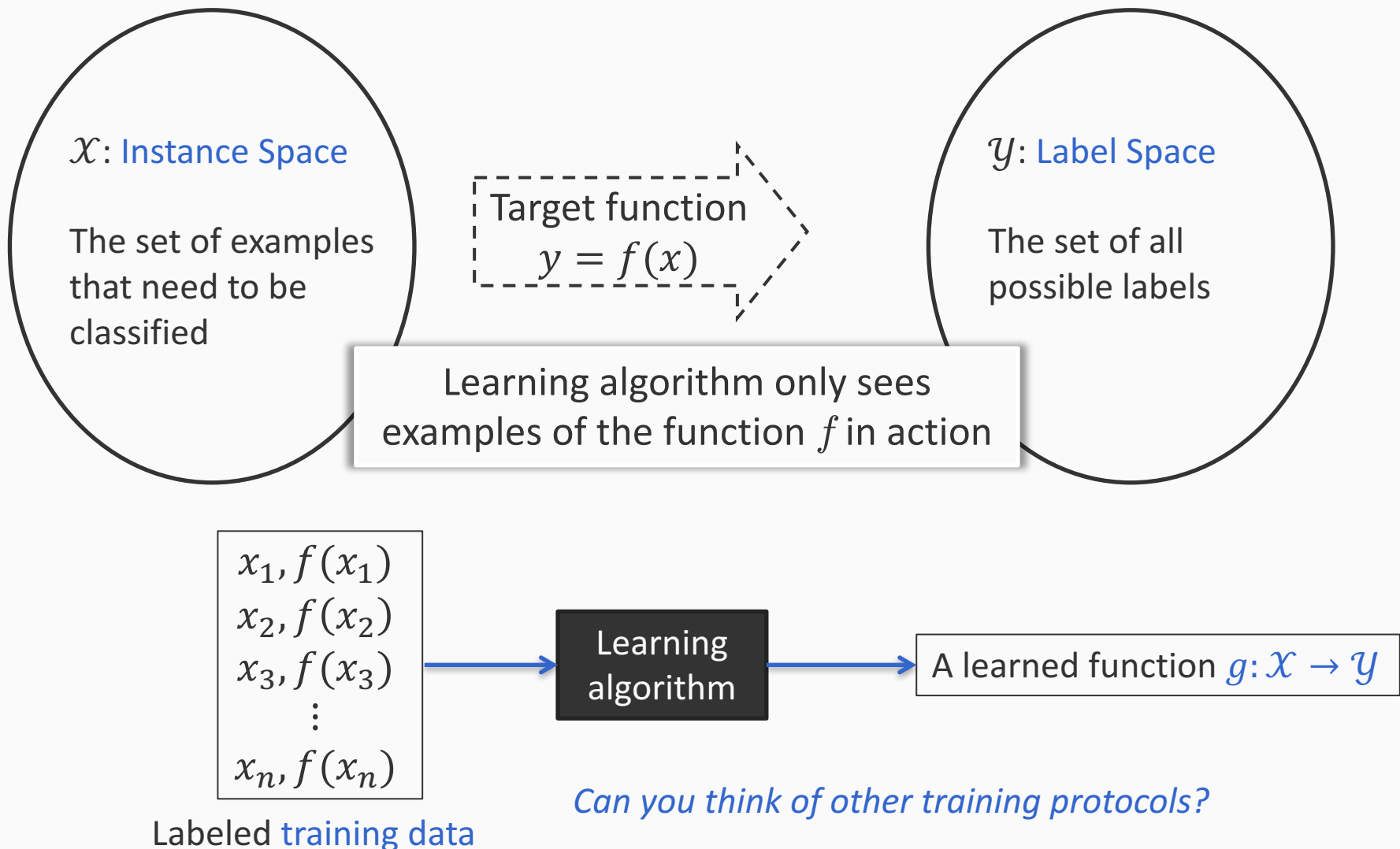
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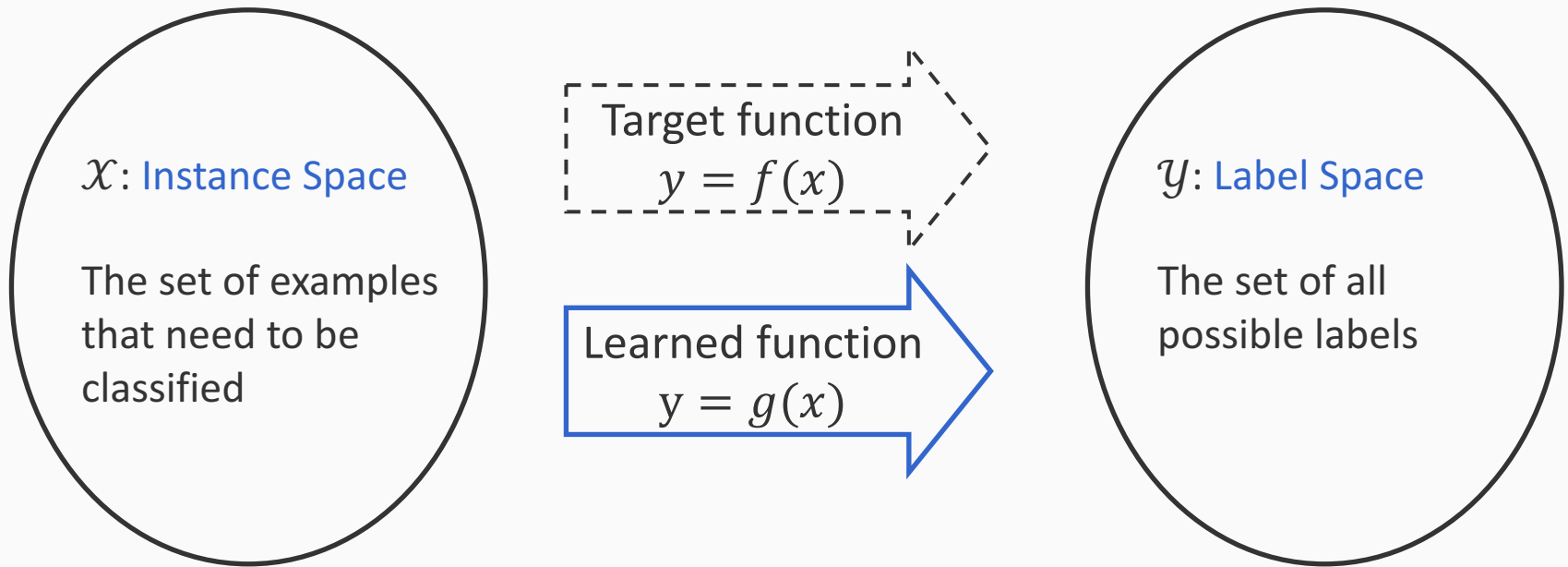
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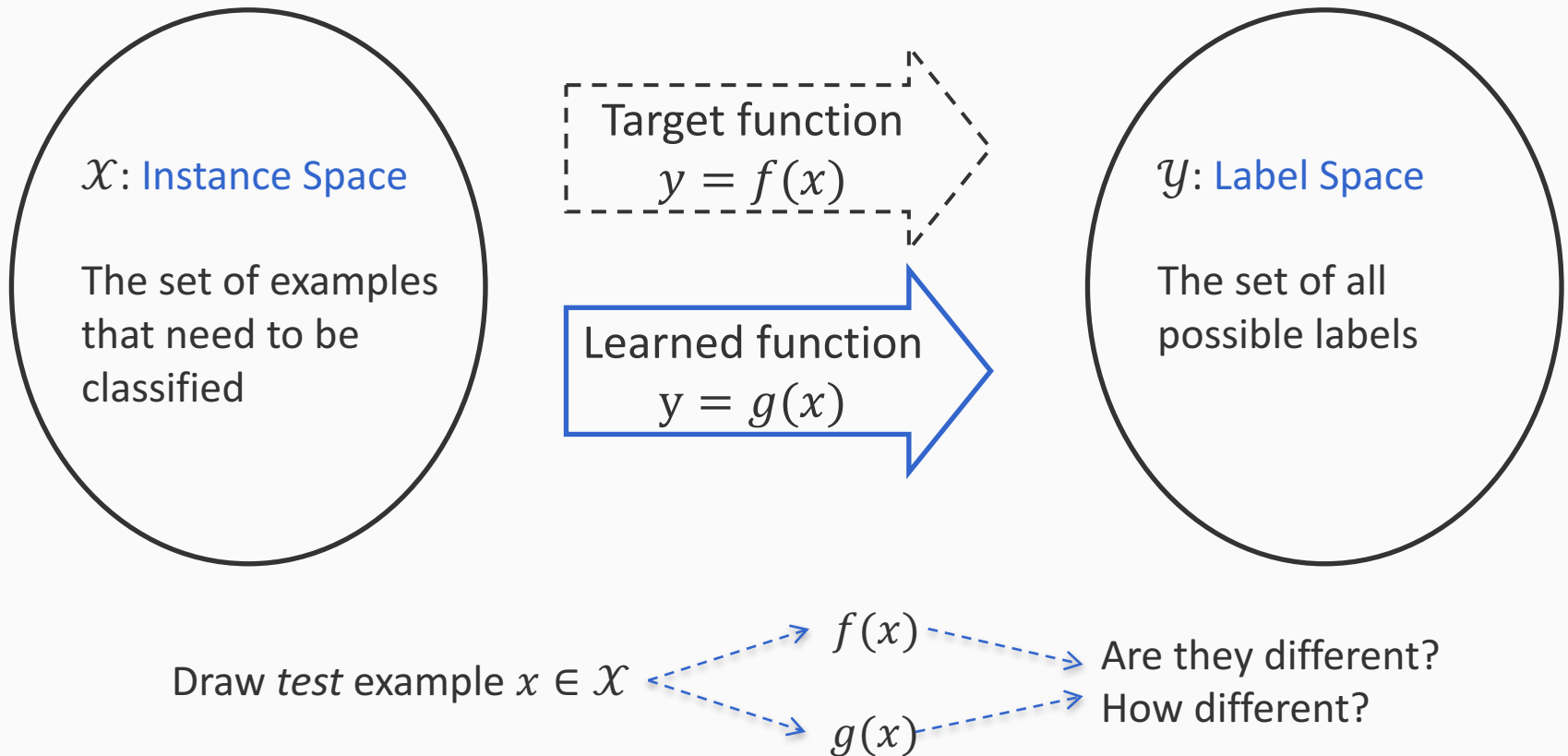
Supervised learning



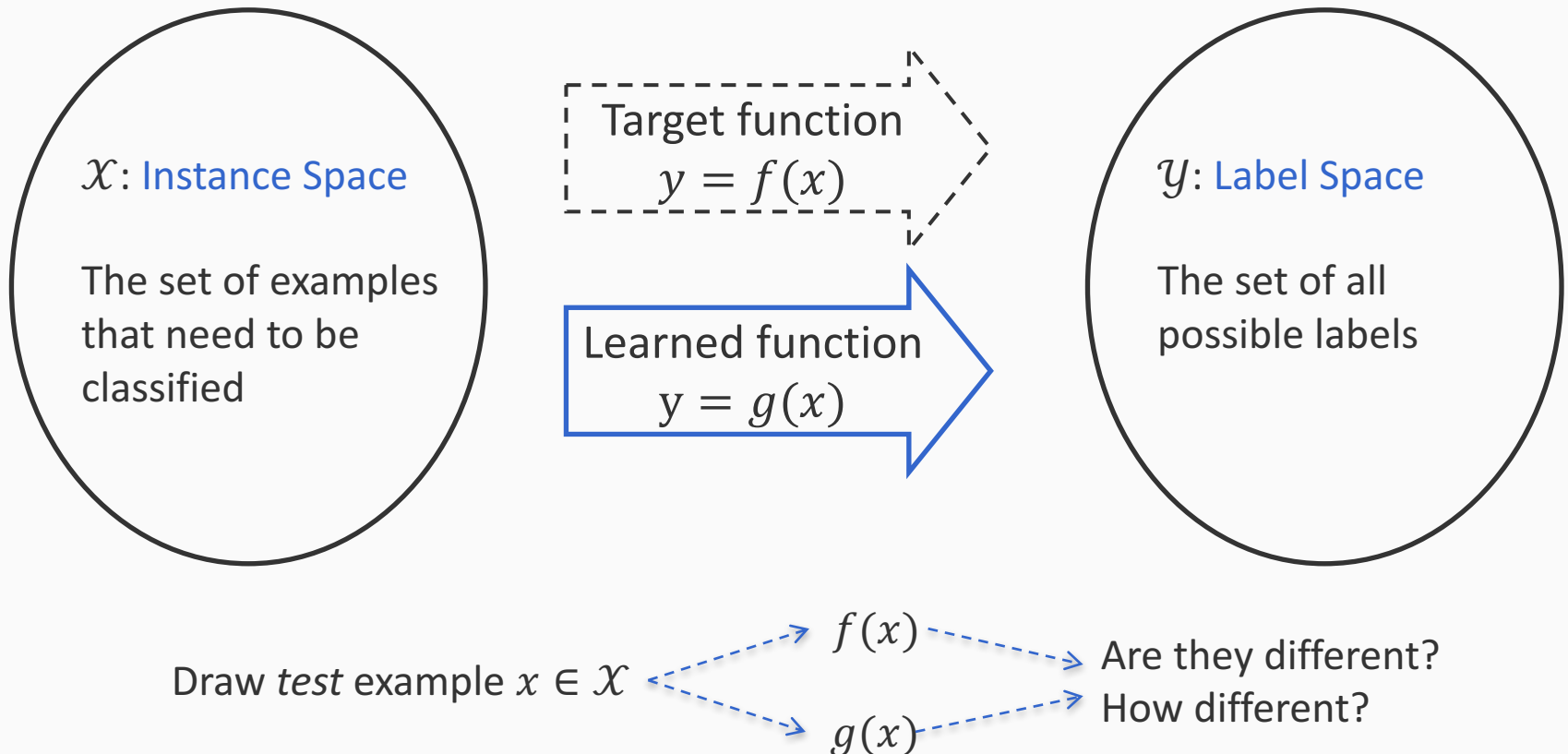
Supervised learning: Evaluation



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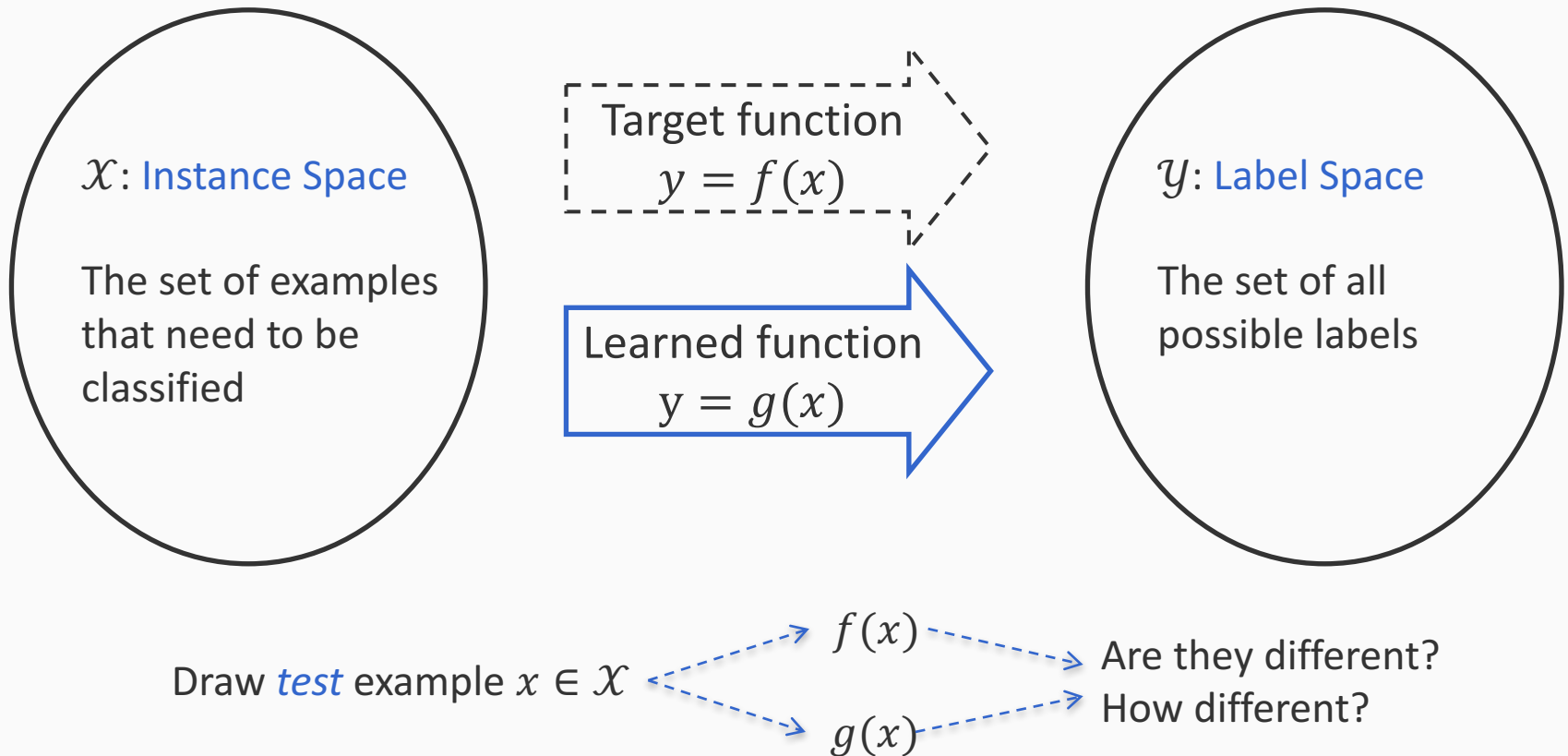
Supervised learning: Evaluation



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

Aggregate these results to get a quality measure

Supervised learning: Evaluation



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

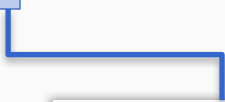
Can we use these test examples during the training phase?

Supervised learning: General setting

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

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The function
 f is unknown

Supervised learning: General setting

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

Typically the input x is represented as *feature vectors*

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

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The label determines the kind of problem we have

- **Binary classification:** label space = $\{-1, 1\}$
- **Multiclass classification:** label space = $\{1, 2, 3, \dots, K\}$
- **Regression:** label space = \mathbb{R}

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Questions?

Examples of binary classification

(the label space consists of two elements)

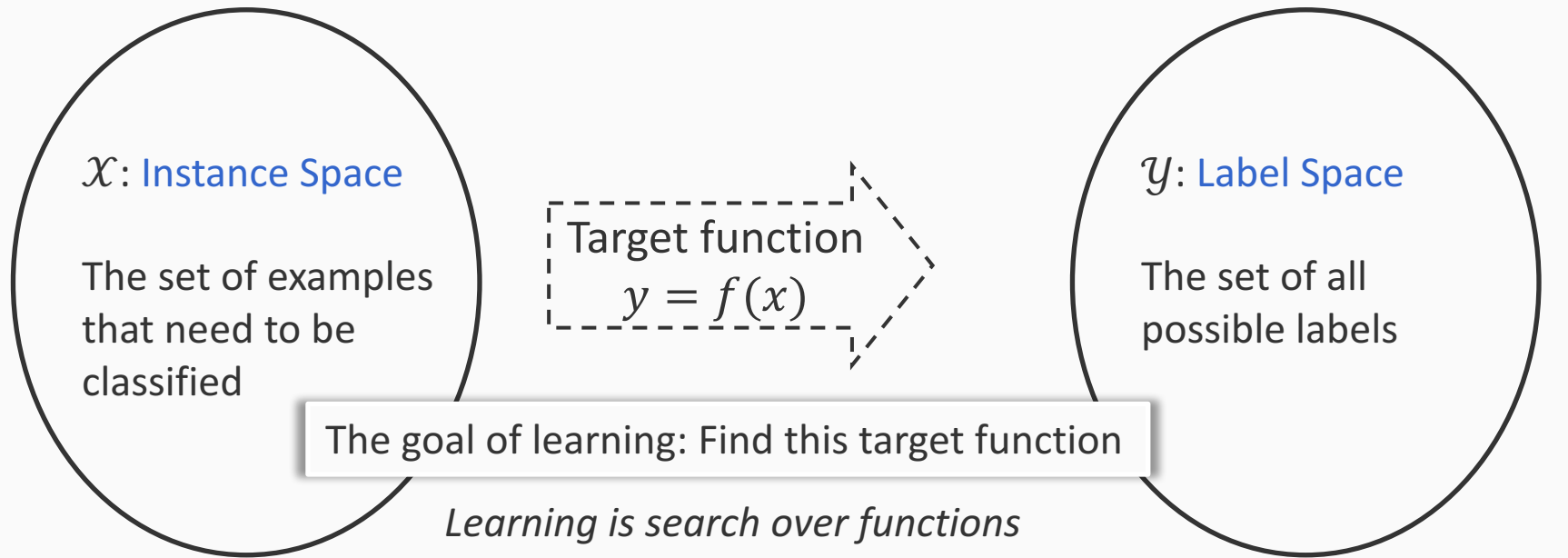
- Spam filtering
 - Is an email spam or not?
- Recommendation systems
 - Given user's movie preferences, will she like a new movie?
- Anomaly detection
 - Is a smartphone app malicious?
 - Is a Twitter user a bot?
- Authorship identification
 - Were these two documents written by the same person?
- Time 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?
2. What is our **label space**?
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3. What is our **hypothesis space**?
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5. What is our **loss function** or **evaluation metric**?
What is success?

1. The Instance Space \mathcal{X}



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

Eg: {Spam, Not-Spam}, {+, -}, etc.

1. The Instance Space \mathcal{X}

\mathcal{X} : Instance Space

The set of examples
that need to be
classified

The goal of

Learn

Eg: The set of all possible
names, documents,
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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

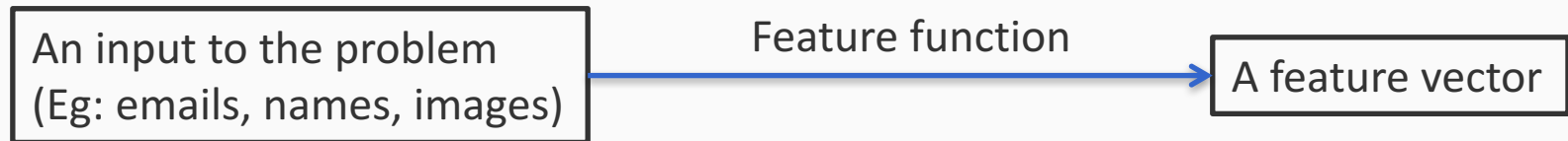
- **Example:** Does the email contain the word “free”?

Features could be real valued

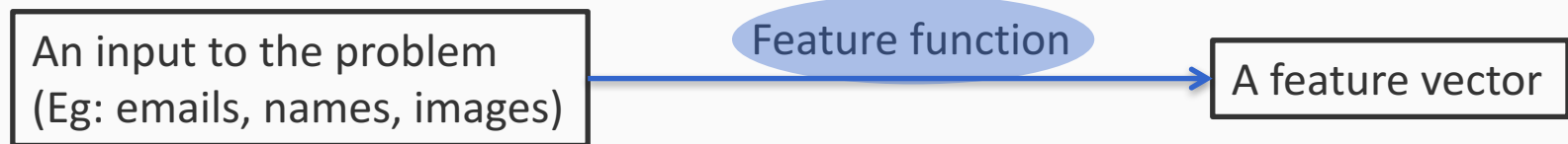
- **Example:** What is the height of the person?
- **Example:** What was the stock price yesterday?

Features could be hand-crafted or themselves learned

Instances as feature vectors



Instances as feature vectors



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

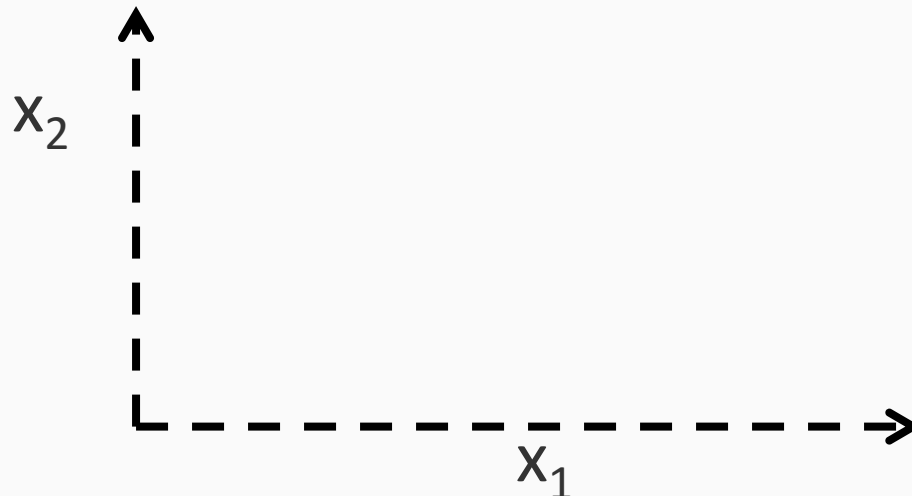
What might be good features for the badges game?

Instances as feature vectors

- Features functions convert inputs to vectors
- The instance space \mathcal{X} *is* a d -dimensional vector space (e.g. \mathbb{R}^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 $x = [x_1, x_2, \dots, x_d]$ is a point in the vector space with d dimensions

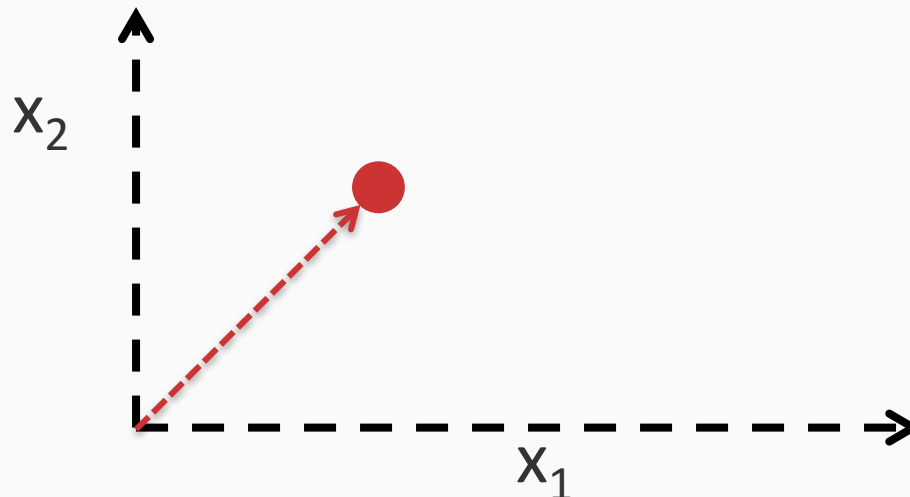
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Feature functions produce feature vectors

When designing feature functions, think of them as templates

- Feature: *“The second letter of the name”*

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- N**a**oki a \rightarrow [*1* 0 0 0 ...]
- A**b**e b \rightarrow [0 *1* 0 0 ...]
- M**a**nning a \rightarrow [*1* 0 0 0 ...]
- S**c**rooge c \rightarrow [0 0 *1* 0 ...]

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26 (One dimension per letter)

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What is the dimensionality of these feature vectors?

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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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- Feature: *“The length of the name”*

- Naoki \rightarrow 5
- Abe \rightarrow 3

Feature functions produce feature vectors

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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 0 ... 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?”

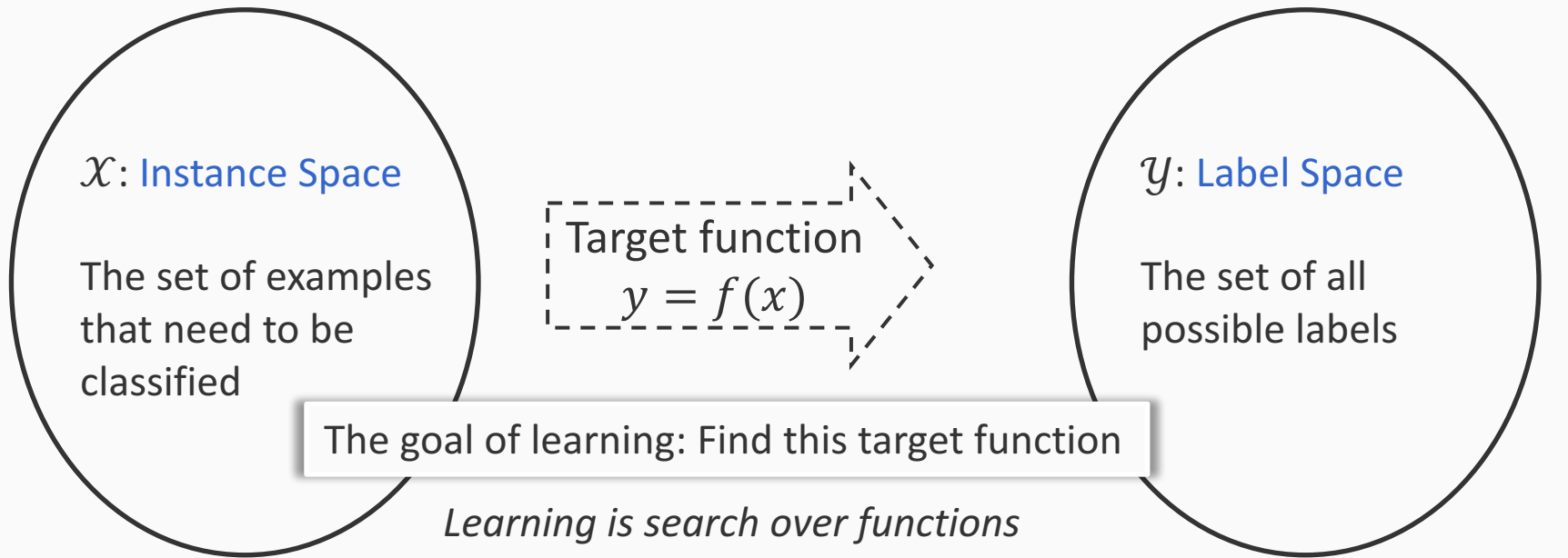
Something to think about: Why would we think that this is a bad feature?

- 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**?
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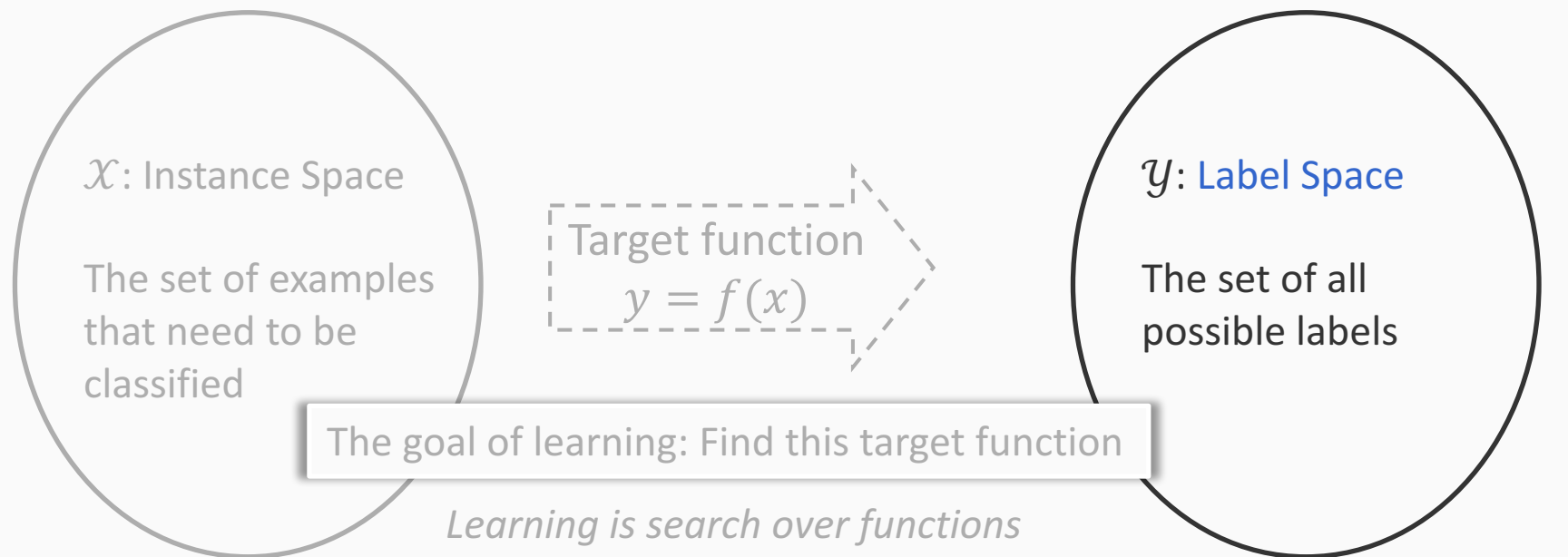
2. The Label Space \mathcal{Y}



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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

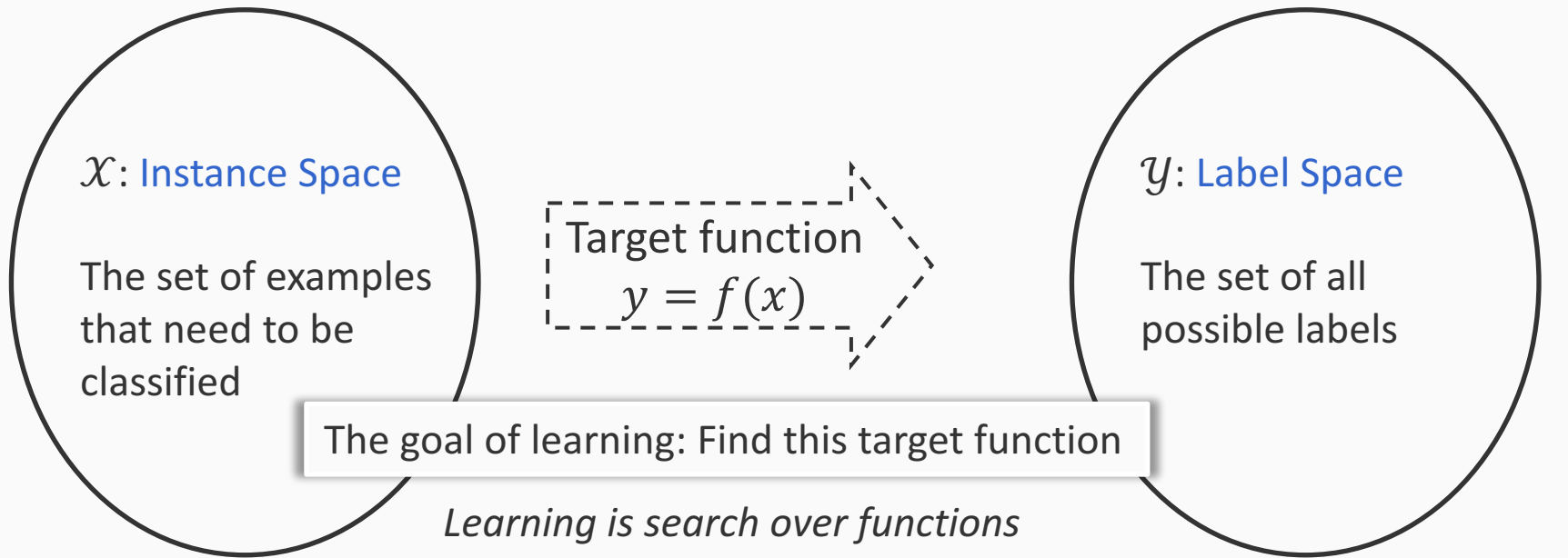
- Ranking

- 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

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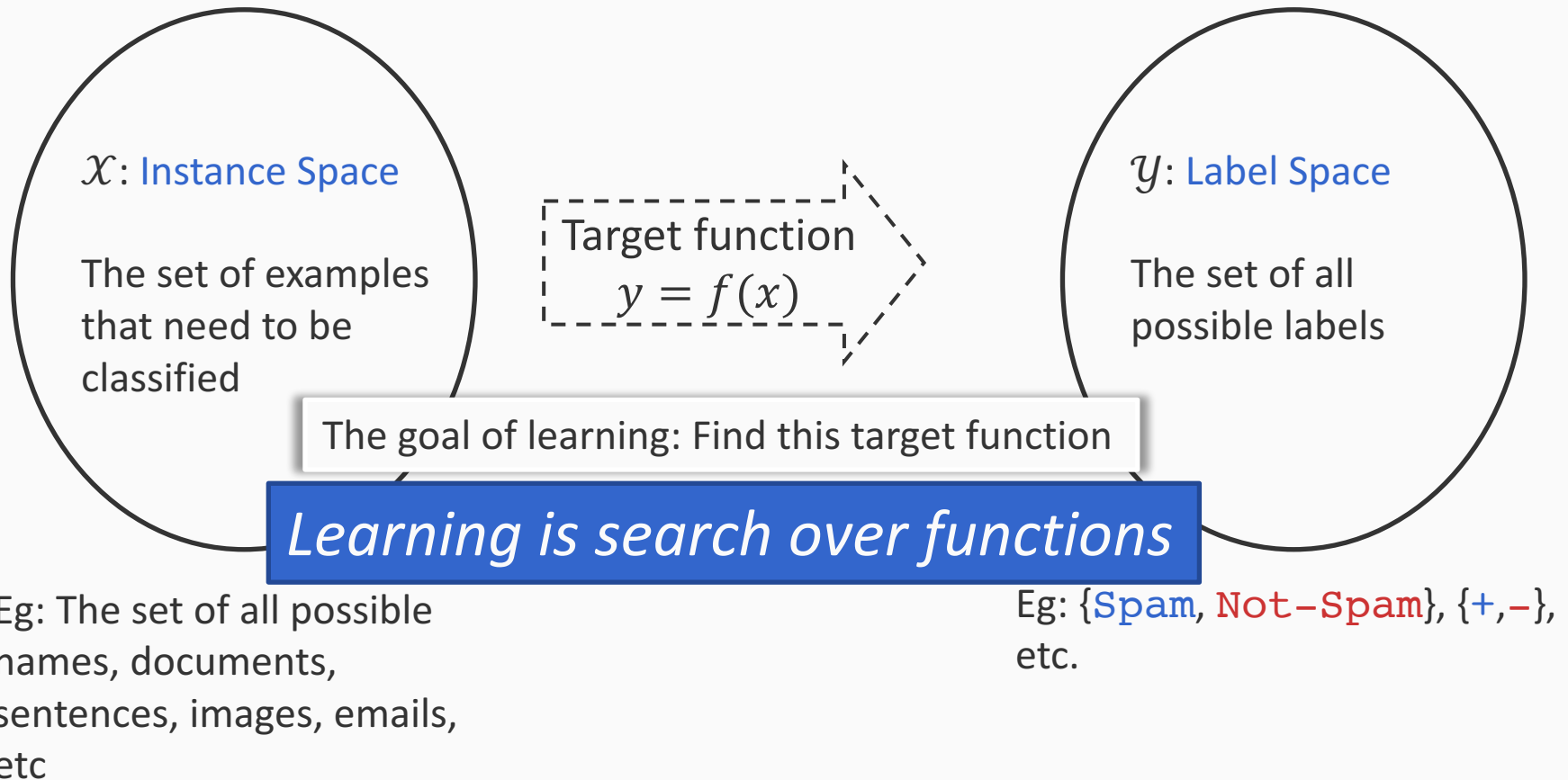
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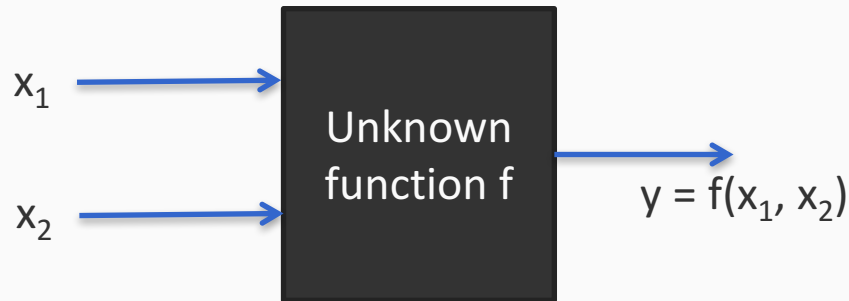
Eg: The set of all possible names, documents, sentences, images, emails, etc

Eg: {Spam, Not-Spam}, {+, -}, etc.

3. The Hypothesis Space



Example of search over functions



| x_1 | x_2 | $y = f(x_1, x_2)$ |
|-------|-------|-------------------|
| 0 | 0 | 0 |
| 0 | 1 | 0 |
| 1 | 0 | 0 |
| 1 | 1 | 1 |

Can you learn this function?

What is it?

Assume that 1 stands for True
0 stands for False

The fundamental problem

Machine learning is ill-posed!



Can you learn this function?

What is it?

| x_1 | x_2 | x_3 | x_4 | 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 |

Is learning possible at all?

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^{16} 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 | |
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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 | 1 | ? |
| 0 | 0 | 1 | 0 | 0 ← |
| 0 | 0 | 1 | 1 | 1 ← |
| 0 | 1 | 0 | 0 | 0 ← |
| 0 | 1 | 0 | 1 | 0 ← |
| 0 | 1 | 1 | 0 | 0 ← |
| 0 | 1 | 1 | 1 | ? |
| 1 | 0 | 0 | 0 | ? |
| 1 | 0 | 0 | 1 | 1 ← |
| 1 | 0 | 1 | 0 | ? |
| 1 | 0 | 1 | 1 | ? |
| 1 | 1 | 0 | 0 | 0 ← |
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We have seen only 7 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

| 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 ← |
| 0 | 1 | 0 | 0 | 0 ← |
| 0 | 1 | 0 | 1 | 0 ← |
| 0 | 1 | 1 | 0 | 0 ← |
| 0 | 1 | 1 | 1 | ? |
| 1 | 0 | 0 | 0 | ? |
| 1 | 0 | 0 | 1 | 1 ← |
| 1 | 0 | 1 | 0 | ? |
| 1 | 0 | 1 | 1 | ? |
| 1 | 1 | 0 | 0 | 0 ← |
| 1 | 1 | 0 | 1 | ? |
| 1 | 1 | 1 | 0 | ? |
| 1 | 1 | 1 | 1 | ? |

Is learning possible at all?

- 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^{16} functions.

| 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 ← |
| 0 | 1 | 0 | 0 | 0 ← |
| 0 | 1 | 0 | 1 | 0 ← |
| 0 | 1 | 1 | 0 | 0 ← |
| 0 | 1 | 1 | 1 | 0 ← |
| 1 | 0 | 0 | 0 | ? |
| 1 | 0 | 0 | 1 | 1 ← |
| 1 | 0 | 1 | 0 | ? |
| 1 | 0 | 1 | 1 | ? |
| 1 | 1 | 0 | 0 | 0 ← |
| 1 | 1 | 0 | 1 | ? |
| 1 | 1 | 1 | 0 | ? |
| 1 | 1 | 1 | 1 | ? |

How could we possibly learn anything?

- We have seen only 7 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** all possible 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 | x_3 | x_4 | 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 |

Example

Hypothesis space 1

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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

Always False

x_1

x_2

x_3

x_4

$x_1 \wedge x_2$

$x_1 \wedge x_3$

$x_1 \wedge x_4$

Rule

$x_2 \wedge x_3$

$x_2 \wedge x_4$

$x_3 \wedge x_4$

$x_1 \wedge x_2 \wedge x_3$

$x_1 \wedge x_2 \wedge x_4$

$x_1 \wedge x_3 \wedge x_4$

$x_2 \wedge x_3 \wedge x_4$

$x_1 \wedge x_2 \wedge x_3 \wedge x_4$

Example

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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 |

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Rule

$x_2 \wedge x_3$

$x_1 \wedge x_2$

$x_1 \wedge x_2 \wedge x_3$

$x_1 \wedge x_2 \wedge x_4$

$x_1 \wedge x_3 \wedge x_4$

$x_2 \wedge x_3 \wedge x_4$

$x_1 \wedge x_2 \wedge x_3 \wedge x_4$

Exercise: How many simple conjunctions are possible when there are n inputs instead of 4?

Example

Hypothesis space 1

Simple conjunctions

Is there a *consistent* hypothesis in this space?

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

| x_1 | x_2 | x_3 | x_4 | 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

x_1

x_2

x_3

x_4

$x_1 \wedge x_2$

$x_1 \wedge x_3$

$x_1 \wedge x_4$

Rule

$x_2 \wedge x_3$

$x_2 \wedge x_4$

$x_3 \wedge x_4$

$x_1 \wedge x_2 \wedge x_3$

$x_1 \wedge x_2 \wedge x_4$

$x_1 \wedge x_3 \wedge x_4$

$x_2 \wedge x_3 \wedge x_4$

$x_1 \wedge x_2 \wedge x_3 \wedge x_4$

Example

Hypothesis space 1

Simple conjunctions

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

| x_1 | x_2 | x_3 | x_4 | 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 |
| x_2 | 0100 | $x_3 \wedge x_4$ | 1001 |
| x_3 | 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

Hypothesis space 1

Simple conjunctions

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

| x_1 | x_2 | x_3 | x_4 | 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 |
| <p>No simple conjunction explains the data! (Confirm each counterexample by going through the list afterwards)</p> <p>Our hypothesis space is too small and the true function we were looking for is not in it. ☹️</p> | | | |
| 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 |

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 - ...
- How do we pick a hypothesis space?
 - Using some prior knowledge (or by guessing)

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 - *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)
- 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 $\{x_1, x_3, x_4\}$ are 1, then the output is 1.

Otherwise, the output is 0.

Is there a consistent hypothesis in this space?

| x_1 | x_2 | x_3 | x_4 | 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 |

Exercise: Check if there is one

First, how many m-of-n rules are there for four variables?

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

Much of the rest
of this semester