

CIS 519/419

Applied Machine Learning

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Slides were created by Dan Roth (for CIS519/419 at Penn or CS446 at UIUC), Eric Eaton for CIS519/419 at Penn, or from other authors who have made their ML slides available.

CIS419/519 Spring '18

Course Overview

- Introduction: Basic problems and questions
- A detailed example: Linear classifiers; key algorithmic idea
- Two Basic Paradigms:
 - Discriminative Learning & Generative/Probabilistic Learning
- Learning Protocols:
 - Supervised; Unsupervised; Semi-supervised
- Algorithms
 - Gradient Descent
 - Decision Trees
 - Linear Representations: (Perceptron; SVMs; Kernels)
 - Neural Networks/Deep Learning
 - Probabilistic Representations (naïve Bayes)
 - Unsupervised /Semi supervised: EM
 - Clustering; Dimensionality Reduction
- Modeling; Evaluation; Real world challenges
- Ethics

CIS519 on the web

- Check our class website:
 - Schedule, slides, videos, policies
 - <http://www.seas.upenn.edu/~cis519/spring2018/>
 - Sign up, participate in our Piazza forum:
 - Announcements and discussions
 - <http://piazza.com/upenn/spring2018/cis419519>
 - Check out our team
 - Office hours
 - Canvas:
 - Notes, homework and videos will be open.
 - [Optional] Discussion Sessions:
 - Starting this Wednesday, 5:30PM: Python Tutorial
 - Active Learning Class, 3401 Wing B/C
- Scribing the Class [Good writers; Latex]?



What is Learning

- The Badges Game.....
 - This is an example of the key learning protocol: supervised learning
- First question: Are you sure you got it?
 - Why?

Training data

- + Naoki Abe
- Myriam Abramson
- + David W. Aha
- + Kamal M. Ali
- Eric Allender
- + Dana Angluin
- Chidanand Apte
- + Minoru Asada
- + Lars Asker
- + Javed Aslam
- + Jose L. Balcazar
- Cristina Baroglio
- + Peter Bartlett
- Eric Baum
- + Welton Becket
- Shai Ben-David
- + George Berg
- + Neil Berkman
- + Malini Bhandaru
- + Bir Bhanu
- + Reinhard Blasig
- Avrim Blum
- Anselm Blumer
- + Justin Boyan
- + Carla E. Brodley
- + Nader Bshouty
- Wray Buntine
- Andrey Burago
- + Tom Bylander
- + Bill Byrne
- Claire Cardie
- + John Case
- + Jason Catlett
- Philip Chan
- Zhixiang Chen
- Chris Darken

The Badges game

-  
- Conference attendees to the 1994 Machine Learning conference were given **name badges labeled with + or -**.
- What function was used to assign these labels?

Raw test data

Shivani Agarwal
Gerald F. DeJong
Chris Drummond
Yolanda Gil
Attilio Giordana
Jiarong Hong

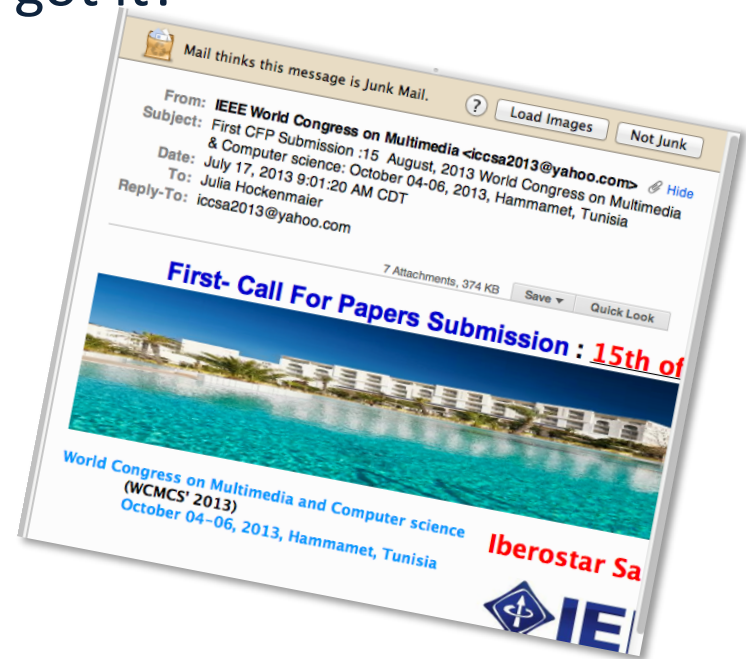
J. R. Quinlan
Priscilla Rasmussen
Dan Roth
Yoram Singer
Lyle H. Ungar

Labeled test data

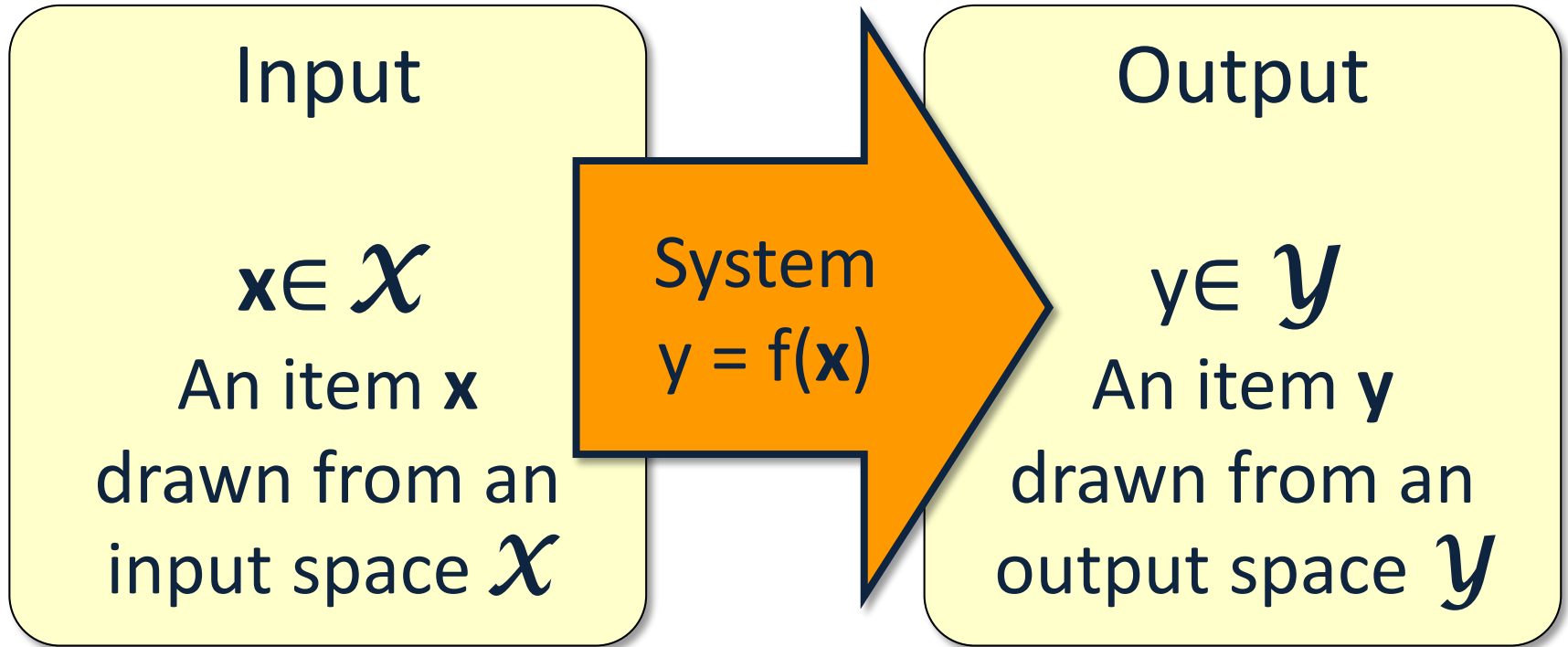
- ? Shivani Agarwal
- + Gerald F. DeJong
- Chris Drummond
- + Yolanda Gil
- Attilio Giordana
- + Jiarong Hong
- J. R. Quinlan
- Priscilla Rasmussen
- + Dan Roth
- + Yoram Singer
- Lyle H. Ungar

What is Learning

- The Badges Game.....
 - This is an example of the key learning protocol: supervised learning
- First question: Are you sure you got it?
 - Why?
- Issues:
 - Which problem was easier?
 - Prediction or Modeling?
 - Representation
 - Problem setting
 - Background Knowledge
 - When did learning take place?
 - **Algorithm:** can you write a program that takes this data as input and predicts the label for your name?

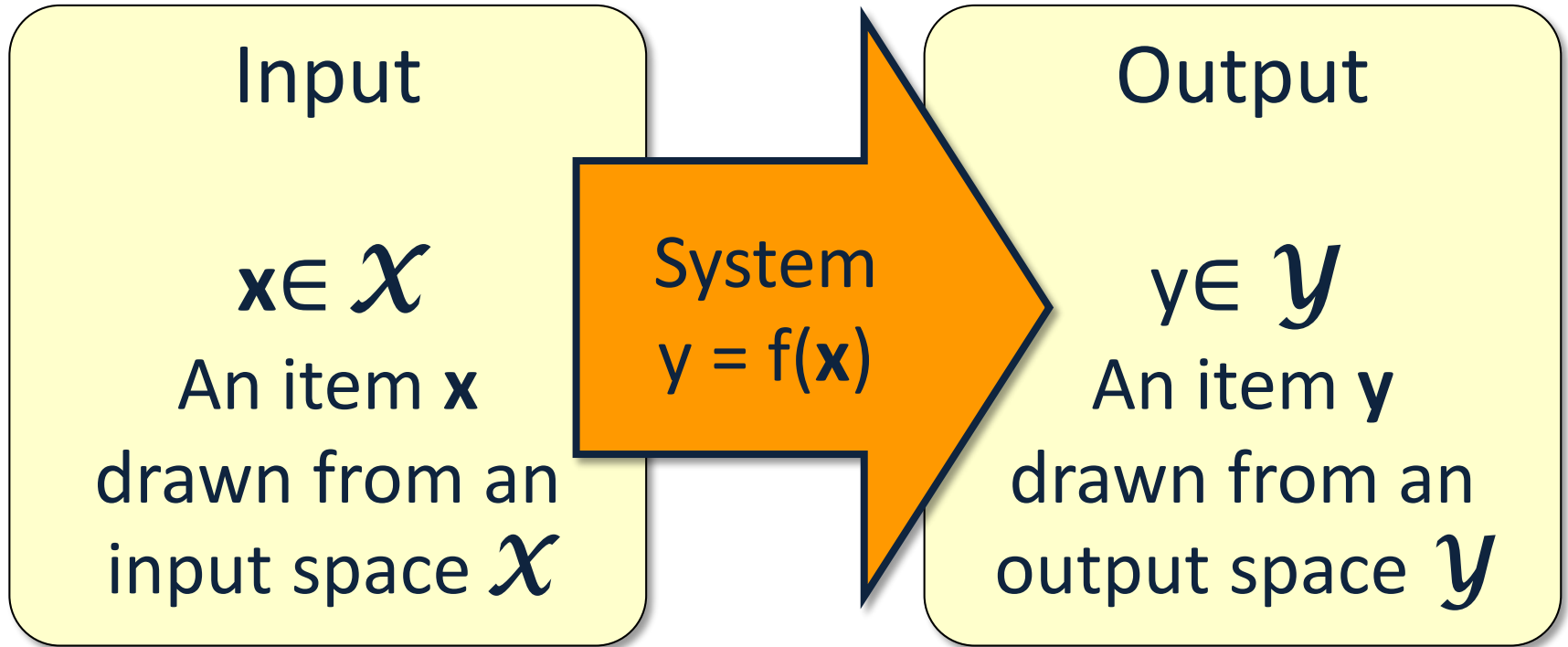


Supervised Learning



- We consider systems that apply a function $f()$ to input items \mathbf{x} and return an output $\mathbf{y} = f(\mathbf{x})$.

Supervised Learning

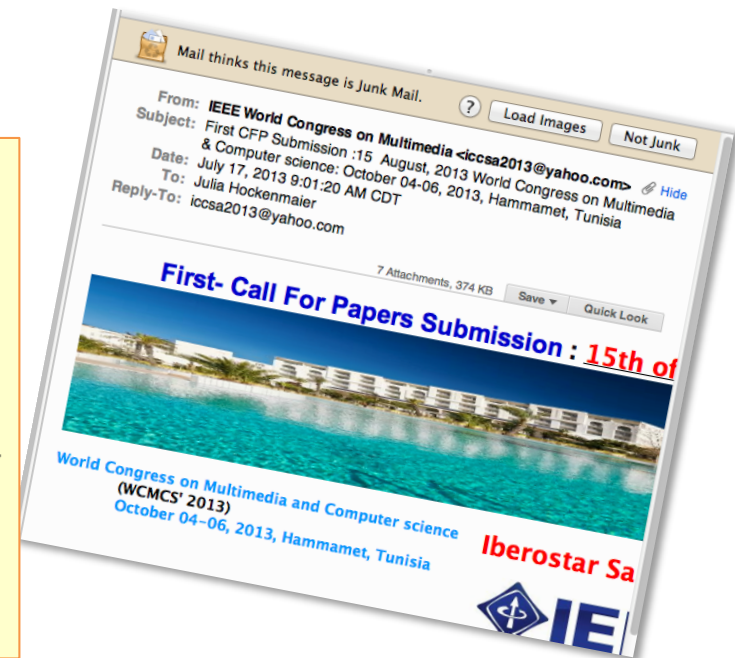


- In (supervised) machine learning, we deal with systems whose $f(x)$ is learned from examples.

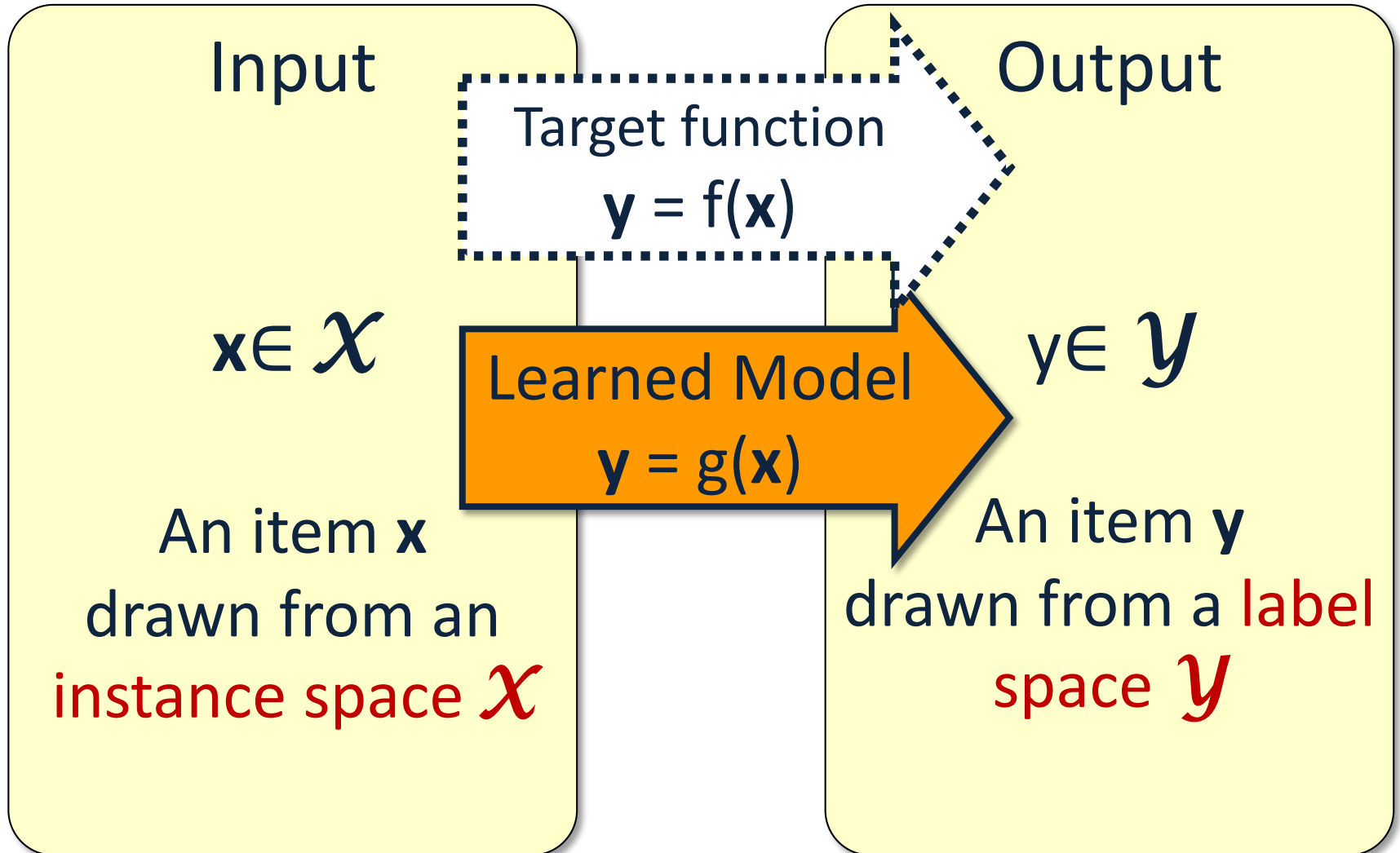
Why use learning?

- We typically use machine learning when the function $f(x)$ we want the system to apply is unknown to us, and we cannot “think” about it. The function could actually be simple.

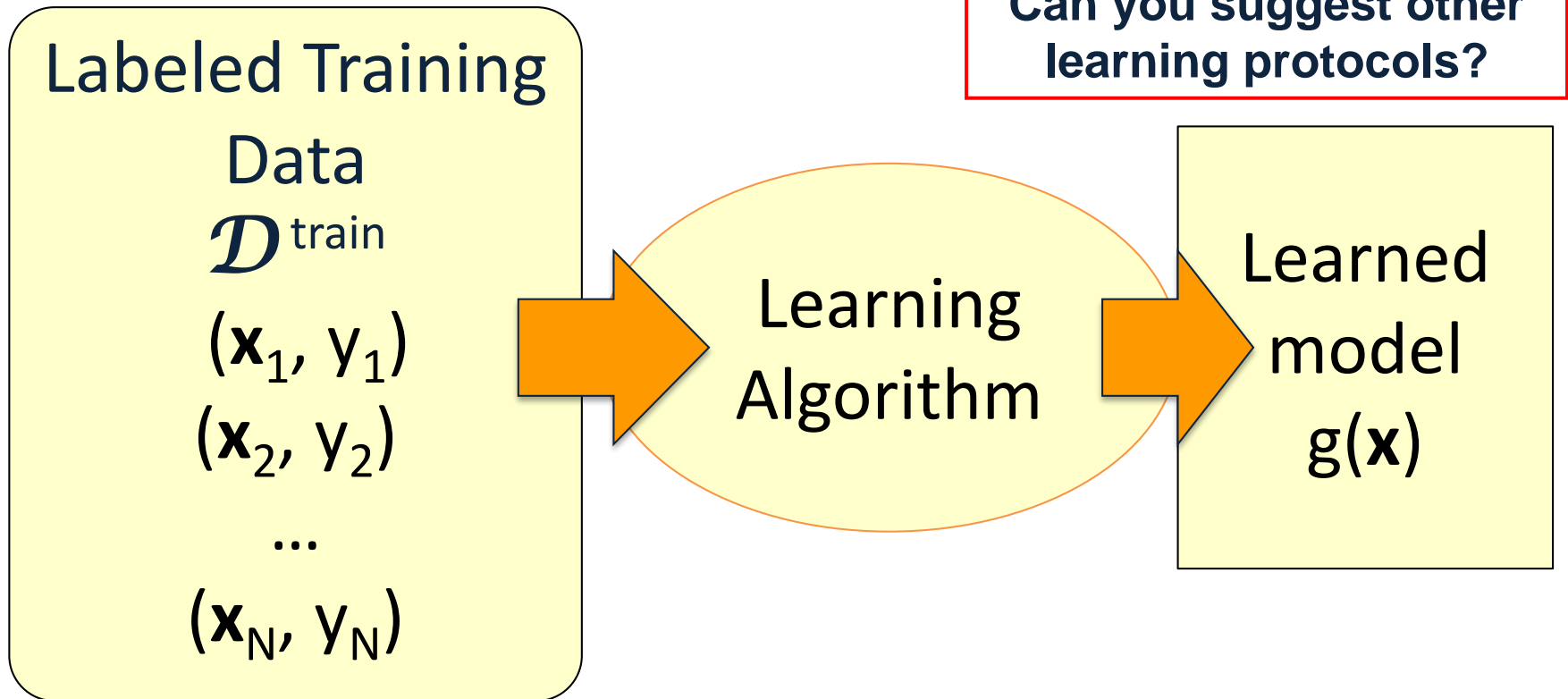
(ENGLAND, June, 1989) - Christopher Robin is alive and well. He lives in England. He is the same person that you read about in the book, Winnie the Pooh. As a boy, Chris lived in a pretty home called Cotchfield Farm. When Chris was three years old, his father wrote a poem about him. The poem was printed in a magazine for others to read. Mr. Robin then wrote a book. He made up a fairy tale land where Chris lived. His friends were animals. There was a bear called Winnie the Pooh. There was also an owl and a young pig, called a piglet. All the animals were stuffed toys that Chris owned. Mr. Robin made them come to life with his words. The places in the story were all near Cotchfield Farm. Winnie the Pooh was written in 1925. Children still love to read about Christopher Robin and his animal friends. Most people don't know he is a real person who is grown now. He has written two books of his own. They tell what it is like to be famous.



Supervised learning



Supervised learning: Training



- Give the learner examples in $\mathcal{D}^{\text{train}}$
- The learner returns a model $g(\mathbf{x})$

$g(\mathbf{x})$ is the model we'll use in our application

Supervised learning: Testing

Labeled
Test Data

$\mathcal{D}^{\text{test}}$

(\mathbf{x}'_1, y'_1)

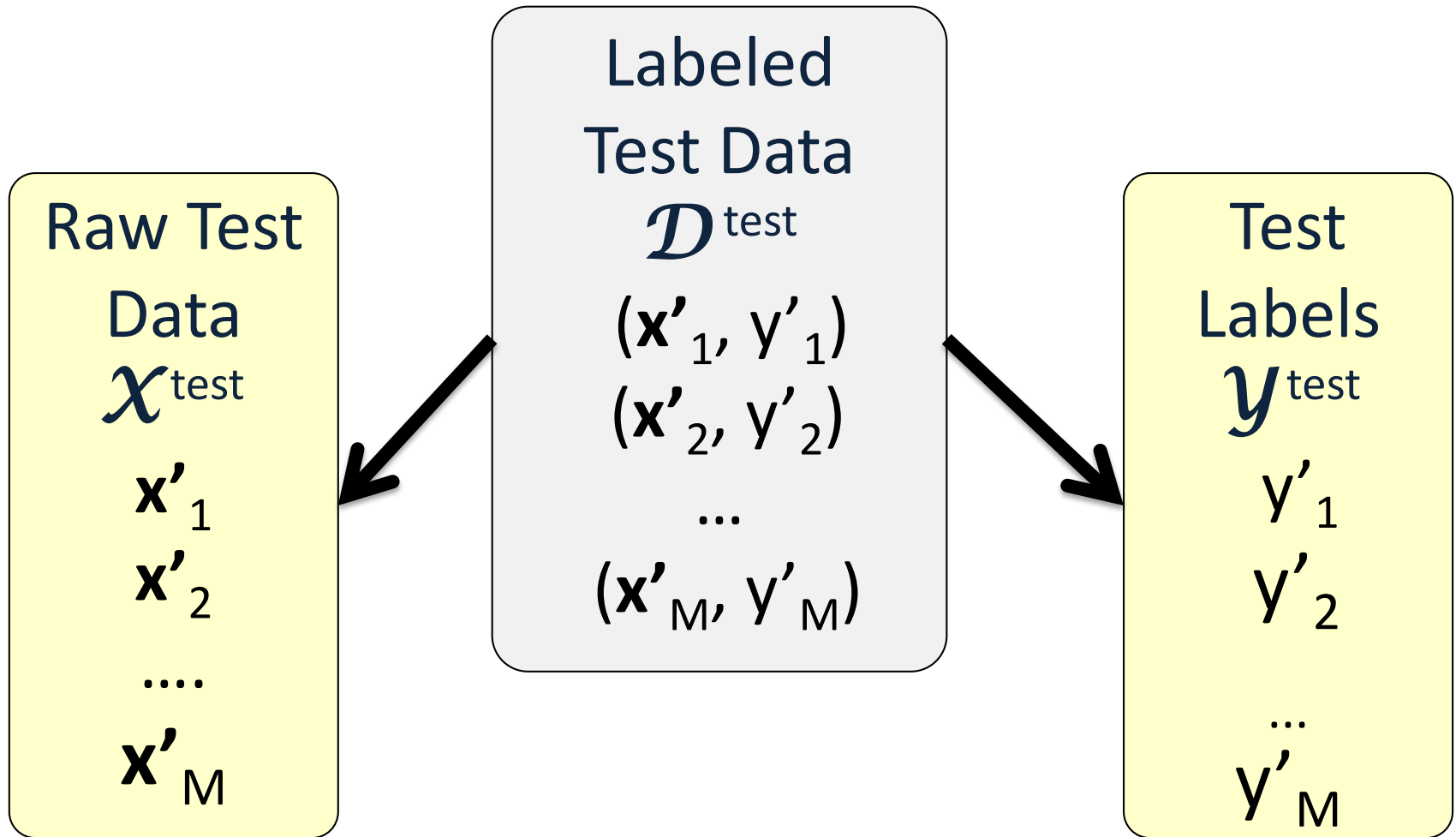
(\mathbf{x}'_2, y'_2)

...

(\mathbf{x}'_M, y'_M)

- Reserve some labeled data for testing

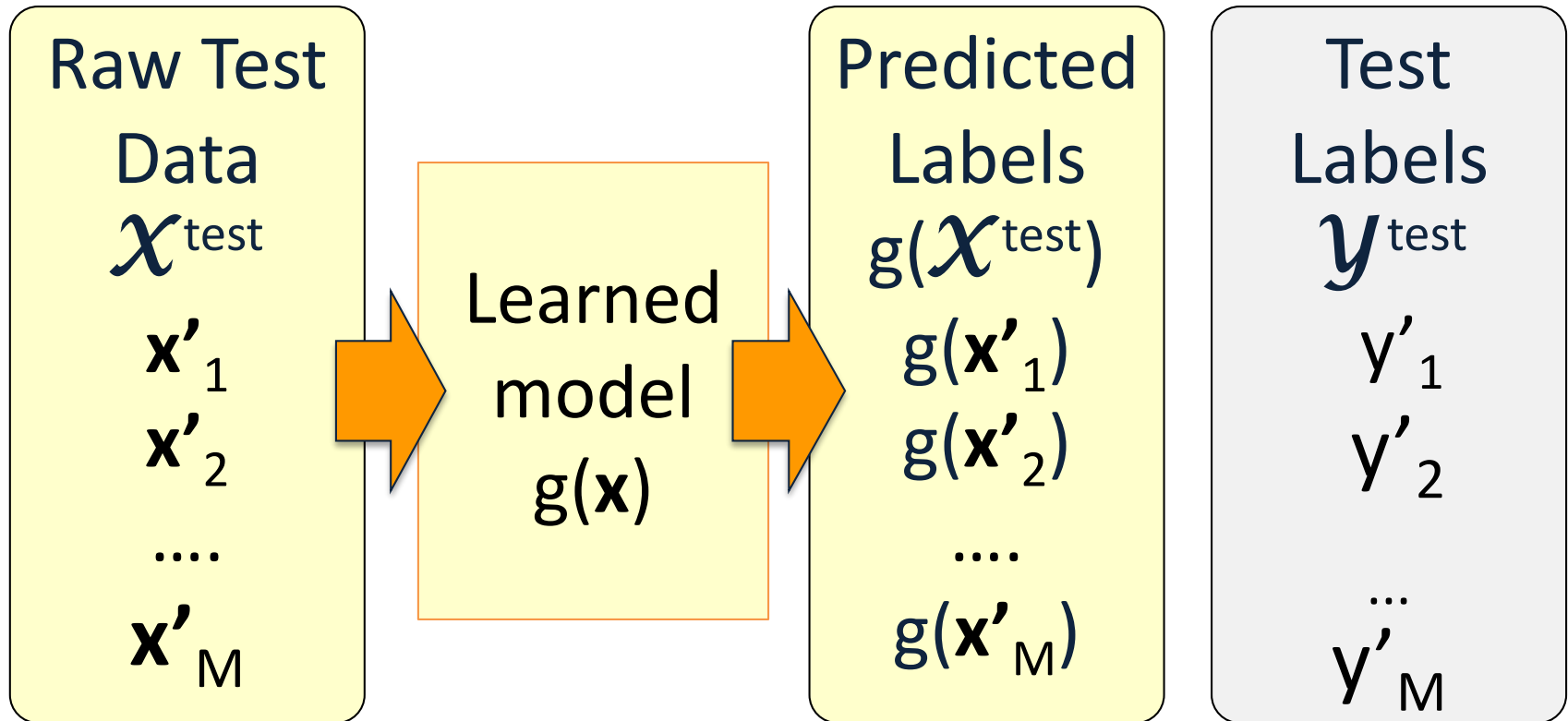
Supervised learning: Testing



Supervised learning: Testing

- Apply the model to the raw test data
- Evaluate by comparing predicted labels against the test labels

Can you **use** the test data otherwise?



Supervised Learning : Examples

- Disease diagnosis
 - x : Properties of patient (symptoms, lab tests)
 - f : Disease (or maybe: recommended therapy)
- Part-of-Speech tagging
 - x : An English sentence (e.g., The can will rust)
 - f : The part of speech of a word in the sentence
- Face recognition
 - x : Bitmap picture of person's face
 - f : Name the person (or maybe: a property of)
- Automatic Steering
 - x : Bitmap picture of road surface in front of car
 - f : Degrees to turn the steering wheel

Many problems that do not seem like classification problems can be decomposed to classification problems.

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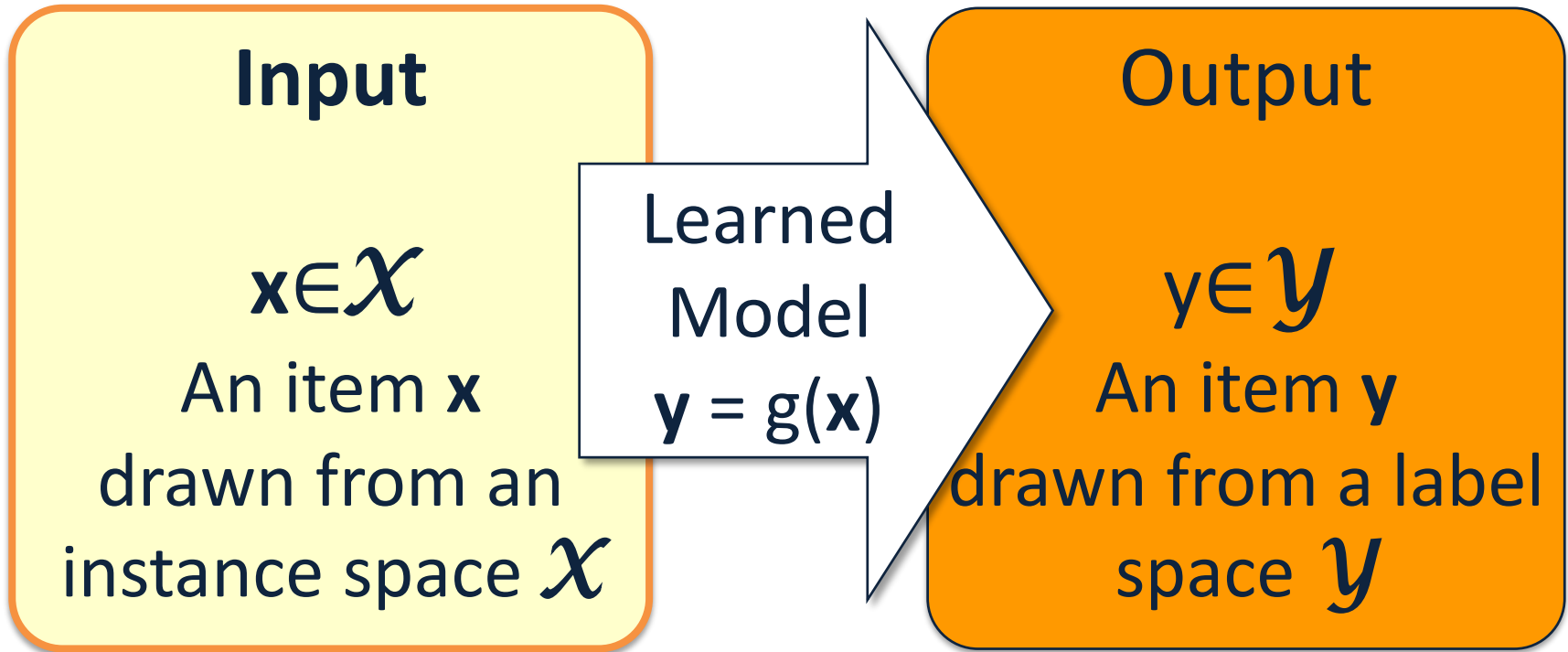
Key Issues in Machine Learning

- Modeling
 - How to formulate application problems as machine learning problems ? How to represent the data?
 - Learning Protocols (where is the data & labels coming from?)
- Representation
 - What functions should we learn (hypothesis spaces) ?
 - How to map raw input to an instance space?
 - Any rigorous way to find these? Any general approach?
- Algorithms
 - What are good algorithms?
 - How do we define success?
 - Generalization Vs. over fitting
 - The computational problem

Using supervised learning

- What is our instance space?
 - Gloss: What kind of features are we using?
- What is our label space?
 - Gloss: What kind of learning task are we dealing with?
- What is our hypothesis space?
 - Gloss: What kind of functions (models) are we learning?
- What learning algorithm do we use?
 - Gloss: How do we learn the model from the labeled data?
- What is our loss function/evaluation metric?
 - Gloss: How do we measure success? What drives learning?

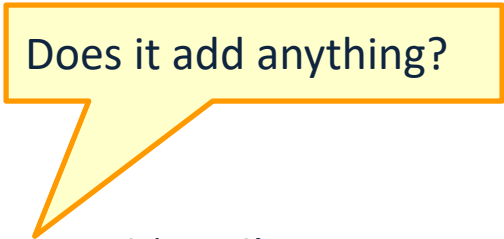
1. The instance space \mathcal{X}



- Designing an appropriate instance space \mathcal{X} is crucial for how well we can predict y .

1. The instance space \mathcal{X}

- When we apply machine learning to a task, we first need to define the instance space \mathcal{X} .
- Instances $x \in \mathcal{X}$ are defined by features:
 - Boolean features:
 - Does this email contain the word 'money'?
 - Does this email contains the word 'money' and the word 'send'?
 - Numerical features:
 - How often does 'money' occur in this email?
 - What is the width/height of this bounding box?
 - What is the length of the first name?



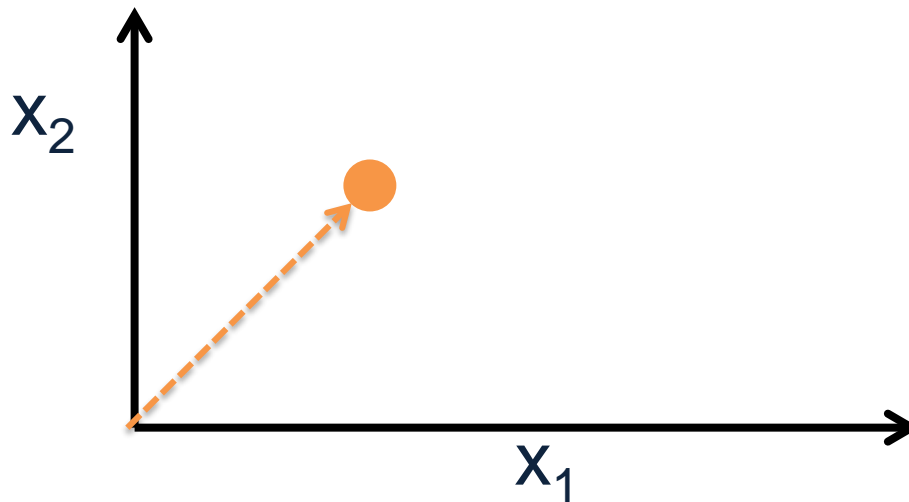
Does it add anything?

What's X for the Badges game?

- Possible features:
 - Gender/age/country of the person?
 - Length of their first or last name?
 - Does the name contain letter 'x'?
 - How many vowels does their name contain?
 - Is the n-th letter a vowel?
 - Height;
 - Shoe size

\mathcal{X} as a vector space

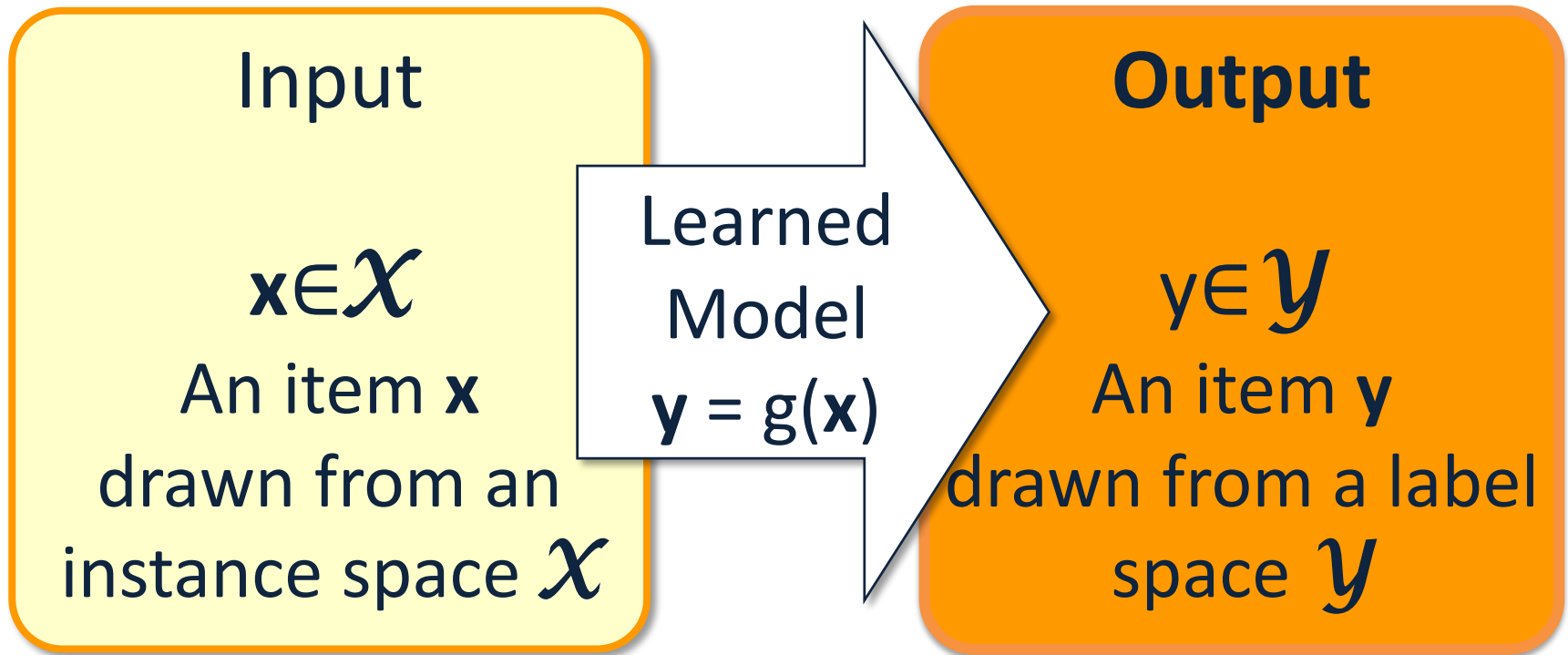
- \mathcal{X} is an N-dimensional vector space (e.g. \mathbb{R}^N)
 - Each dimension = one feature.
- Each \mathbf{x} is a **feature vector** (hence the boldface \mathbf{x}).
- Think of $\mathbf{x} = [x_1 \dots x_N]$ as a point in \mathcal{X} :



Good features are essential

- The choice of features is crucial for how well a task can be learned.
 - In many application areas (language, vision, etc.), a lot of work goes into designing suitable features.
 - This requires domain expertise.
- Think about the badges game – what if you were focusing on visual features?
- We can't teach you what specific features to use for your task.
 - But we will touch on some general principles

2. The label space \mathcal{Y}



- The label space \mathcal{Y} determines *what kind of supervised learning task* we are dealing with

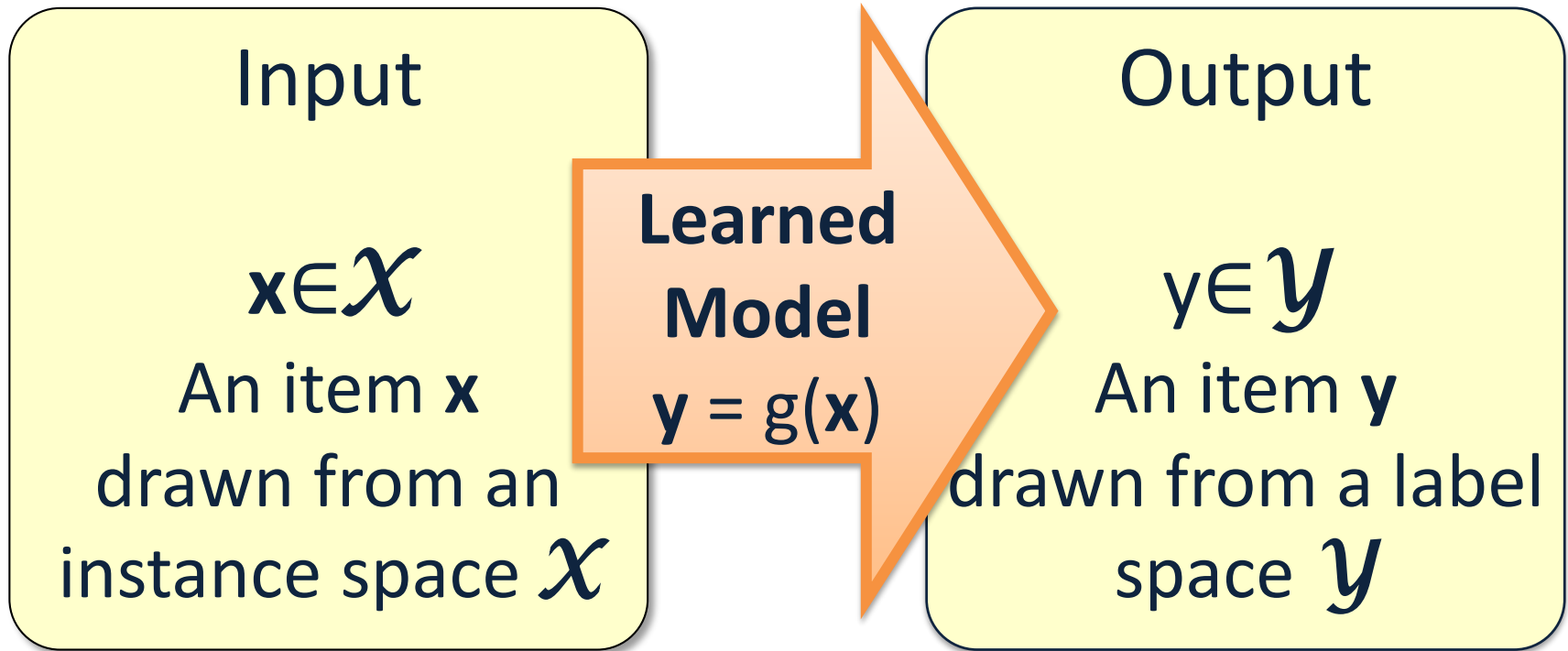
Supervised learning tasks I

- Output labels $y \in Y$ are categorical:
 - Binary classification: Two possible labels
 - Multiclass classification: k possible labels
- Output labels $y \in Y$ are **structured objects** (sequences of labels, parse trees, etc.)
- Structure learning

Supervised learning tasks II

- Output labels $y \in Y$ are numerical:
 - Regression (linear/polynomial):
 - Labels are continuous-valued
 - Learn a linear/polynomial function $f(x)$
 - Ranking:
 - Labels are ordinal
 - Learn an ordering $f(x_1) > f(x_2)$ over input

3. The model $g(\mathbf{x})$



- We need to choose what *kind* of model we want to learn

A Learning Problem



Example	x_1	x_2	x_3	x_4	y
1	0	0	1	0	0
2	0	1	0	0	0
3	0	0	1	1	1
4	1	0	0	1	1
5	0	1	1	0	0
6	1	1	0	0	0
7	0	1	0	1	0

Can you learn this function?
What is it?

Hypothesis Space

Complete Ignorance:

There are $2^{16} = 65536$ possible functions over four input features.

We can't figure out which one is correct until we've seen every possible input-output pair.

After observing seven examples we still have 2^9 possibilities for f

Is Learning Possible?

Example	X1	X2	X3	X4	Y
1	0	0	0	0	?

- There are $|Y|^{|X|}$ possible functions $f(\mathbf{x})$ from the instance space X to the label space Y .
- Learners typically consider **only a subset of the functions from X to Y** , called the hypothesis space H . $H \subseteq |Y|^{|X|}$

	1	0	1	1	?
	1	1	0	0	0
	1	1	0	1	?
	1	1	1	0	?
16	1	1	1	1	?

Hypothesis Space (2)

1	0	0	1	0	0	
2	0	1	0	0		0
3	0	0	1	1		1
4	1	0	0	1		1
5	0	1	1	0		0
6	1	1	0	0		0
7	0	1	0	1		0

Simple Rules: There are only 16 simple **conjunctive rules**
of the form $y = x_i \wedge x_j \wedge x_k$

Rule	Counterexample
------	----------------

$y=c$	
X_1	1100 0
X_2	0100 0
X_3	0110 0
X_4	0101 1
$X_1 \wedge X_2$	1100 0
$X_1 \wedge X_3$	0011 1
$X_1 \wedge X_4$	0011 1

Rule	Counterexample
------	----------------

$X_2 \wedge X_3$	0011 1
$X_2 \wedge X_4$	0011 1
$X_3 \wedge X_4$	1001 1
$X_1 \wedge X_2 \wedge X_3$	0011 1
$X_1 \wedge X_2 \wedge X_4$	0011 1
$X_1 \wedge X_3 \wedge X_4$	0011 1
$X_2 \wedge X_3 \wedge X_4$	0011 1
$X_1 \wedge X_2 \wedge X_3 \wedge X_4$	0011 1

No simple rule explains the data. The same is true for **simple clauses**.

Hypothesis Space (5)

Don't worry, this function is actually a neural network...

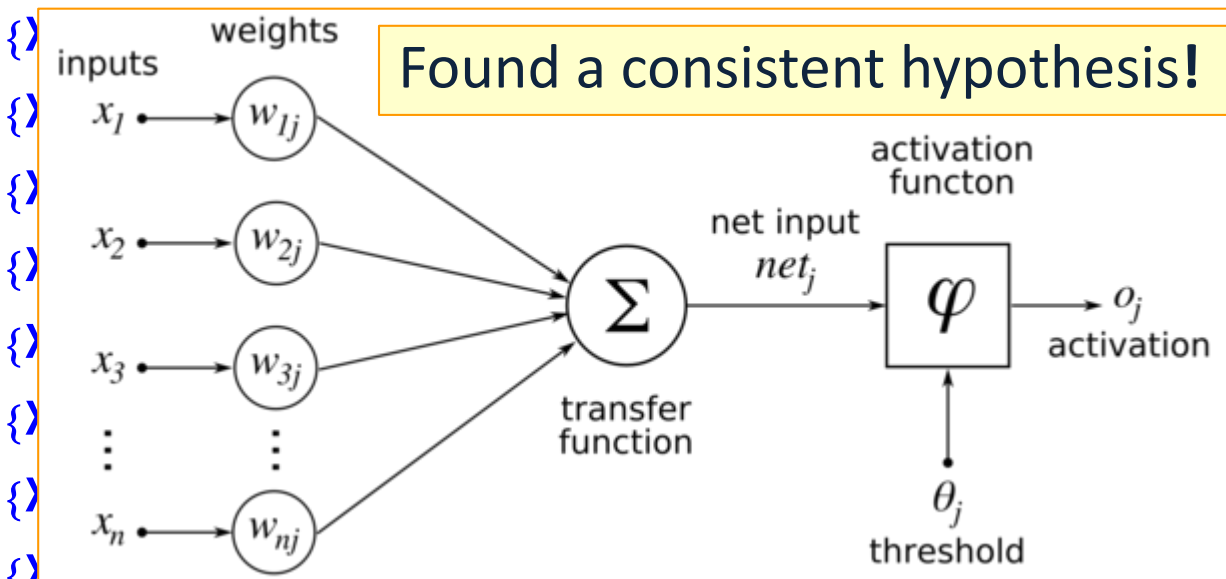
Notation: 2 variables from the set on the left. **Value:** Index of the counterexample.

1	0	0	0	0	0
2	0	1	0	0	0
3	0	0	1	1	1
4	1	0	0	1	1
5	0	1	0	0	0
6	1	0	0	0	0
7	0	1	0	1	0

m-of-n rules: There are 32 possible rules of the form "y = 1 if and only if at least m of the following n variables are 1"

variables 1-of 2-of 3-of 4-of

variables 1-of 2-of 3-of 4-of



2	3	-	-
4	4	-	-
1	3	3	-
2	3	3	-
1	***	3	-
1	5	3	-
1	5	3	3

Views of Learning

- Learning is the removal of our remaining uncertainty:
 - Suppose we knew that the unknown function was an m-of-n Boolean function, then we could use the training data to infer which function it is.
- Learning requires guessing a good hypothesis class:
 - We can start with a very small class and enlarge it until it contains an hypothesis that fits the data.
- We could be wrong !
 - Our prior knowledge might be wrong:
 - $y=x^4 \wedge \text{one-of}(x_1, x_3)$ is also consistent
 - Our guess of the hypothesis space could be wrong
- If this is the unknown function, then we will make errors when we are given new examples, and are asked to predict the value of the function

General strategies for Machine Learning

- Develop flexible hypothesis spaces:
 - Decision trees, neural networks, nested collections.
- Develop representation languages for restricted classes of functions:
 - Serve to limit the expressivity of the target models
 - E.g., Functional representation (n-of-m); Grammars; linear functions; stochastic models;
 - Get flexibility by augmenting the feature space
- In either case:
 - Develop algorithms for finding a hypothesis in our hypothesis space, that fits the data
 - And hope that they will generalize well

Administration

- The class is still full.
- We had a first Python session yesterday.
 - We will continue next week.
- Discussion sessions will be held each week on
 - Tuesday, 6:30
 - Wednesday, 5:30PM: Python
 - Active Learning Class, 3401 Walnut, 401B
 - The next two will still be about Python. We'll move to give other complementary material that is relevant to the class and the HW.
 - Both sessions will be identical
- Anyone wants to go but cannot make any of these?
- Questions?
 - Please ask/comment during class.

Key Issues in Machine Learning

- Modeling
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An Example: Modeling

I don't know {whether, weather} to laugh or cry

This is the Modeling Step

How can we make this a learning problem?

What is the hypothesis space?

- We will look for a function
 $F: \text{Sentences} \rightarrow \{\text{whether, weather}\}$
- We need to define the domain of this function better.
- **An option**: For each word w in English define a Boolean feature x_w :
 $[x_w = 1]$ iff w is in the sentence
- This maps a sentence to a point in $\{0,1\}^{50,000}$
- In this space: some points are whether points
some are weather points

Learning Protocol?

Supervised? Unsupervised?

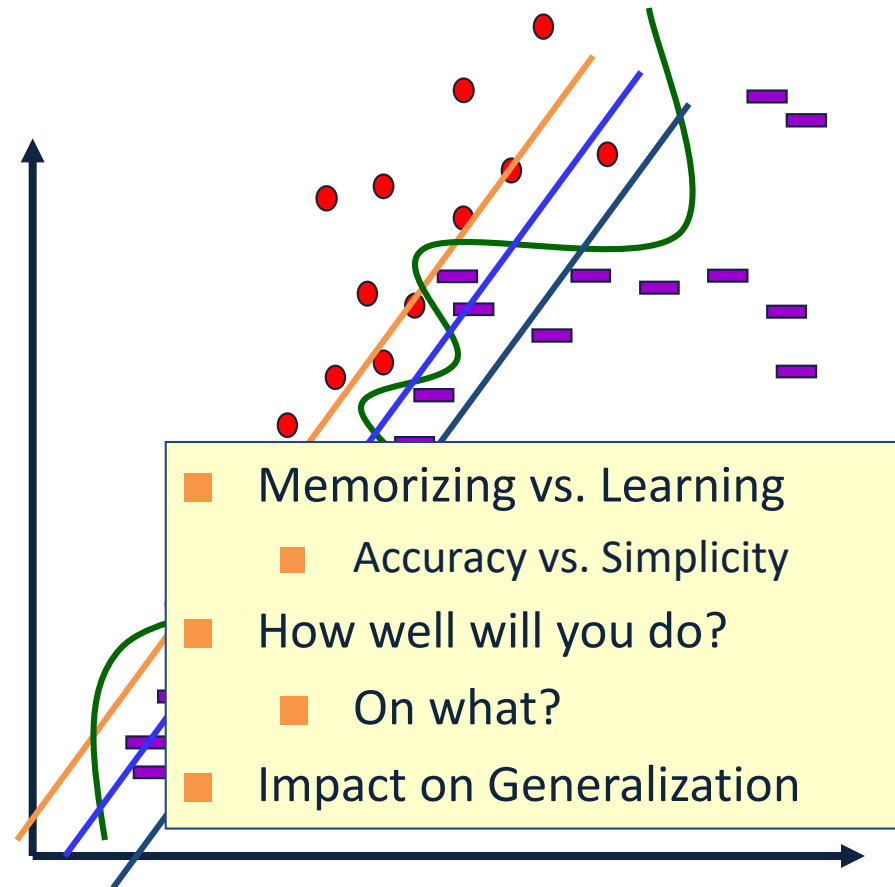
Representation Step: What's Good?

$\text{sgn}(z) = 0$ if $z < 0$;
1 otherwise

$$w^T \cdot x = \sum_{i=1}^n w_i x_i$$

- Learning problem:
Find a function that best separates the data
- What function?
- What's best?
- (How to find it?)

Linear = linear in the feature space
 x = data representation; w = the classifier
(w , x , column vectors of dimensionality n)
 $y = \text{sgn} \{w^T x\}$



- A possibility: Define the learning problem to be:
 - A (linear) function that best separates the data

Expressivity

$$f(x) = \text{sgn} \{w^T \cdot x - \theta\} = \text{sgn} \left\{ \sum_{i=1}^n w_i x_i - \theta \right\}$$

- Many functions are Linear

Probabilistic Classifiers as well

- Conjunctions:

- $y = x_1 \wedge x_3 \wedge x_5$

- $y = \text{sgn}\{1 \cdot x_1 + 1 \cdot x_3 + 1 \cdot x_5 - 3\};$

$$w = (1, 0, 1, 0, 1) \theta=3$$

- At least m of n:

- $y = \text{at least 2 of } \{x_1, x_3, x_5\}$

- $y = \text{sgn}\{1 \cdot x_1 + 1 \cdot x_3 + 1 \cdot x_5 - 2\};$

$$w = (1, 0, 1, 0, 1) \theta=2$$

- Many functions are not

- Xor: $y = (x_1 \wedge x_2) \vee (\neg x_1 \wedge \neg x_2)$

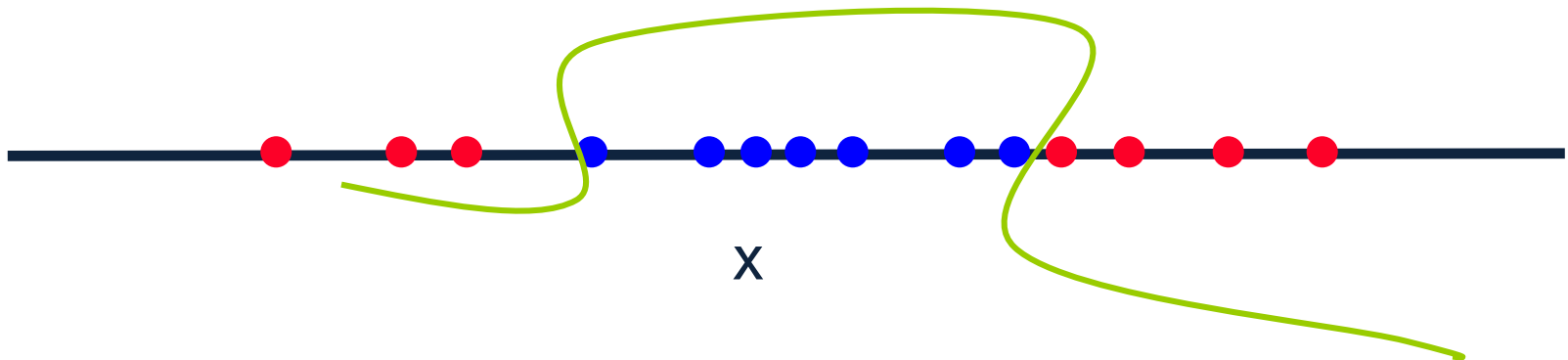
- Non trivial DNF: $y = (x_1 \wedge x_2) \vee (x_3 \wedge x_4)$

- But can be made linear

- Note: all the variables above are Boolean variables

Functions Can be Made Linear

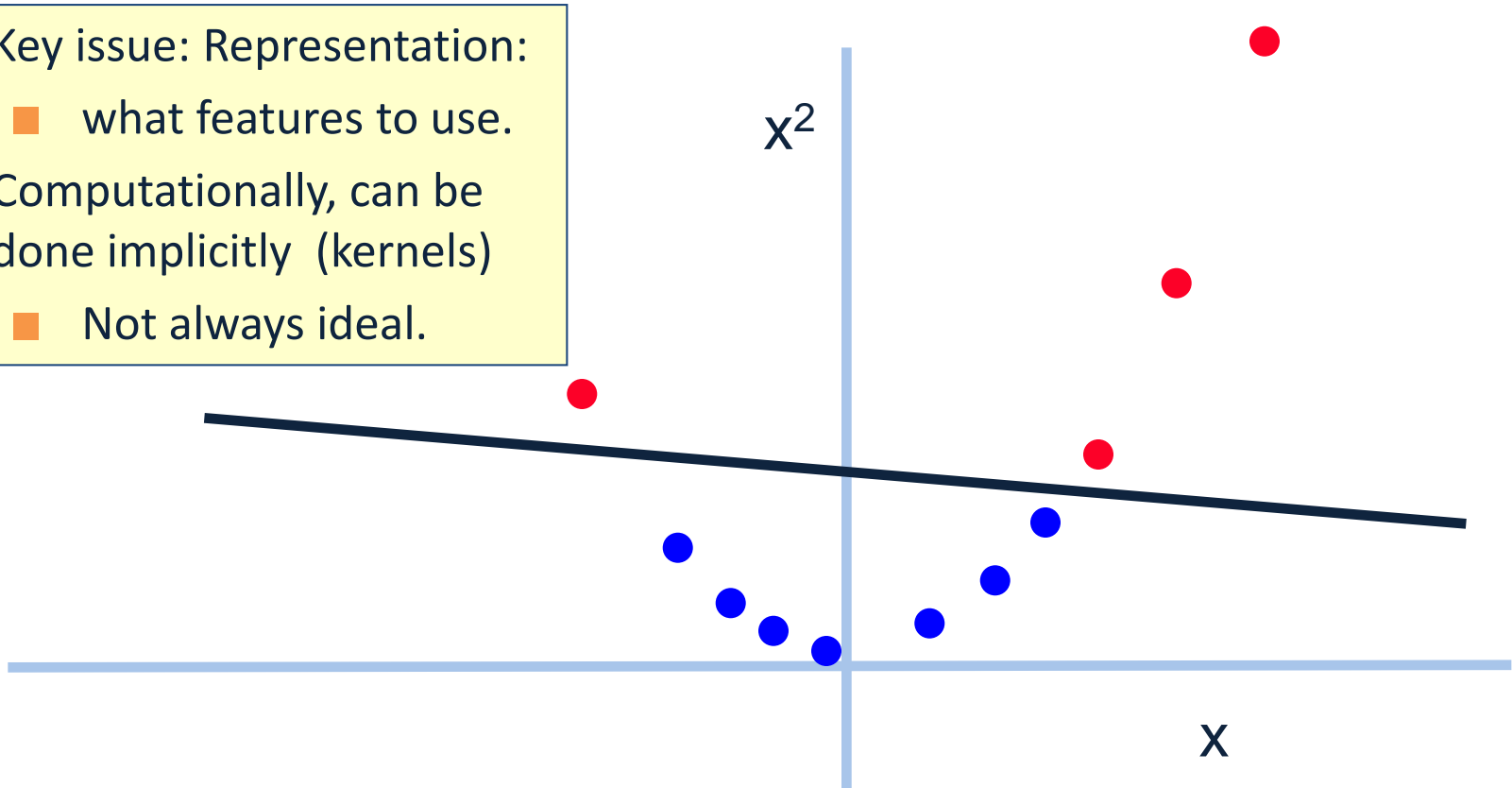
- Data are not linearly separable in one dimension
- Not separable if you insist on using a specific class of functions (e.g., linear)



Blown Up Feature Space

- Data are separable in $\langle x, x^2 \rangle$ space

- Key issue: Representation:
 - what features to use.
- Computationally, can be done implicitly (kernels)
 - Not always ideal.

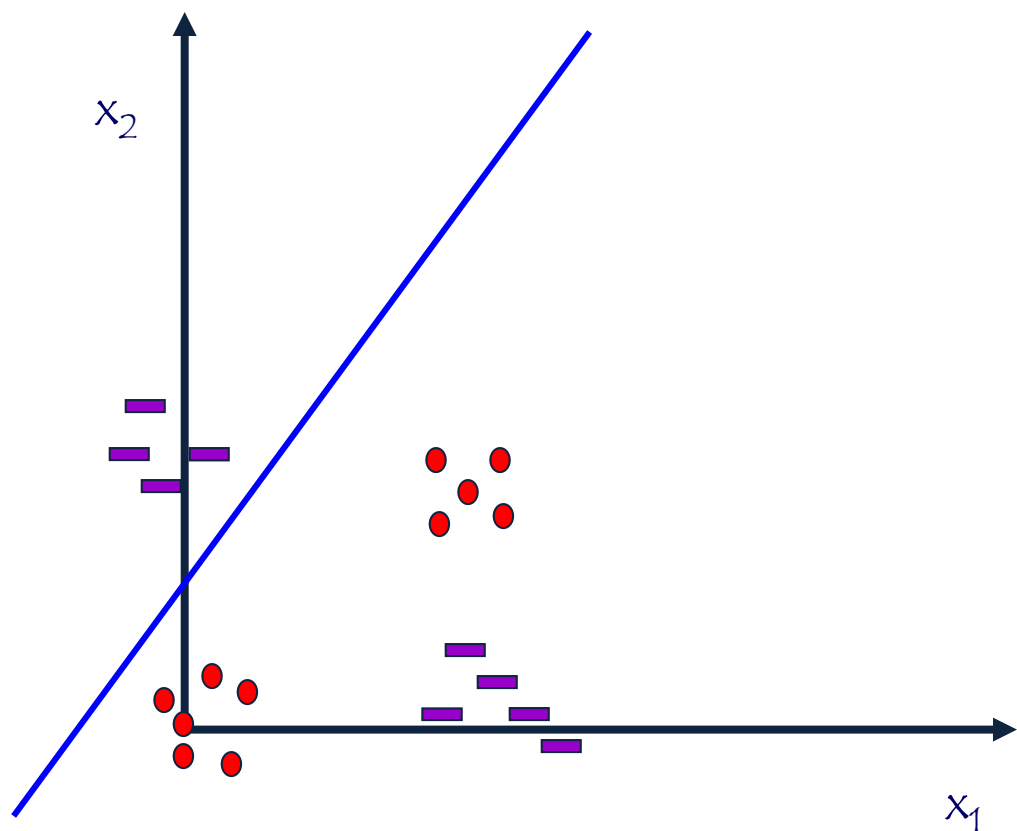


Exclusive-OR (XOR)

- $(x_1 \wedge x_2) \vee (\neg\{x_1\} \wedge \neg\{x_2\})$
- In general: a parity function.

- $x_i \in \{0,1\}$
- $f(x_1, x_2, \dots, x_n) = 1$
iff $\sum x_i$ is even

This function is not
linearly separable.



Functions Can be Made Linear

A real Weather/Whether example

Discrete Case

$x_1 x_2 x_4 \vee x_2 x_4 x_5 \vee x_1 x_3 x_7$

$y_3 \vee y_4 \vee y_7$
New discriminator is functionally simpler

Whether

1. The instance space \mathcal{X}

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 - What is the length of the first name?

Does it add anything?

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New Space: $Y = \{y_1, y_2, \dots\} = \{x_i, x_i x_j, x_i x_j x_k, \dots\}$

Representation (1)

Feature Types:

(what does the algorithm know about the input):

1. relative position (+/-1) has this **pos/w**
2. Conjunctions of size two
3. word **w** occurs in (-2,+2) window around target

Note: 4 feature types; many features

The feature resulting from instantiating the type in the given data

Some statistics (not part of the learning process; just for the understanding of the problem)

```
1p=Det 0.972222 0 34
1w=the 0.961538 0 24
-1p=Punc 1p=Pro 0.96 0 23
-1p=V 1p=Adv 0.96 0 23
or 0.959184 3 93
1p=Adj 0.957447 1 44
not 0.956522 1 43
-1p=V 1p=Pro 0.956522 0 21
1p=Det 2p=Ns 0.954545 0 20
-1p=V 1p=Det 0.954545 0 20
1w=he 0.952381 0 19
-1p=Prep 1p=Pro 0.952381 0 19
-2w=to -1p=V 0.952381 0 19
1p=Pro 2p=Vpp 0.947368 0 17
question 0.947368 0 17
1p=Pro 0.946237 4 87
-1w=, 1p=Pro 0.944444 0 16
-1p=Punc 0.941176 2 47
should 0.941176 0 15
1w=they 0.941176 0 15
-1p=V 1w=the 0.941176 0 15
-1p=Ns 1p=Adj 0.9375 0 14
1p=Pro 2p=Was 0.9375 0 14
1p=Pro 2p=Vpt 0.9375 0 14
-1p=Punc 1p=Adj 0.9375 0 14
-2p=Ns -1p=Punc 0.933333 1 27
1p=Adj 2p=Prep 0.933333 0 13
1p=Ns 2p=Vpp 0.933333 0 13
-1p=Conj 1p=Pro 0.933333 0 13
you 0.933333 0 13
1p=Ns 2p=Was 0.933333 0 13
1w=it 0.933333 0 13
-1p=Punc 1p=Prep 0.933333 0 13
-1w=, 1p=Adj 0.928571 0 12
-1p=Punc 1p=Ns 0.928571 1 25
-1p=V 1p=Adj 0.928571 0 12
1p=Ns 2w=was 0.928571 0 12
```

Representation (2)

Extracting features from the data:

(what does the algorithm know about the input):

1. relative position (+/-1); pos/w
2. Conjunctions of size two

Note: 2 feature types; many features

For each feature type, the data gives rise to multiple features; you don't know which, before you see the data.

But << whether >> the murder of El Benefactor in Ciudad Trujillo means freedom for the people of the Caribbean fiefdom is a question that cannot now be answered .

If Russian pupils have to take these languages , how come American students have a choice << whether >> or not to take a language , but have to face so many exceptions ? ?

The rescue squad is to be praised immensely for the fine work they do in all kinds of << weather >> .

Besides the lack of an adequate ethical dimension to the Governor's case , one can ask seriously << whether >> our lead over the Russians in quality and quantity of nuclear weapons is so slight as to make the tests absolutely necessary .

It is another question << whether >> `` they '' -- or a single general , off in a corner of China , secure for a few (galvanizing ? ?

And little Zeme North , a Dora with real spirit and verve , was fascinating << whether >> she was singing of her love for Floyd , the cop who becomes sewer commissioner and then is promoted into garbage , or just dancing to display her exuberant feelings .

A few drops of rain just before midnight , when Sarah Vaughan was in the midst of her first number , scattered the more timid members of the audience briefly , but at this hour and with Sarah on the stand , most of the listeners didn't care << whether >> they got wet .

Expressed differently : if the price for becoming a faithful follower of Jesus Christ is some form of self-destruction , << whether >> of the body or of the mind -- sacrificium corporis , sacrificium intellectus -- then there is no alternative but that the price remain unpaid .

Thus , if what is at issue is << whether >> `` All S is P '' , it is indifferent whether `` Some S is not P '' or `` No S is P '' , since in either case the judgment in question is false .

Thus , if what is at issue is whether `` All S is P '' , it is indifferent << whether >> `` Some S is not P '' or `` No S is P '' , since in either case the judgment in question is false .

Such efforts almost always find themselves compelled to ask << whether >> Adam was created capable of growing old and then older and then still older , in short , whether Adam's life was intended to be part of the process of time .

Such efforts almost always find themselves compelled to ask whether Adam was created capable of growing old and then older and then still older , in short , << whether >> Adam's life was intended to be part of the process of time .

It is idle to ask why we are no longer disturbed if somebody , professing the deepest piety , decides anew that it is of no importance << whether >> or not Christ transformed the water into wine at eleven A.M. on the third of August , A.D. 32 .

Representation (3)

Each **example** corresponds to one target occurrence; all the features for this target are collected into a vector, and the label is added.

Here:

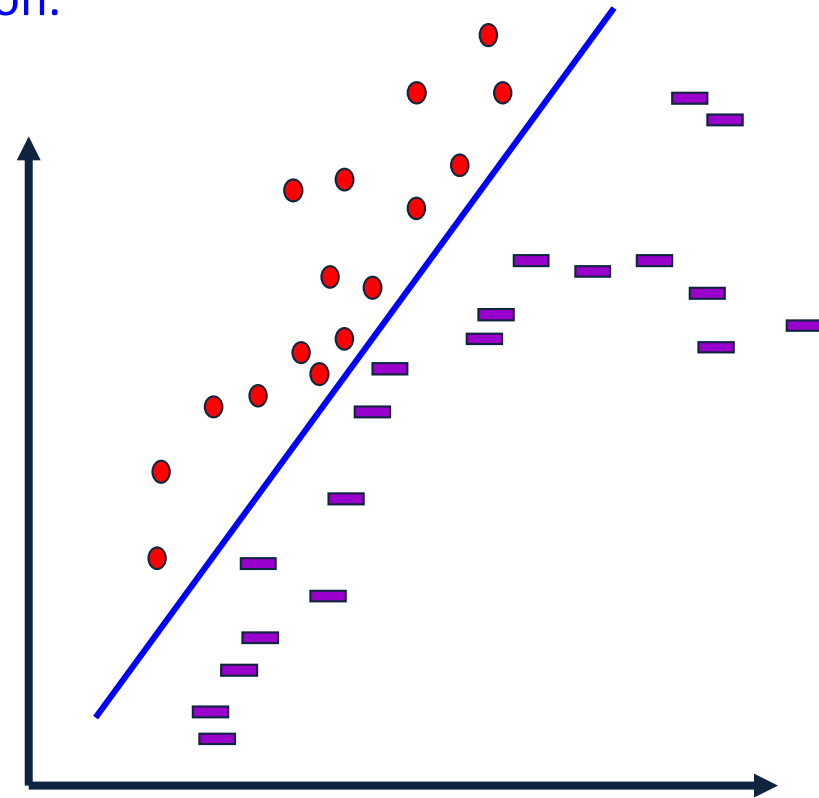
- Sparse Representation of the feature vector. **Why?**
- Variable size: **Why?**

Here the first index (0/1) is the label

1,2,3,11,48,51,82,87,92,105,176,198,199,279,327,413,439,482,498,747,963,964,965,975,1029,1072,1166,1176:
1,6,9,42,43,44,45,47,73,155,157,216,226,238,240,322,441,497,498,757,829,971,978,987,995,1000,1047,1060,1073,1077,1078,1086,1116,1118,1119,1132,1138,1139,1141,1172:
0,57,94,109,112,119,153,305,387,482,759,855,963,964,965,1002,1050,1068,1142,1207,1226:
1,7,52,60,65,141,197,240,469,497,772,963,964,965,989,1045,1067,1072:
1,6,16,57,69,116,137,153,156,201,213,280,302,304,322,325,432,468,497,830,986,987,1058,1143:
1,17,26,32,36,46,119,148,157,239,292,299,322,329,433,474,497,919,963,964,978,1001,1045,1061,1071,1116,1131,1209:
1,8,15,17,20,25,57,103,116,224,370,414,458,497,719,956,963,964,987,1068:
1,6,21,27,29,41,58,67,69,155,238,271,304,460,497,963,964,1027,1111:
1,54,69,78,91,100,110,115,153,156,195,250,283,302,305,325,497,656,753,756,833,957,977,986,1065,1066:
1,6,9,37,69,153,156,302,305,325,443,497,597,729,986,1013,1040,1065,1111,1116:
1,7,12,32,36,39,89,116,152,154,157,222,240,329,827,938,943,963,1045,1188:
1,21,27,41,67,68,98,121,133,162,232,240,329,489,497,886,963,964,965,1045:
1,6,9,42,43,44,45,47,69,155,156,157,216,238,441,497,757,833,954,963,964,966,968,971,987,995,1040,1078,1086,1101,1118,1143,1172:
1,6,7,21,24,27,29,35,38,41,56,58,61,67,87,125,156,157,223,232,238,455,489,497,774,1203:
1,6,8,17,62,99,116,147,156,220,237,240,275,276,284,298,322,326,486,497,499,559,561,961,963,964,970,1039:
1,6,13,17,28,62,90,93,101,103,119,147,158,161,169,194,237,240,275,276,305,322,323,326,482,487,491,497,961,963,970,987,1029,1045:
1,2,3,6,11,21,27,41,48,61,67,87,98,121,125,133,162,204,217,229,256,305,322,329,439,497,517,630,964,965:
1,6,8,14,17,75,89,103,116,119,154,156,157,182,229,296,497,499,536,679,684,700,784,888,927,966,971,976,987,1040,1058,1086,1106,1143,1190:
1,99,116,117,205,212,237,305,322,455,499,601,943,989,999,1068,1071,1091,1127:
0,119,217,440,487,491,497,743,791,847,938,987,1016,1046,1061,1071,1116,1129,1145,1168,1196:
0,305,322,329,482,812,963,964,965,1002,1045,1050,1068,1142,1196,1207:
0,37,49,127,153,172,201,324,354,490,497,498,531,689,908,963,964,965,966,972,987,994,1000,1007,1028,1045,1047,1049,1052,1056,1057,1065,1066,1072,1081,1086,1094,1116,1117,1120,1122,1135,1138,1140,1143,1204:
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1,7,9,57,73,80,157,197,226,237,240,295,356,437,442,484,493,497,893,917,1067,1072,1101,1120:
1,9,57,356,428,453,485,493,497,893,963,964,965,1032,1045,1072,1120:
1,6,7,21,24,29,38,61,69,80,87,157,208,211,238,295,304,364,419,437,442,606,628,739,776,803,963,964,965,1220:

Third Step: How to Learn?

- A possibility: Local search
 - Start with a linear threshold function.
 - ➔ ■ See how well you are doing.
 - Correct
 - Repeat until you converge.
- There are other ways that do not search directly in the hypotheses space
 - Directly compute the hypothesis

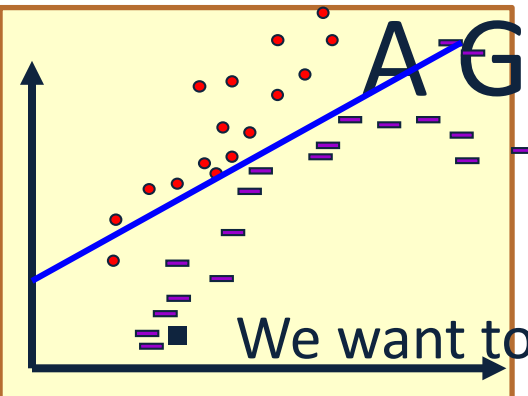


A General Framework for Learning

- Goal: predict an unobserved output value $y \in Y$ based on an observed input vector $x \in X$
- Estimate a functional relationship $y \sim f(x)$ from a set $\{(x, y)_i\}_{i=1, n}$
- Most relevant - **Classification**: $y \in \{0, 1\}$ (or $y \in \{1, 2, \dots, k\}$)
 - (But, within the same framework can also talk about **Regression**, $y \in \mathcal{R}$)
- What do we want $f(x)$ to satisfy?
 - We want to minimize the **Risk**: $L(f()) = E_{x, y}([f(x) \neq y])$
 - Where: $E_{x, y}$ denotes the expectation with respect to the true distribution.

Simple **loss function**: # of mistakes
[...] is a indicator function

A General Framework for Learning (II)



We want to minimize the Loss: $L(f()) = E_{X,Y}([f(X) \neq Y])$

- Where: $E_{X,Y}$ denotes the expectation with respect to the true distribution.

Side note: If the distribution over $X \times Y$ is known, predict: $y = \operatorname{argmax}_y P(y|x)$
This is the best possible (the optimal Bayes' error).

- We cannot minimize this loss
- Instead, we try to minimize the **empirical** classification error.
- For a set of training examples $\{(x_i, y_i)\}_{i=1,m}$
- Try to minimize: $L'(f()) = 1/m \sum_i [f(x_i) \neq y_i]$ (m=# of examples)
 - (Issue I: why/when is this good enough? Not now)
- This minimization problem is typically NP hard.
- To alleviate this computational problem, minimize a new function – a convex upper bound of the classification error function

$$I(f(x), y) = [f(x) \neq y] = \{1 \text{ when } f(x) \neq y; 0 \text{ otherwise}\}$$

Algorithmic View of Learning: an Optimization Problem

- A **Loss Function** $L(f(x), y)$ measures the penalty incurred by a classifier f on example (x, y) .
- There are many different loss functions one could define:
 - Misclassification Error:

$$L(f(x), y) = 0 \text{ if } f(x) = y; \quad 1 \text{ otherwise}$$

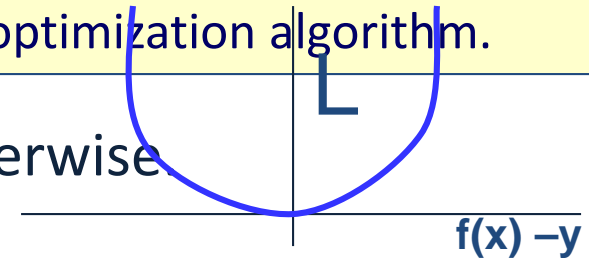
- Squared Loss:

$$L(f(x), y) = (f(x) - y)^2$$

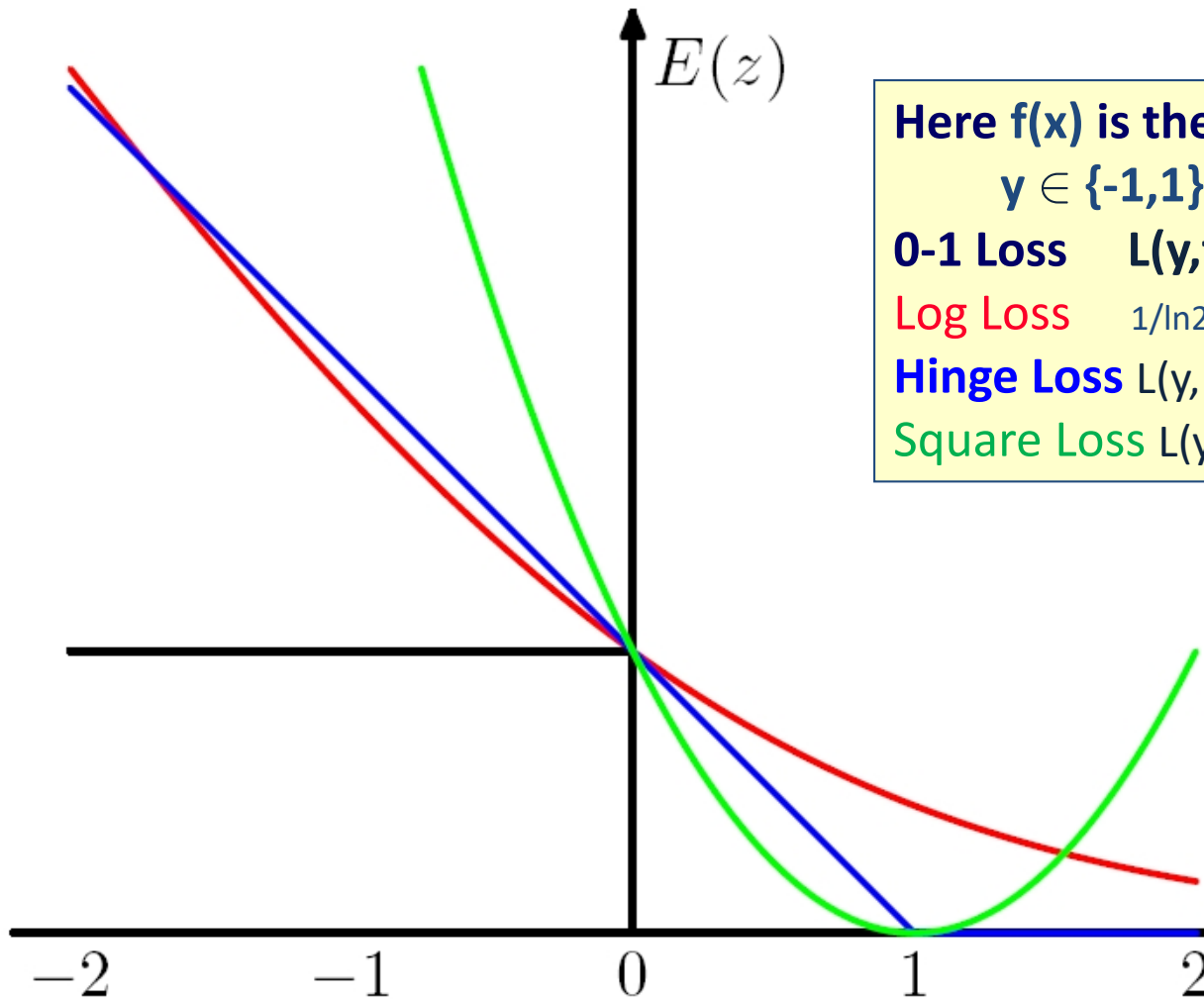
- Input dependent loss:

$$L(f(x), y) = 0 \text{ if } f(x) = y; \quad c(x) \text{ otherwise}$$

A continuous convex loss function allows a simpler optimization algorithm.



Loss



Here $f(x)$ is the prediction $\in \mathcal{R}$
 $y \in \{-1, 1\}$ is the correct value

0-1 Loss $L(y, f(x)) = \frac{1}{2} (1 - \text{sgn}(yf(x)))$

Log Loss $\frac{1}{\ln 2} \log (1 + \exp\{-yf(x)\})$

Hinge Loss $L(y, f(x)) = \max(0, 1 - y f(x))$

Square Loss $L(y, f(x)) = (y - f(x))^2$

0-1 Loss x axis = $yf(x)$
Log Loss = x axis = $yf(x)$
Hinge Loss: x axis = $yf(x)$
Square Loss: x axis = $(y - f(x) + 1)$

Administration

- The class is still full.
- We will continue with Python sessions this week.
 - Tuesday, 6:30
 - Wednesday, 5:30PM
 - Active Learning Class, 3401 Walnut, 401B
- We'll move to give other complementary material that is relevant to the class and the HW.
 - Both sessions will be identical
- HW 1 will be released on Thursday
- Quiz 1 will be released on Friday
 - Deadline: Monday 11:59pm .
- Questions?
 - Please ask/comment during class.

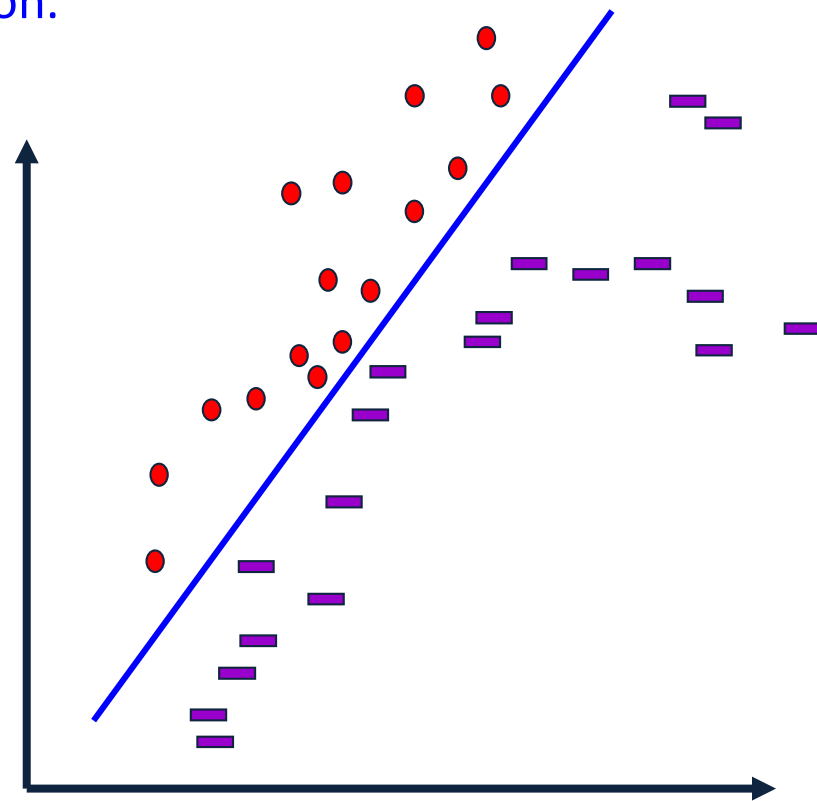
Example

Putting it all together:

A Learning Algorithm

Third Step: How to Learn?

- A possibility: Local search
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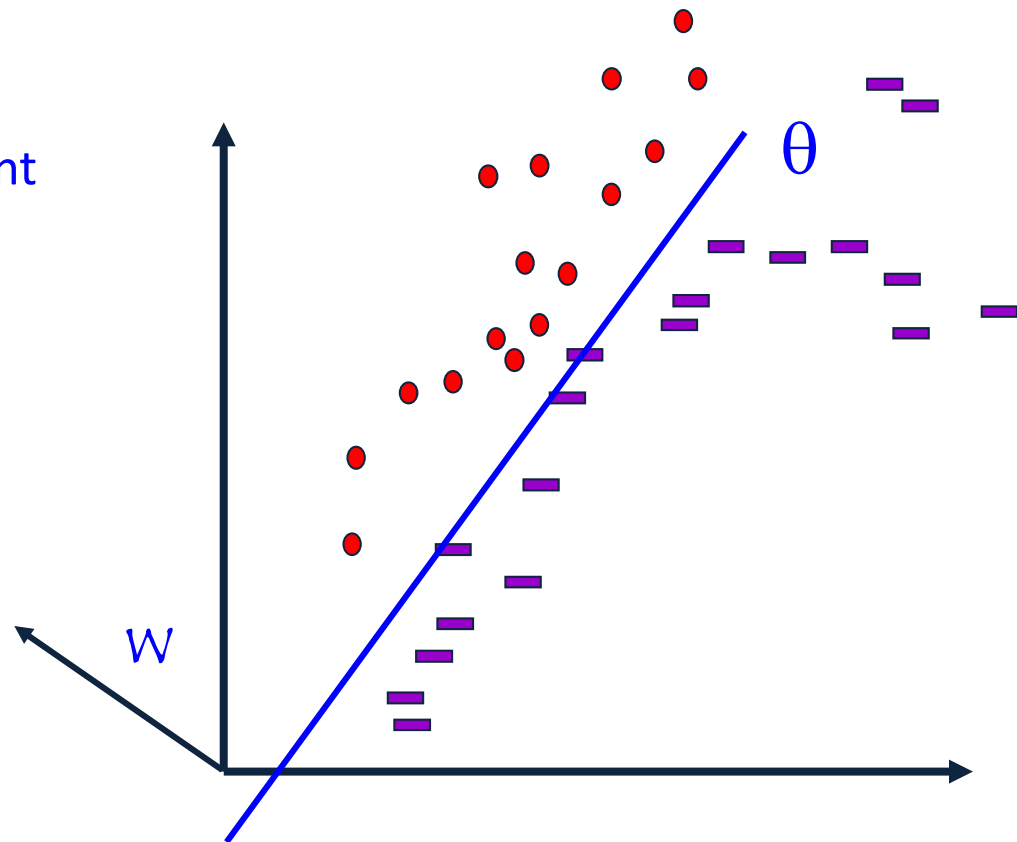


Learning Linear Separators

(LTU=Linear Threshold Unit)

$$f(x) = \text{sgn} \{w^T \cdot x - \theta\} = \text{sgn} \left\{ \sum_{i=1}^n w_i x_i - \theta \right\}$$

- $x^T = (x_1, x_2, \dots, x_n) \in \{0, 1\}^n$
is the feature based
encoding of the data point
- $w^T = (w_1, w_2, \dots, w_n) \in \mathcal{R}^n$
is the target function.
- θ determines the shift
with respect to the origin



Canonical Representation

$$f(x) = \text{sgn} \{w^T \cdot x - \theta\} = \text{sgn} \left\{ \sum_{i=1}^n w_i x_i - \theta \right\}$$

- **Note:** $\text{sgn} \{w^T \cdot x - \theta\} = \text{sgn} \{w'^T \cdot x'\}$
- Where:
 - $x' = (x, -1)$ and $w' = (w, \theta)$
- Moved from an n dimensional representation to an $(n+1)$ dimensional representation, but now can look for hyperplanes that go through the origin.
- Basically, that means that we learn both w and θ

General Learning Principle

The Risk (Err) E :
a function of w

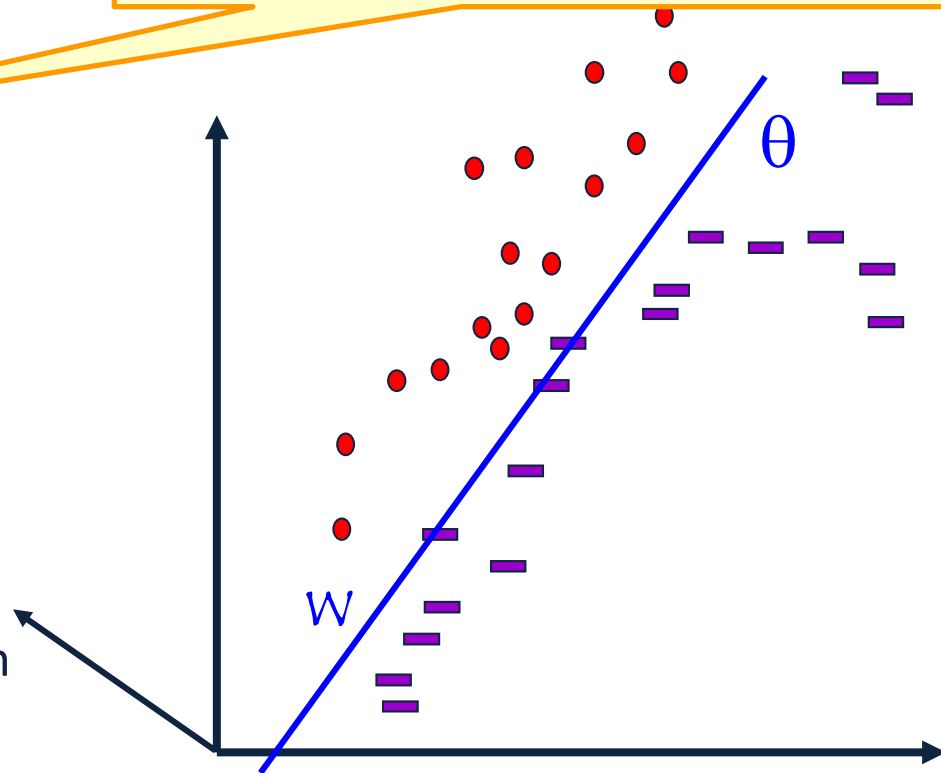
- **Our goal** is to find a w that *minimizes* the expected risk
- We cannot do it.
- **Instead**, we approximate $E(w)$ using a finite training set of independent samples (x_i, y_i)

$$E(w) \approx \frac{1}{m} \sum_{1,m} Q(x_i, y_i, w)$$

- To find the *minimum*, we use a **batch gradient descent** algorithm
- That is, we successively compute estimates w^t of the optimal parameter vector w :

$$w^{t+1} = w^t - \nabla E(w) = w^t - \frac{1}{m} \sum_{1,m} \nabla Q(x_i, y_i, w)$$

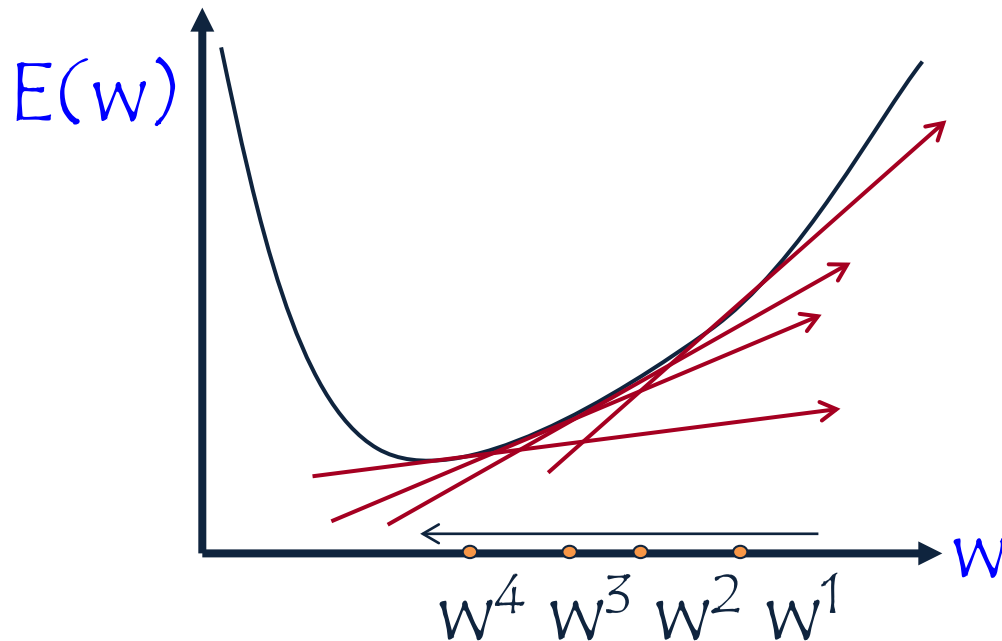
The loss Q : a function of x , w and y



t here is "time"
or "iteration" #

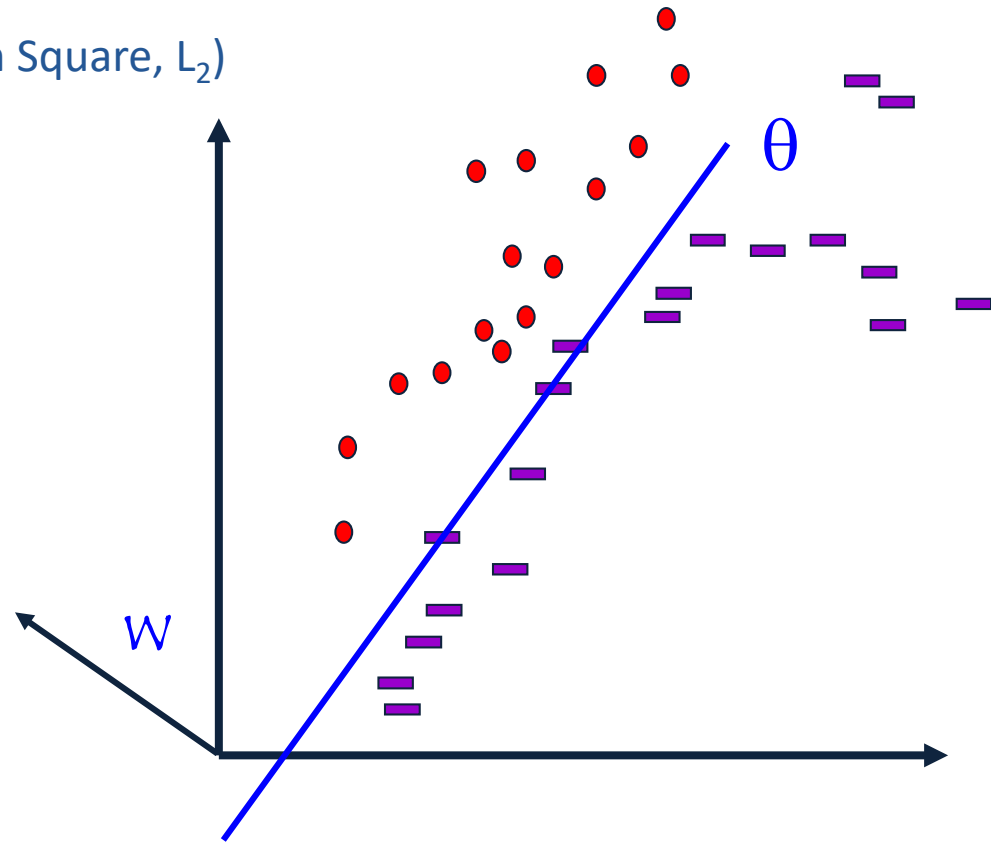
Gradient Descent

- We use gradient descent to determine the weight vector that minimizes $E(w)$ ($= \text{Err}(w)$);
- Fixing the set D of examples, $E = \text{Err}$ is a function of w
- At each step, the weight vector is modified in the direction that produces the steepest descent along the error surface.



LMS: An Optimization Algorithm

- Our Hypothesis Space is the collection of **Linear Threshold Units**
- Loss function:
 - Squared loss: LMS (Least Mean Square, L_2)
 - $Q(x, y, w) = \frac{1}{2} (w^T x - y)^2$



LMS: An Optimization Algorithm

- i (subscript) – vector component; j (superscript) - time; d – example #)

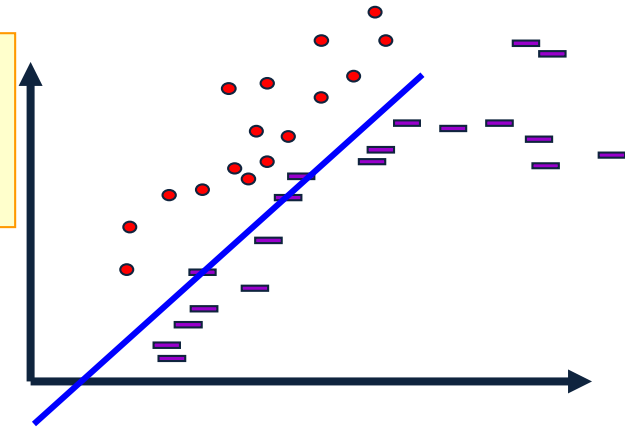
Assumption: $x \in \mathbb{R}^n$; $u \in \mathbb{R}^n$ is the target weight vector; the target (label) is $t_d = u^T \cdot x$. Noise has been added; so, possibly, no weight vector is consistent with the data.

- Let $w^{(j)}$ be the current weight vector we have
- Our prediction on the d -th example x is:

$$O_d = w^{(j)T} \cdot x = \sum_{i=1}^n w_i^{(j)} x_i$$

- Let t_d be the target value for this example)
- The **error** the current hypothesis makes on the data set is:

$$E(w) = \text{Err}(w^j) = \frac{1}{2} \sum_{d \in D} (t_d - O_d)^2$$



Gradient Descent

- To find the best direction in the weight space \mathbf{w} we compute the gradient of E with respect to each of the components of

$$\nabla E(\mathbf{w}) = \left[\frac{\partial E}{\partial w_1}, \frac{\partial E}{\partial w_2}, \dots, \frac{\partial E}{\partial w_n} \right]$$

- This vector specifies the direction that produces the steepest increase in E ;
- We want to modify w in the direction of $-\nabla E(\mathbf{w})$
- Where (with a fixed step size R):

$$\mathbf{w}^t = \mathbf{w}^{t-1} + \Delta \mathbf{w}$$

$$\Delta \mathbf{w} = -R \nabla E(\mathbf{w})$$

Gradient Descent: LMS

- We have: $E(w) = \text{Err}(w^j) = \frac{1}{2} \sum_{d \in D} (t_d - o_d)^2$

- Therefore:
$$\begin{aligned} \frac{\partial E}{\partial w_i} &= \frac{\partial}{\partial w_i} \frac{1}{2} \sum_{d \in D} (t_d - o_d)^2 = \\ &= \frac{1}{2} \sum_{d \in D} \frac{\partial}{\partial w_i} (t_d - o_d)^2 = \\ &= \frac{1}{2} \sum_{d \in D} 2(t_d - o_d) \frac{\partial}{\partial w_i} (t_d - w_d \bullet x_d) = \\ &= \sum_{d \in D} (t_d - o_d) (-x_{id}) \end{aligned}$$

Alg1: Gradient Descent: LMS

- Weight update rule:

$$\Delta w_i = R \sum_{d \in D} (t_d - O_d) x_{id}$$

- Gradient descent algorithm for training linear units:
 - Start with an initial random weight vector
 - For every example d with target value t_d do:
 - Evaluate the linear unit $O_d = w^{(j)T} \cdot x = \sum_{i=1}^n w_i^{(j)} x_i$
 - Update w by adding Δw_i to each component
 - Continue until E below some threshold

This algorithm always converges to a local minimum of $E(w)$, for small enough steps. Here (LMS for linear regression), the surface contains only a single global minimum, so the algorithm converges to a weight vector with minimum error, regardless of whether the examples are linearly separable.

The surface may have local minimum if the loss function is different.

Alg 2: Incremental (Stochastic) Gradient Descent: (LMS)

- Weight update rule:

$$\Delta w_i = R(t_d - O_d)x_{id}$$

Dropped the averaging operation.
Instead of averaging the gradient of the loss over the complete training set, choose at random a sample (x,y) (or a subset of examples) and update w^t

- Gradient descent algorithm for training linear units:
 - Start with an initial random weight vector
 - For every example d with target value t_d do:
 - Evaluate the linear unit $O_d = w^{(j)T} \cdot x = \sum_{i=1}^n w_i^{(j)} x_i$
 - update w by incrementally by adding Δw_i to each component (update without summing over all data)
 - Continue until E below some threshold
- In general - does not converge to global minimum
- Decreasing R with time guarantees convergence
- But, on-line algorithms are sometimes advantageous...

Learning Rates and Convergence

- In the general (non-separable) case the learning rate R must decrease to zero to guarantee convergence.
- The learning rate is called the *step size*. There are more sophisticated algorithms that choose the step size automatically and converge faster.
- Choosing a better starting point also has impact.
- The gradient descent and its stochastic version are very simple algorithms, but almost all the algorithms we will learn in the class can be traced back to gradient decent algorithms for different loss functions and different hypotheses spaces.

Computational Issues

- Assume the data is linearly separable.
- Sample complexity:
 - Suppose we want to ensure that our LTU has an error rate (on new examples) of less than ϵ with high probability (at least $(1-\delta)$)
 - How large does m (the number of examples) must be in order to achieve this ? It can be shown that for n dimensional problems

$$m = O\left(\frac{1}{\epsilon} [\ln(1/\delta) + (n+1) \ln(1/\epsilon)]\right).$$

- Computational complexity: What can be said?
 - It can be shown that there exists a polynomial time algorithm for finding **consistent** LTU (by reduction from linear programming).
 - [Contrast with the NP hardness for 0-1 loss optimization]
 - (On-line algorithms have inverse quadratic dependence on the margin)

Other Methods for LTUs

- Fisher Linear Discriminant:
 - A direct computation method
- Probabilistic methods (naïve Bayes):
 - Produces a stochastic classifier that can be viewed as a linear threshold unit.
- Winnow/Perceptron
 - A multiplicative/additive update algorithm with some sparsity properties in the function space (a large number of irrelevant attributes) or features space (sparse examples)
- Logistic Regression, SVM...many other algorithms