# Machine Learning

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Most slides have been adapted from Bhiksha Raj, 11-785, CMU 2020, Fei Fei Li, cs231n, Stanford 2017, and Soleymani, CE40717, Sharif 2020.

# Schedule

# Machine Learning

# Definition of machine learning

**Tom Mitchell (1998)**

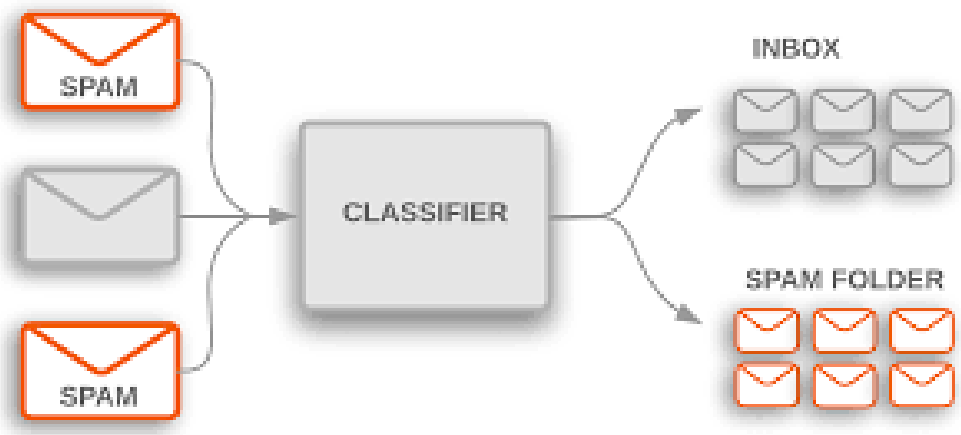
A computer program is said to **learn** from **experience E** with respect to some class of **tasks T** and **performance measure P**, if its performance at tasks in **T**, as measured by **P**, improves with experience **E**.

**Example**

**Task:** Classifying emails as spam or not spam
**Experience:** Watching label of emails as spam or not spam
**Performance metric:** The number (or fraction) of emails correctly classified as spam

# The essence of machine learning

- A pattern exist
- We do not know it mathematically
- We have data on it



# Paradigms of ML

- **Supervised learning**
  Predicting a target variable for which we get to see examples

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  Predicting a target variable for which we get to see examples
- **Unsupervised learning**
  Revealing structure in the observed data
- **Reinforcement learning**
  Partial (indirect) feedback, no explicit guidance
  Given rewards for a sequence of moves to learn a policy and utility functions

# Supervised learning

**Regression**

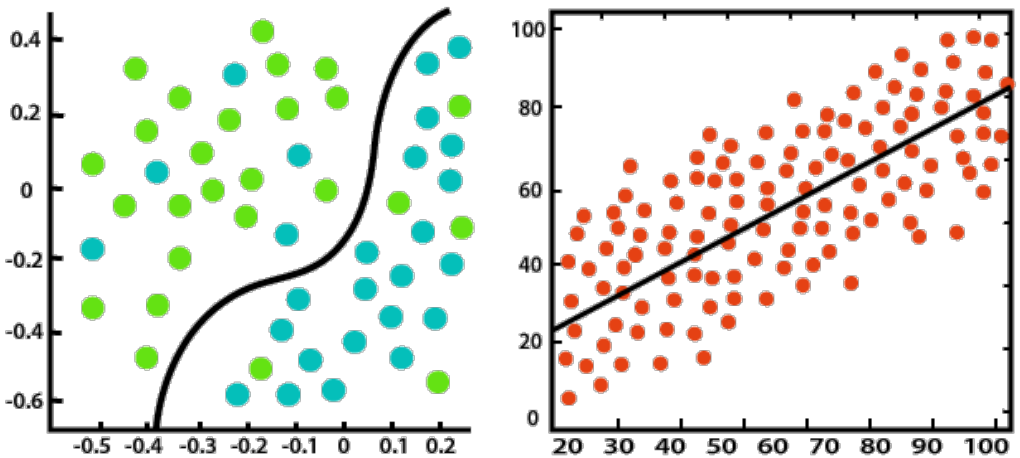
predict a continuous target variable

$$E.g., y \in [0, 1]$$

**Classification**

predict a discrete (unordered) target variable

$$E.g., y \in \{0, 1, 2, ..., 9\}$$




javatpoint.com

# Supervised learning: housing price prediction

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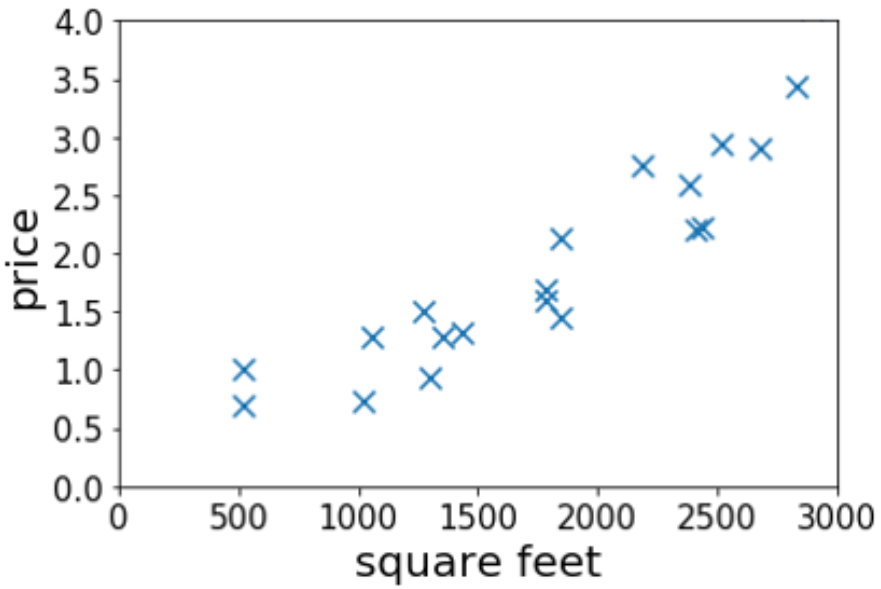

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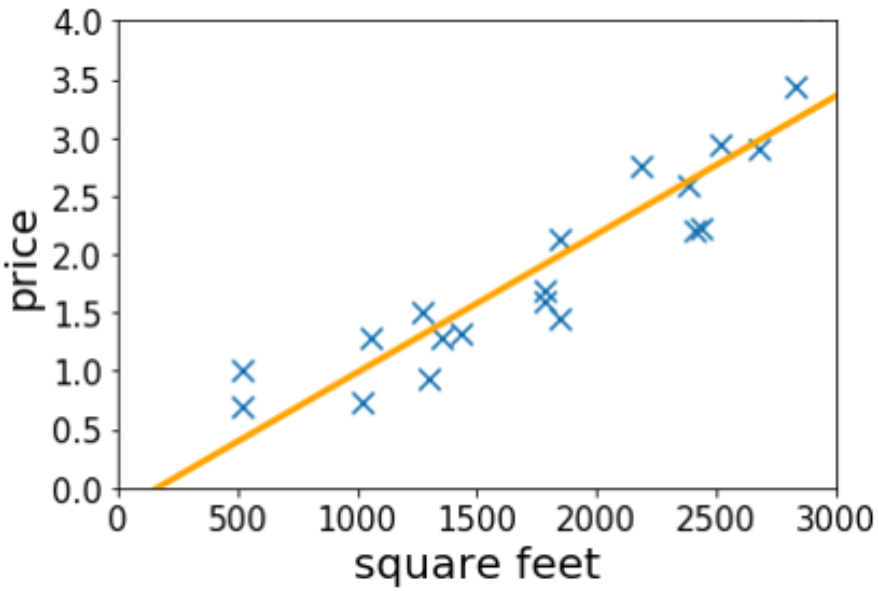

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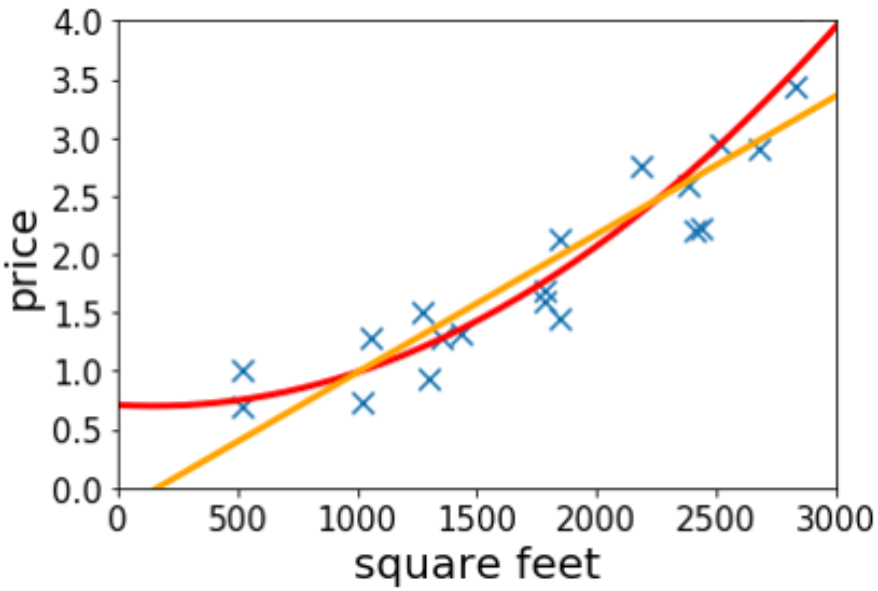

# High-dimensional features

$$\mathbf{x^{(i)}} \in \mathbb{R}^d$$

$$\mathbf{x}^{(i)} = \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ . \\ . \\ . \\ x_d \end{bmatrix}$$

– Size
– Region
– # floors
– Age
.
.
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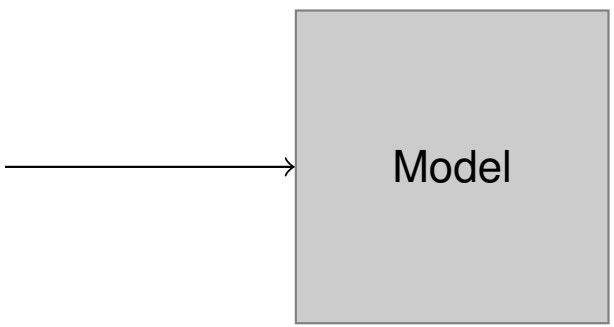

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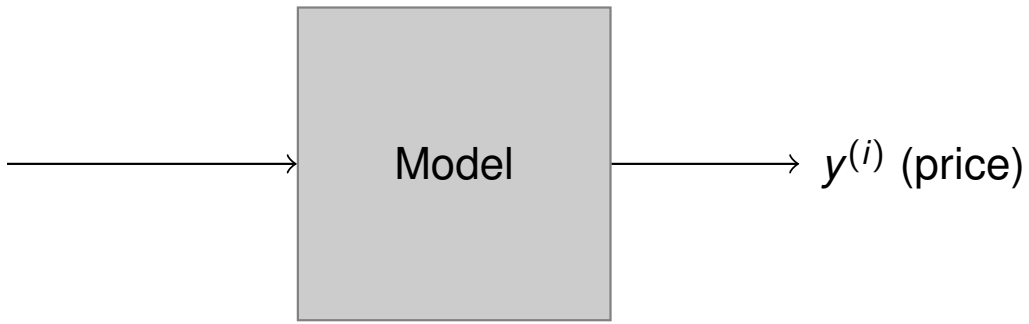
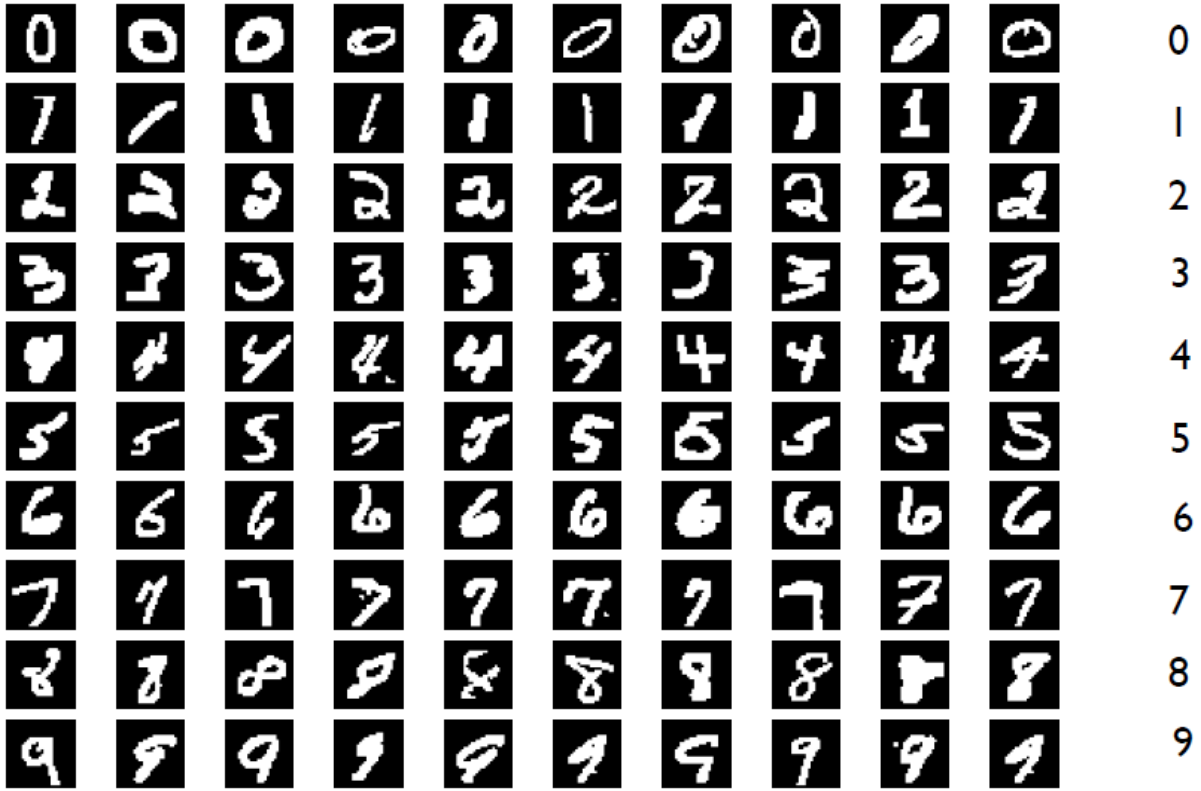


# Image classification




Example images from the MNIST dataset.

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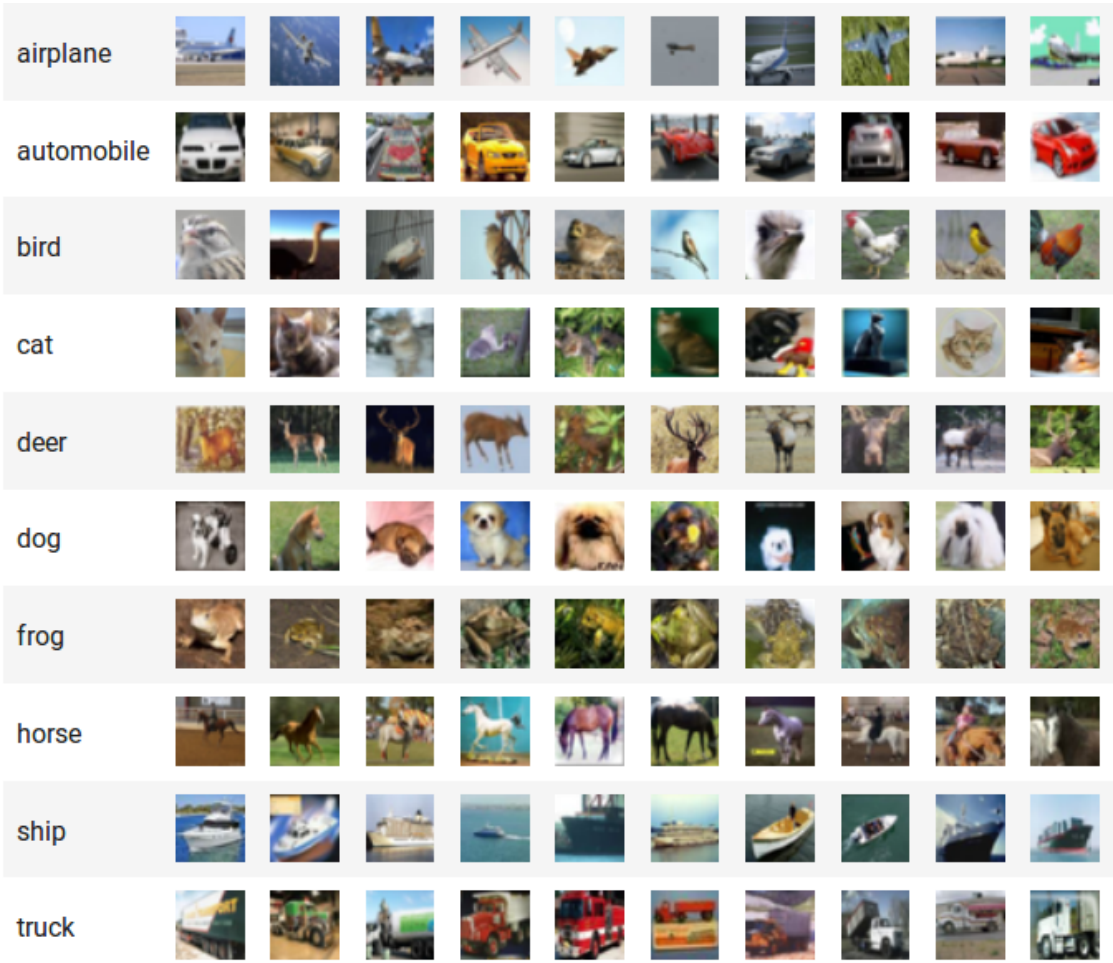



Example images from the CIFAR-10 dataset.

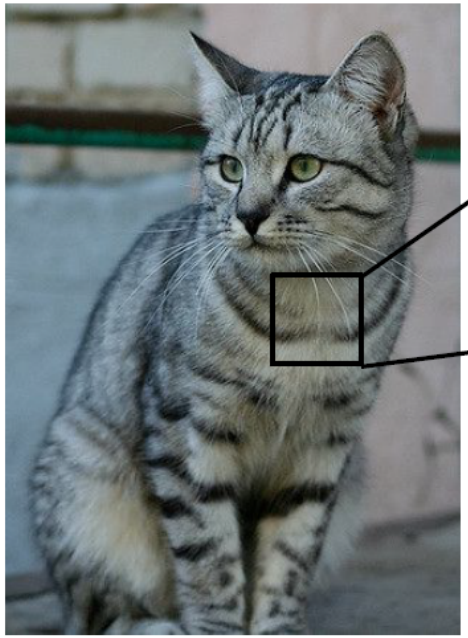
# Image classification



(assume given a set of labels)
{dog, cat, truck, plane, ...}

cat

# Image classification





```
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 [ 91  98 102 106 104  79  98 103  99 105 123 136 110 105  94  85]
 [ 76  85  90 105 128 105  87  95  95  99 115 112 105 103  99  85]
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 [128 137 144 140 109  95  86  70  62  65  63  63  60  73  86 101]
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 [122 164 148 103  71  56  78  83  93 103 119 139 102  61  69  84]]
```

What the computer sees

An image is just a tensor of integers between [0, 255]:

e.g. 800 x 600 x 3
(3 channels RGB)

# Unsupervised learning

**Goal**

Discover the intrinsic structure in the data

**Data**

Dataset contains no labels: $\{x^{(1)}, x^{(2)}, ..., x^{(N)}\}$

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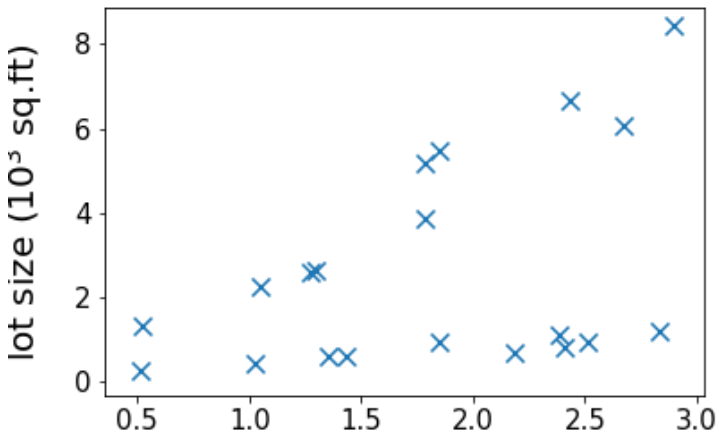


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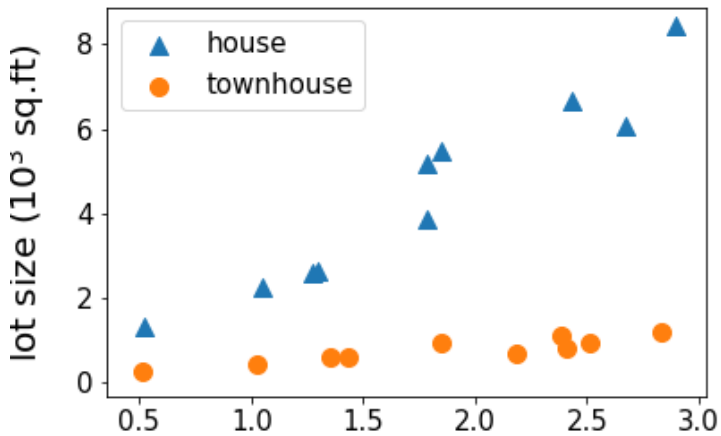

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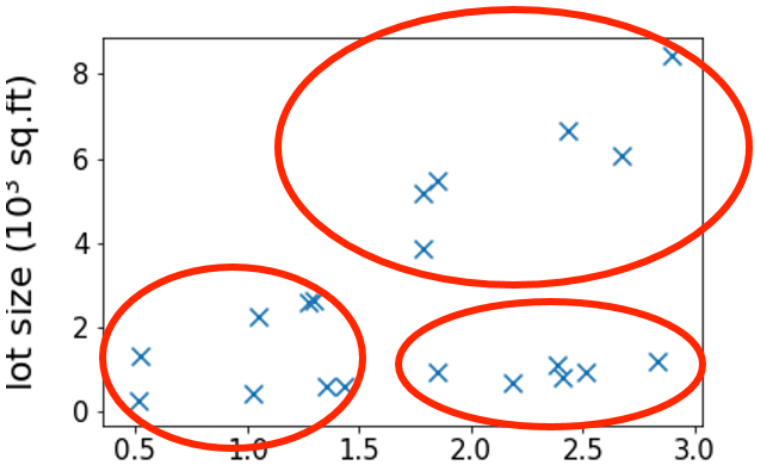


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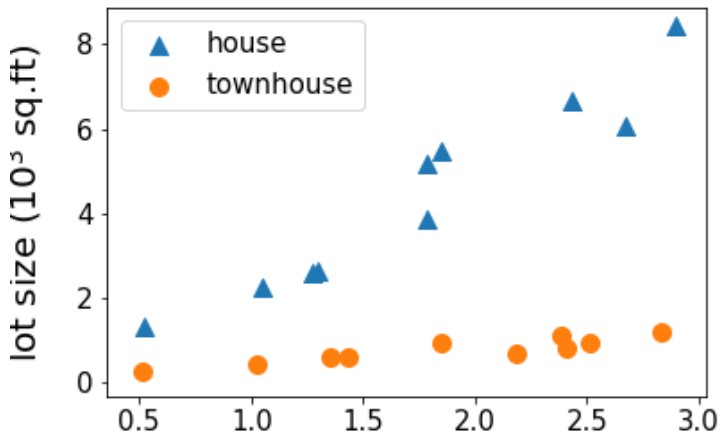

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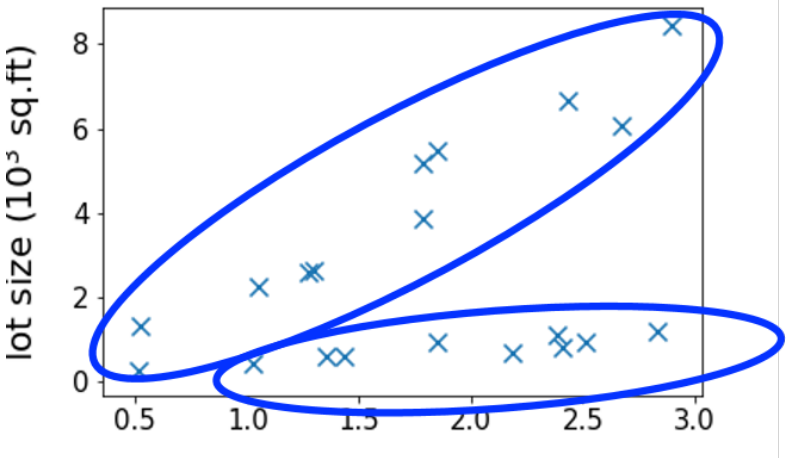


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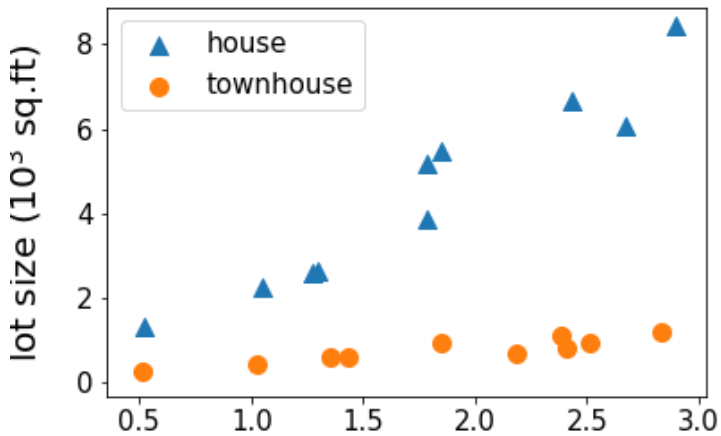


# Unsupervised learning

**Clustering**

- Partitioning of data into groups of similar data points

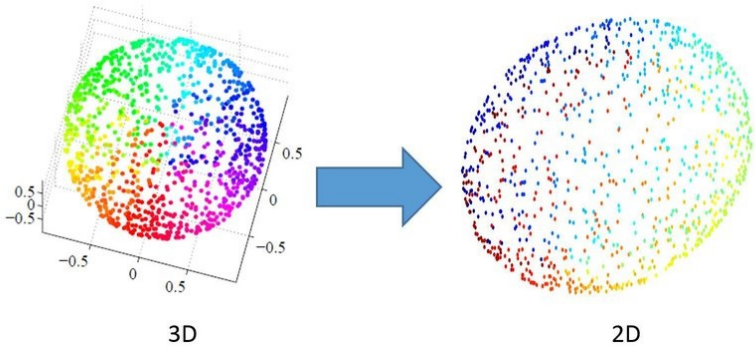
**Dimensionality reduction**

- Data representation using a smaller number of dimensions while preserving (perhaps approximately) some properties of the data

**Synthetic data generation**

- e.g., Variational AutoEncoders (VAE) and Generative Adversarial Networks (GANs),

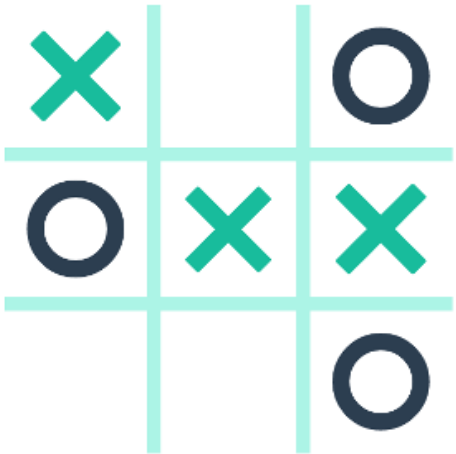
(Karras, 2019)

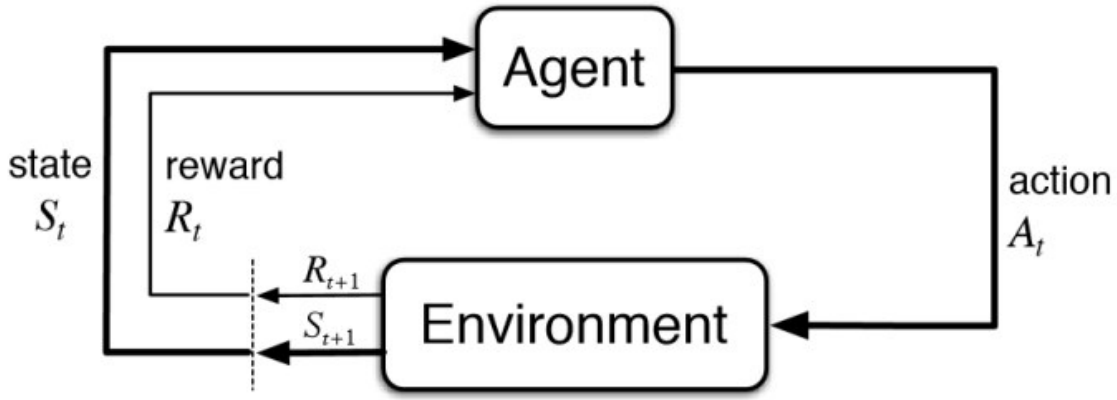


# Reinforcement learning

Provides only an indication as to whether an action is correct or not

Data in supervised learning: (input, correct output)
Data in Reinforcement Learning: (input, some output, a reward for this output)





# Supervised Learning

# Components of supervised learning (function approximation)

**Concept**

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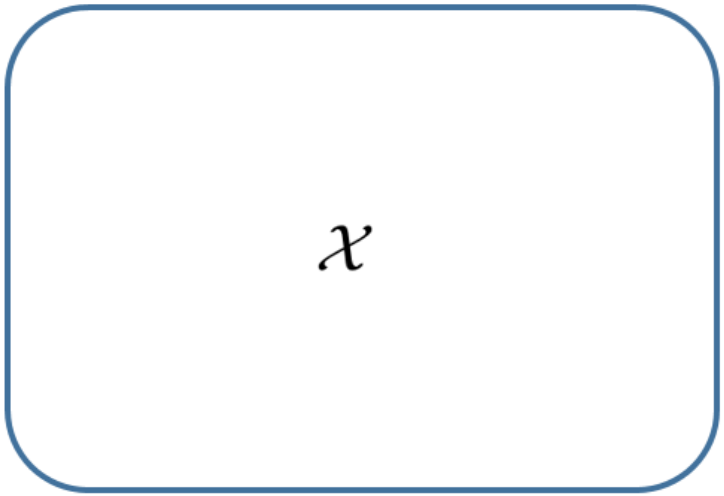

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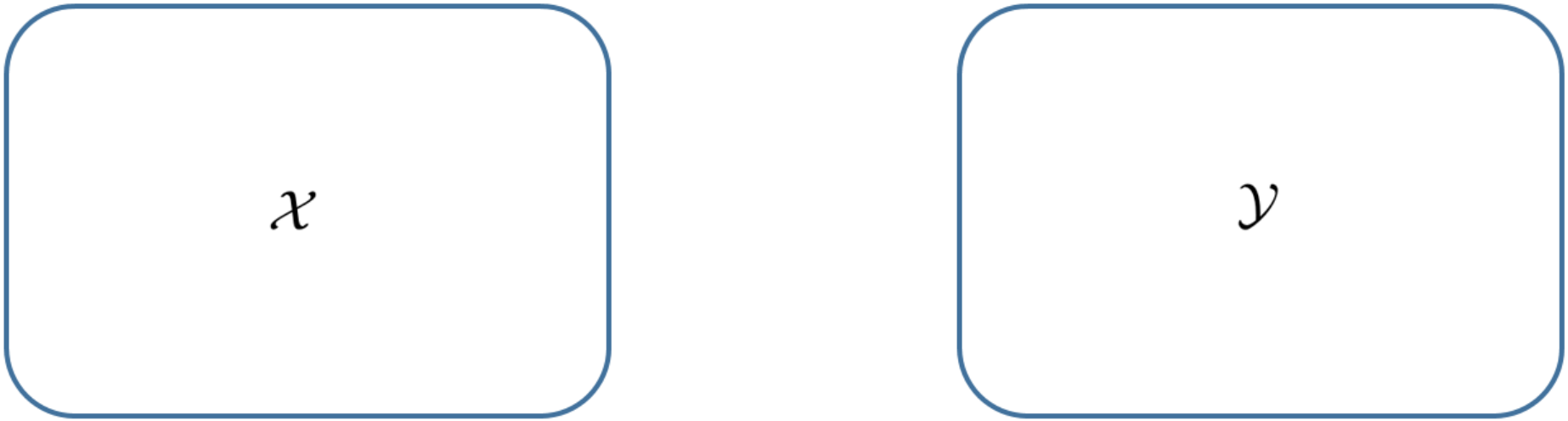

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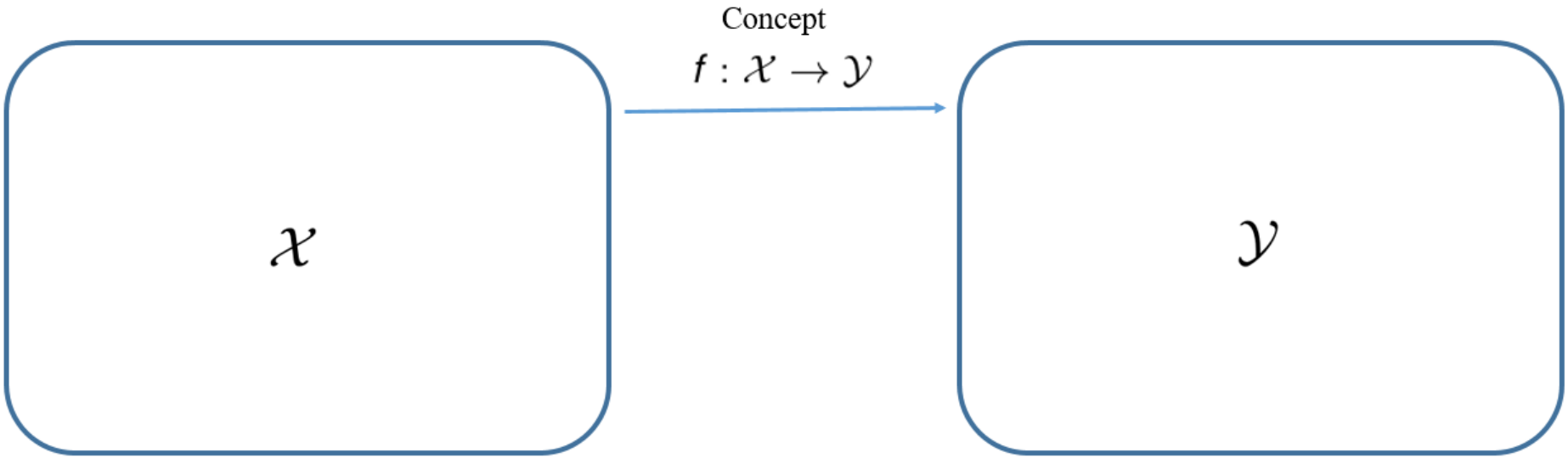

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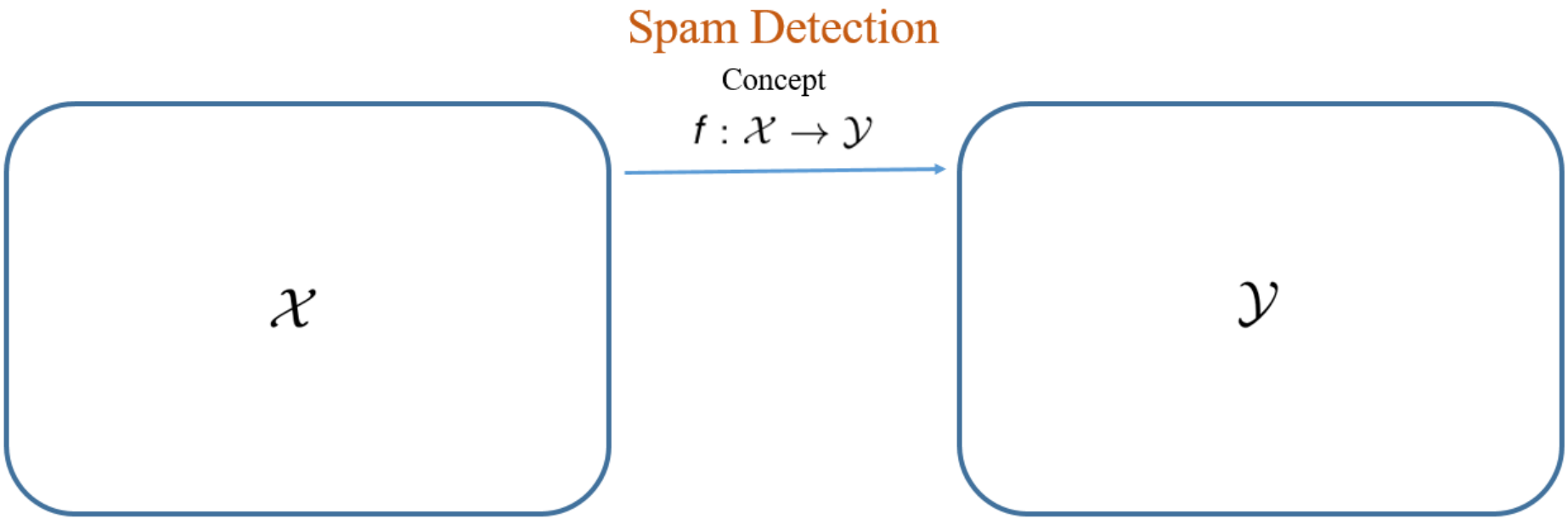

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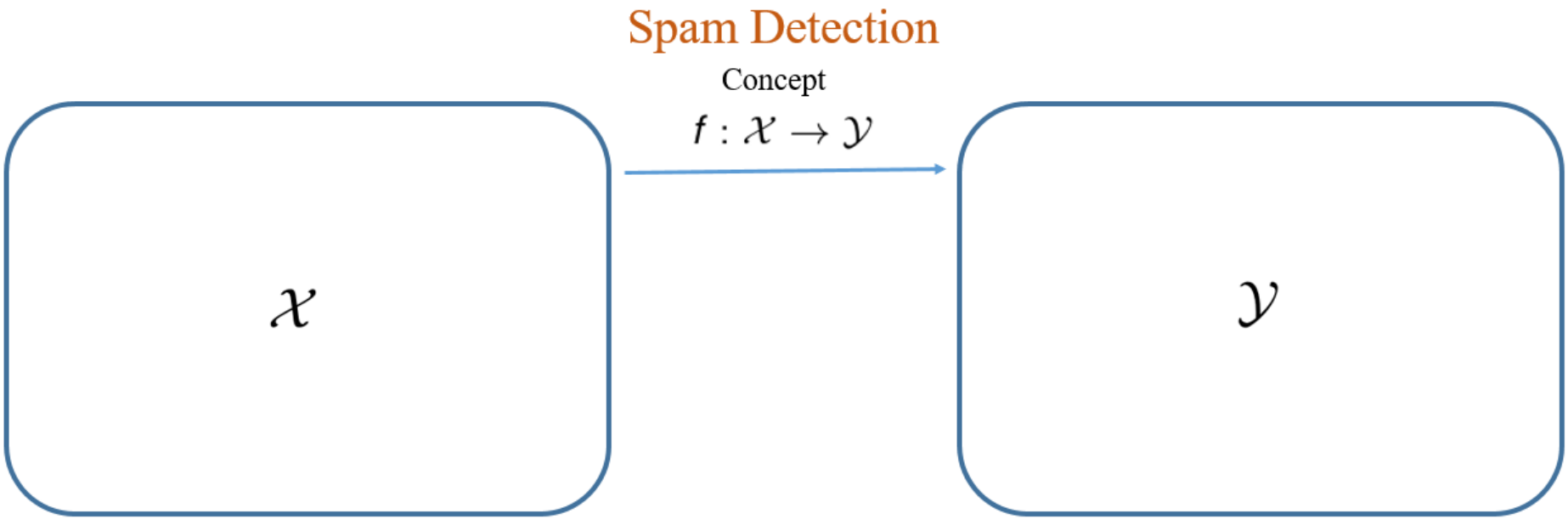


20 binary features:

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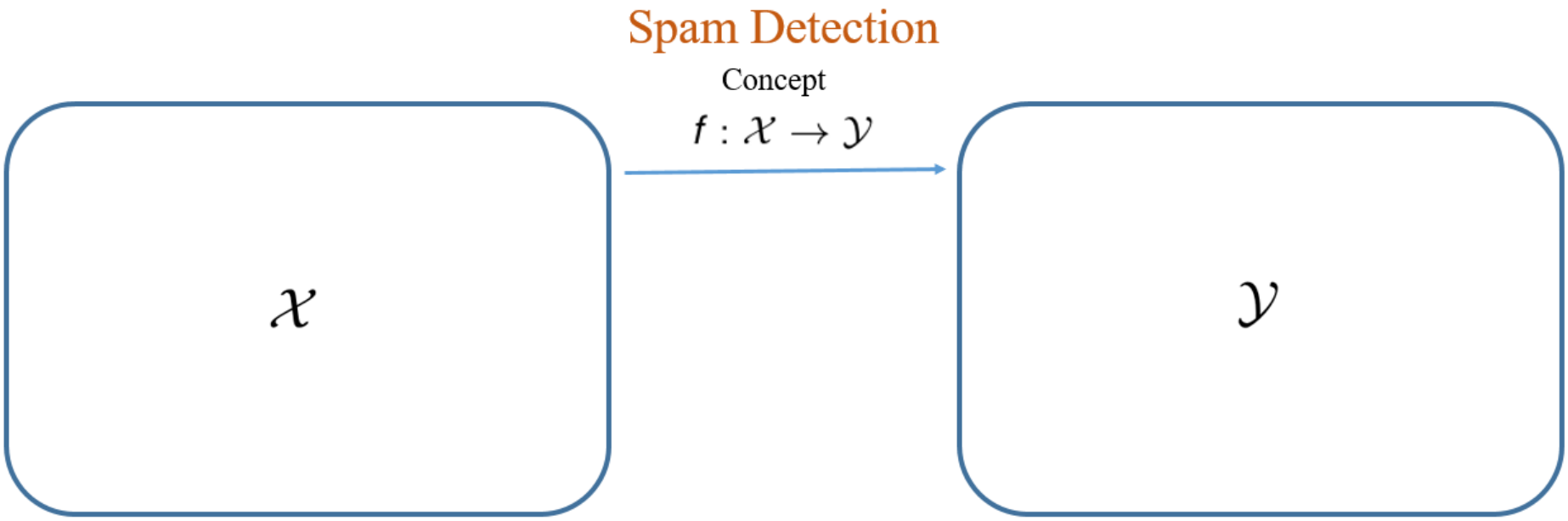


20 binary features: $|\mathcal{X}| = 2^{20}$

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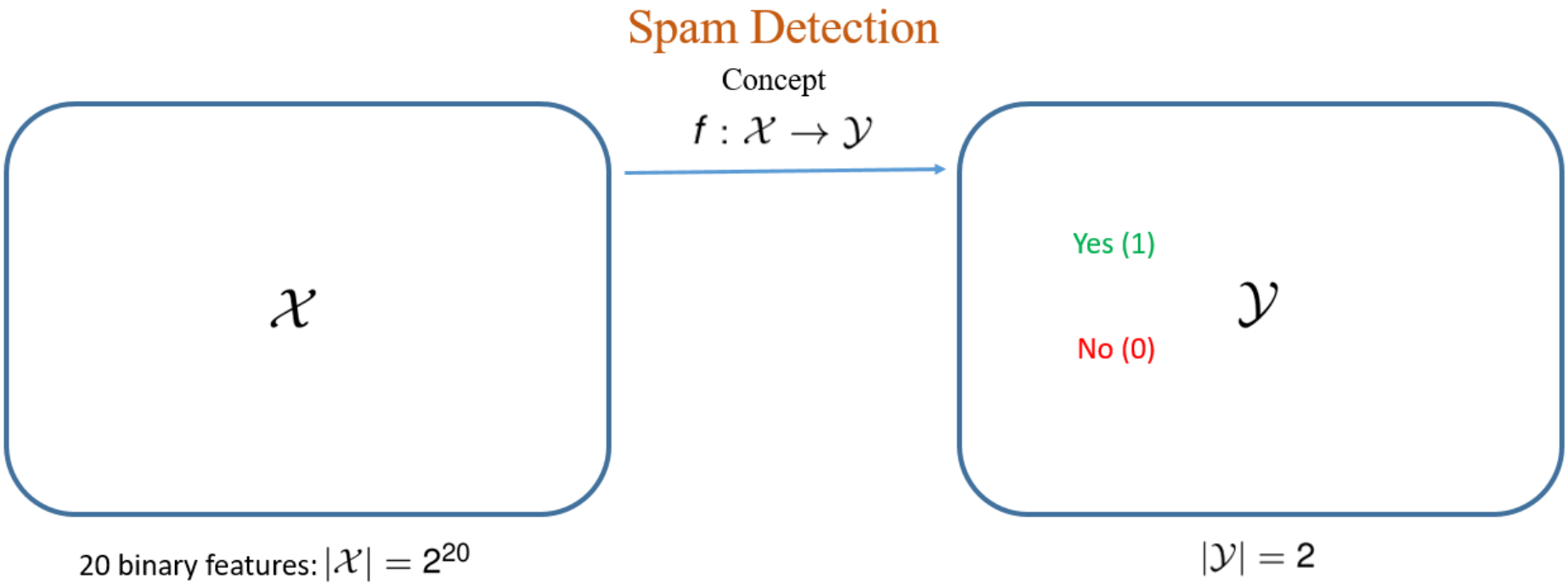

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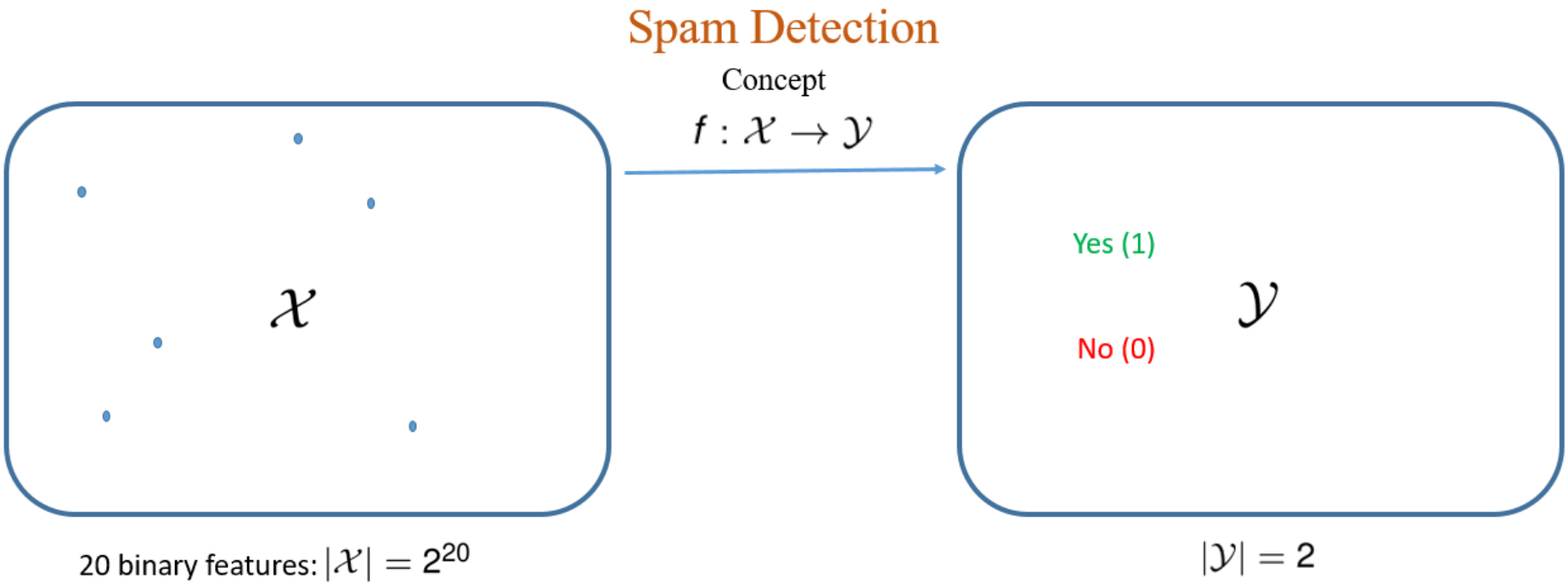

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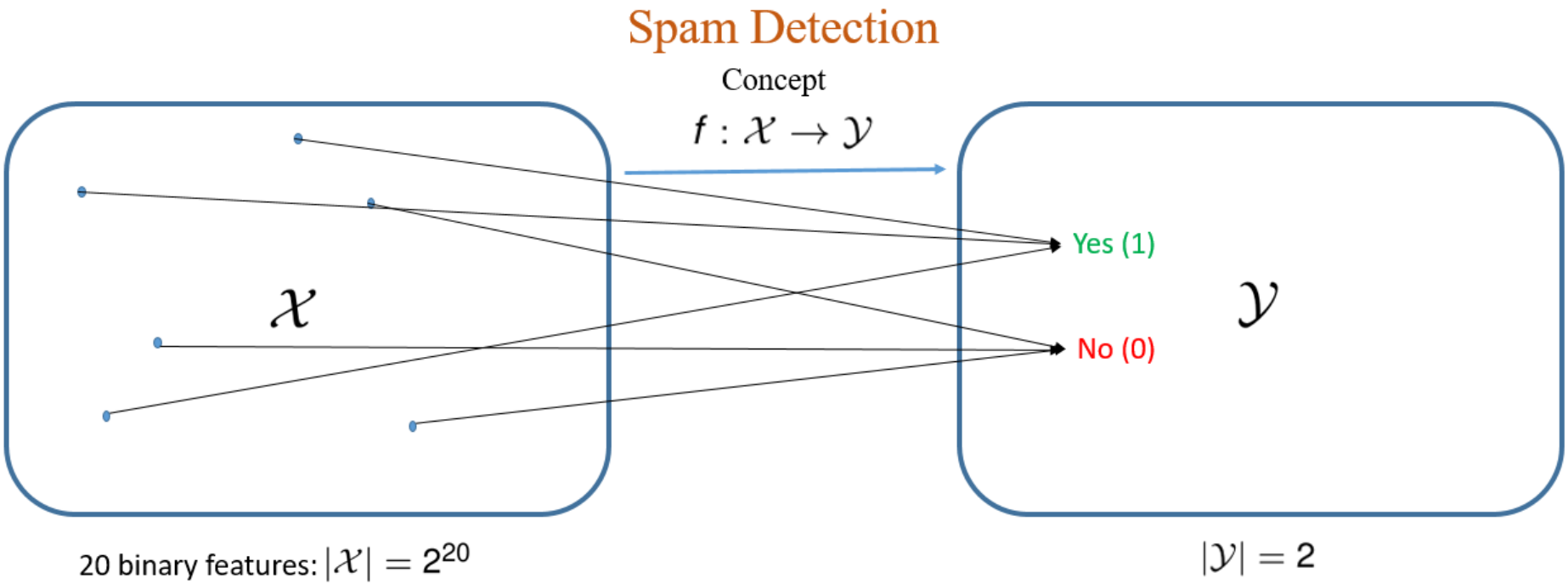

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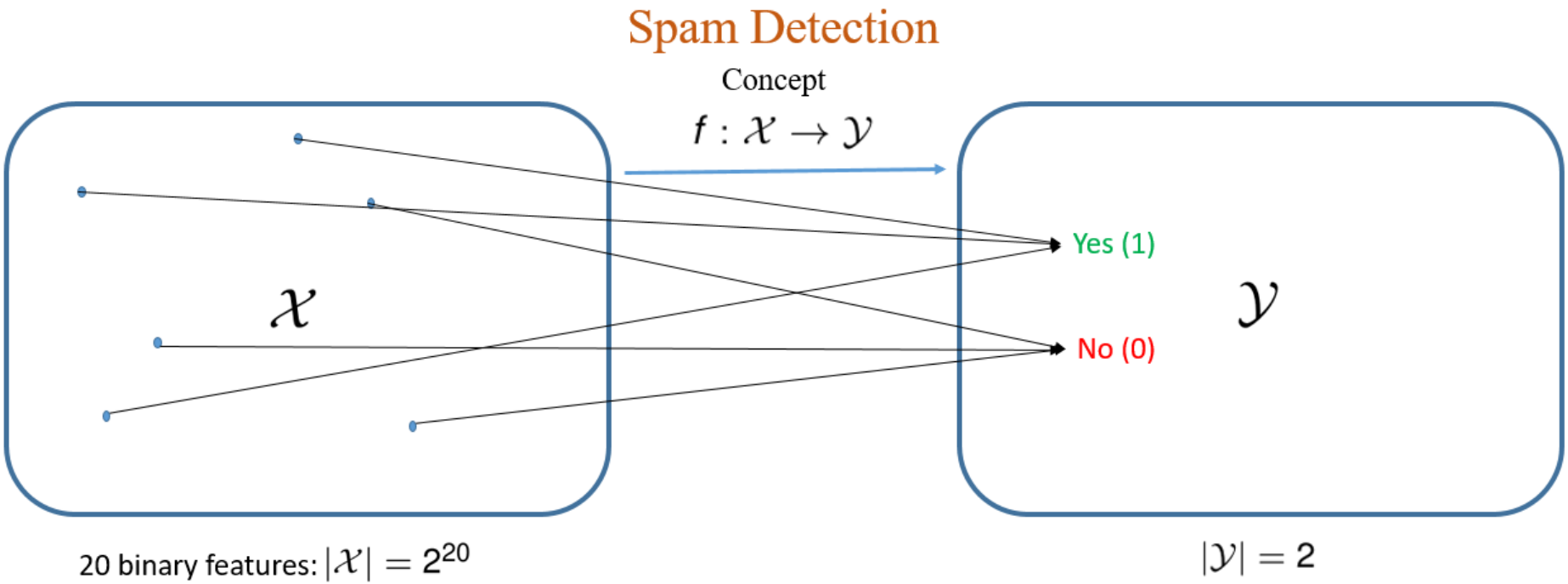


Goal: finding function $h : \mathcal{X} \to \mathcal{Y}$ that approximates the target function $f$

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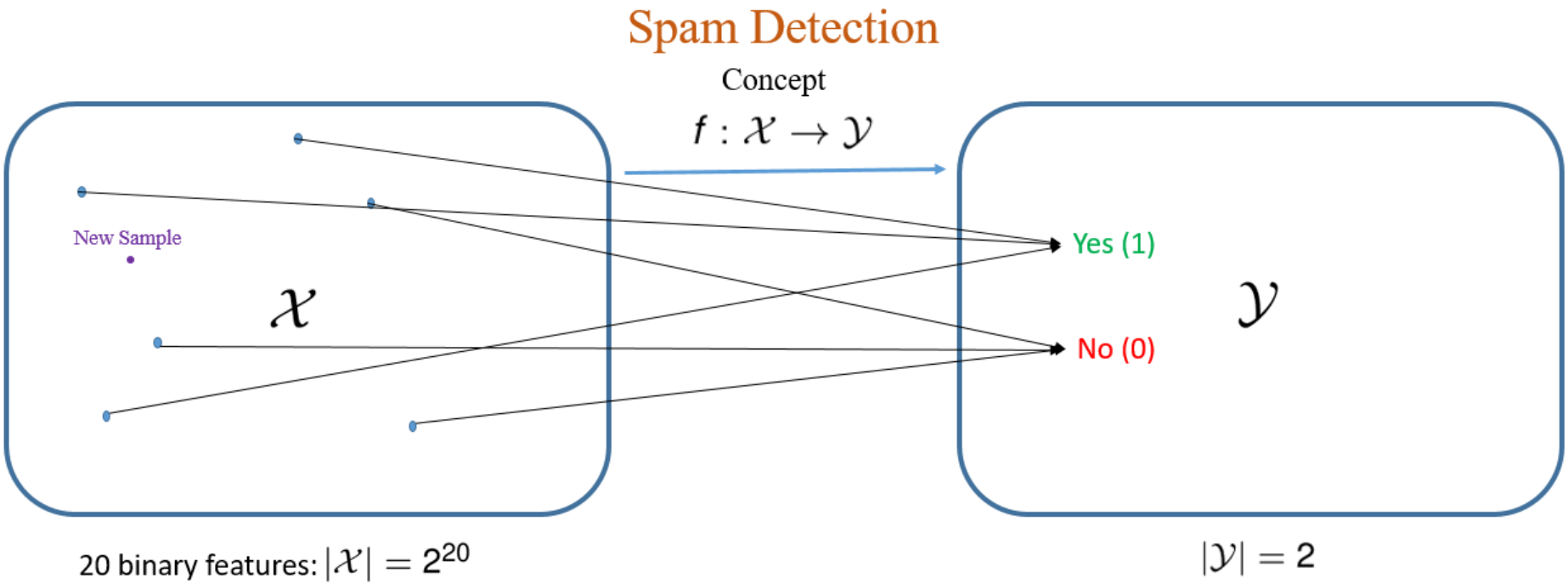


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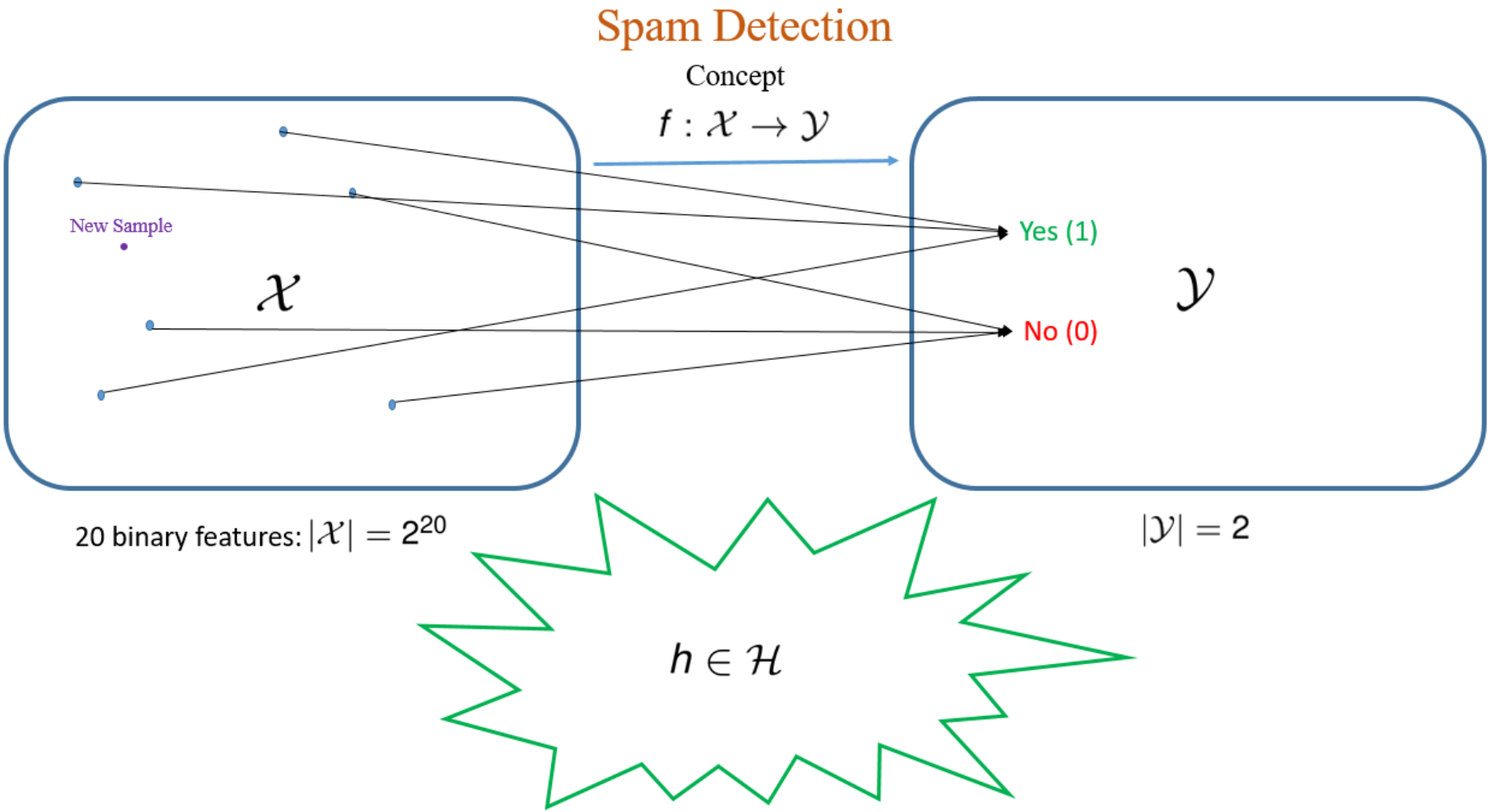


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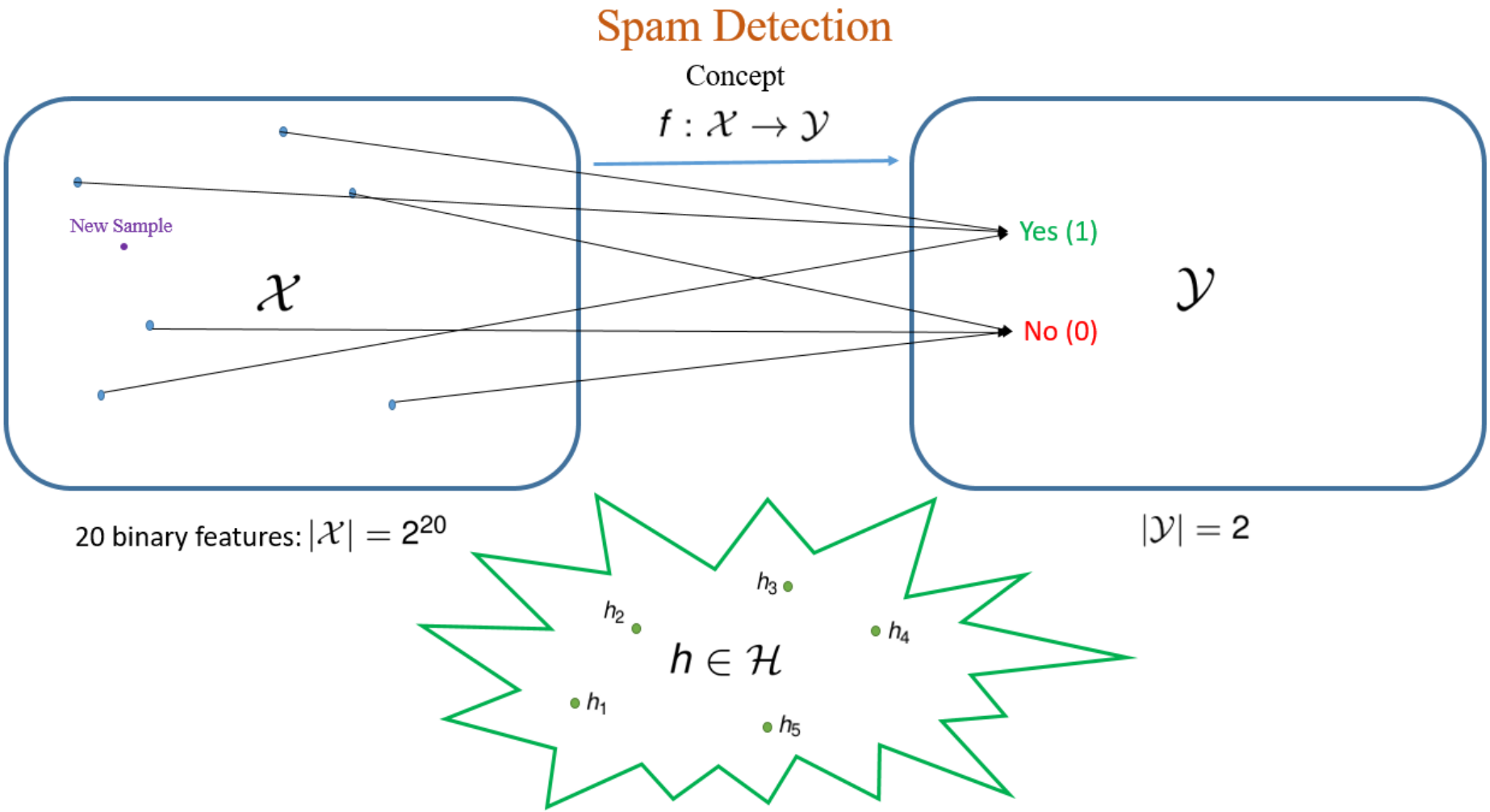

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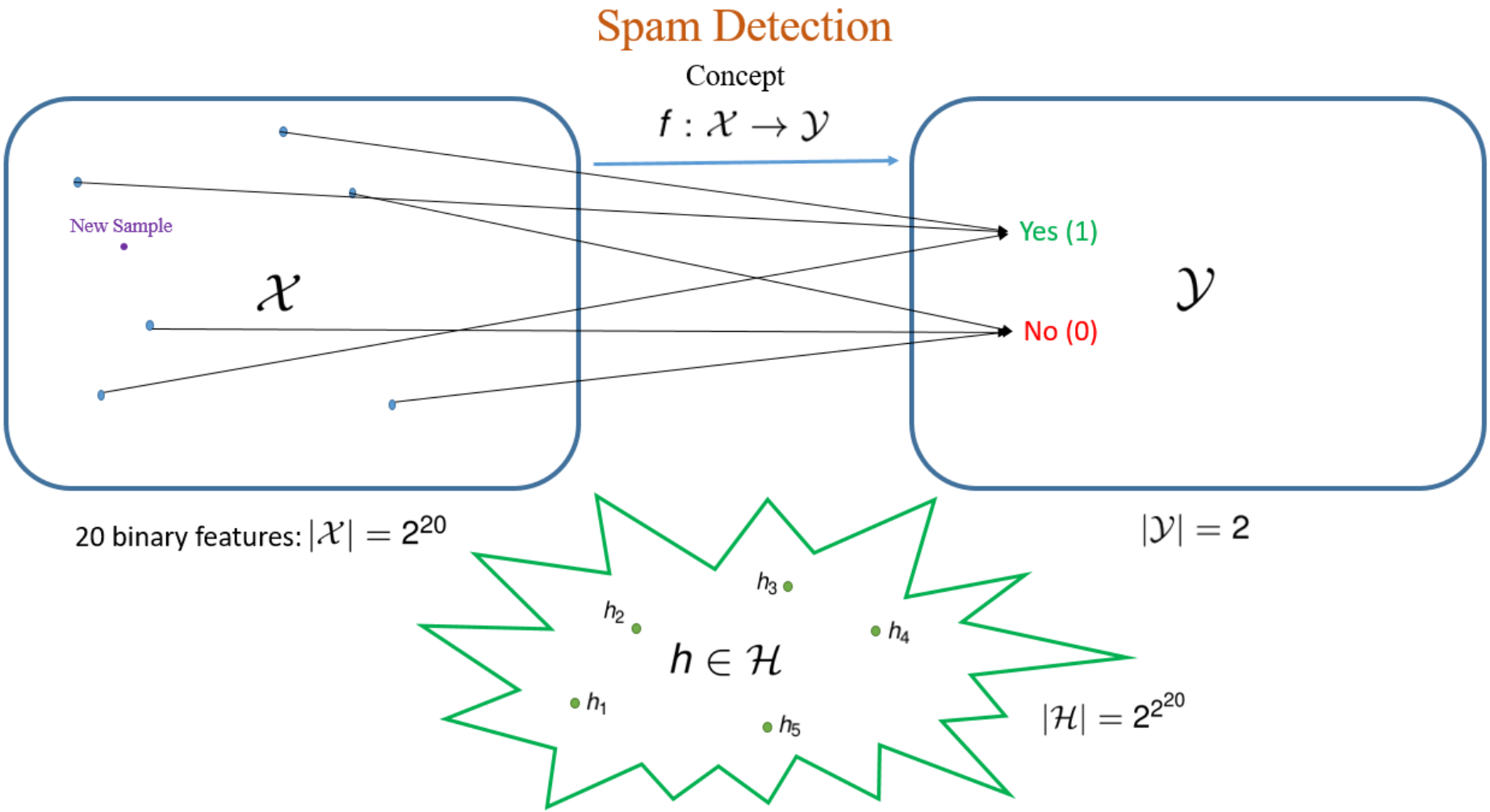


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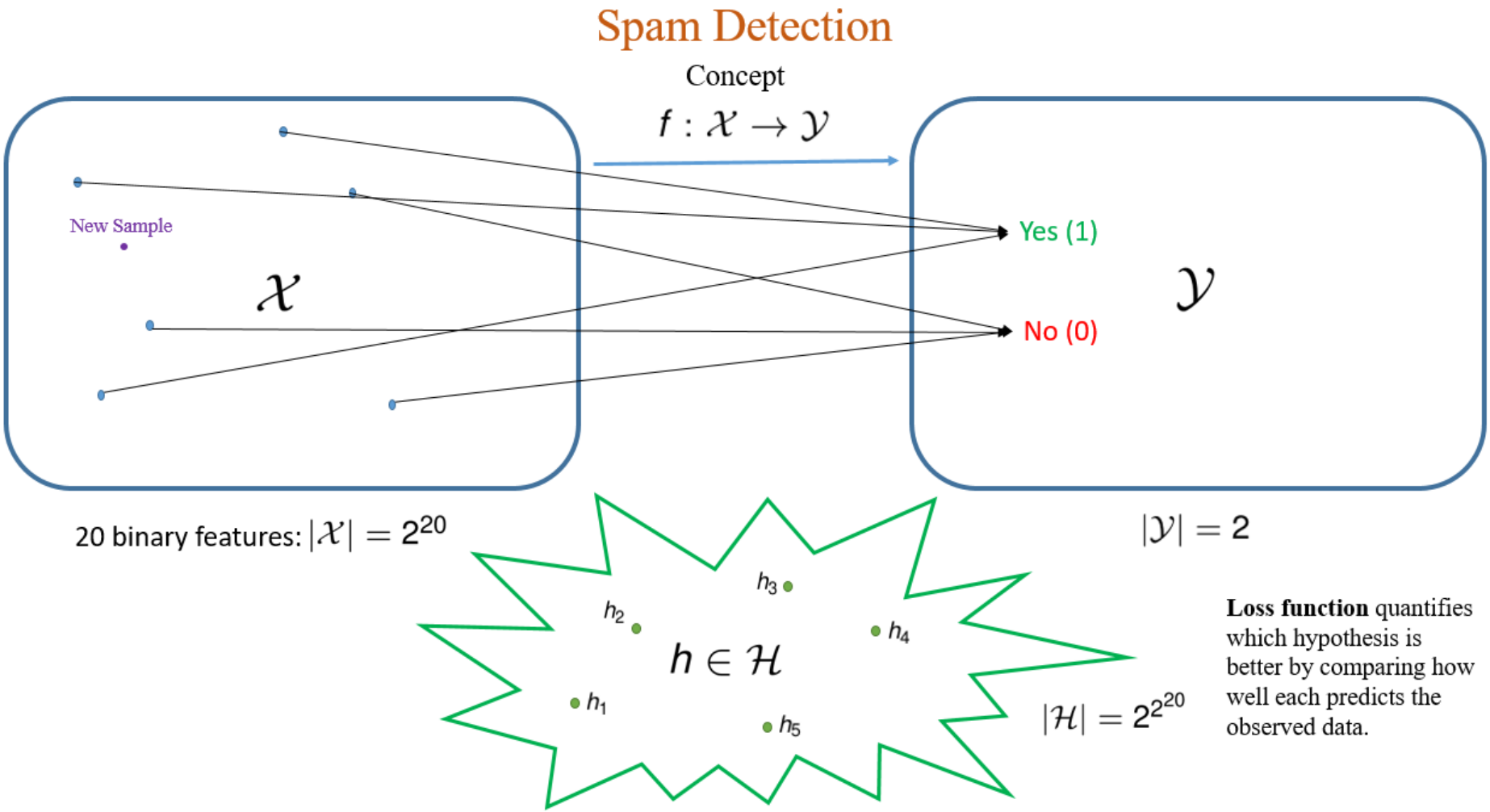

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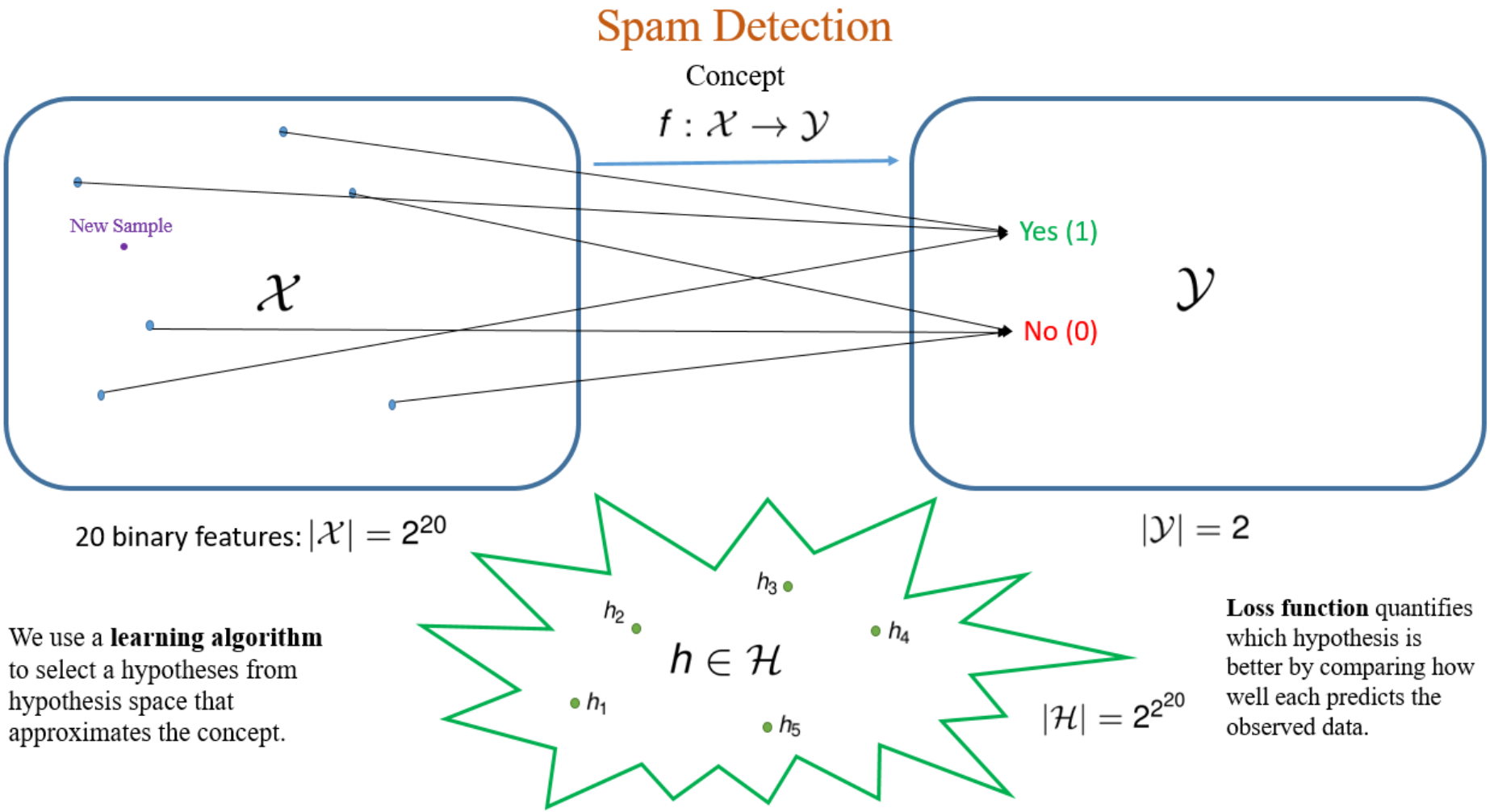



We use a **learning algorithm** to select a hypotheses from hypothesis space that approximates the concept.

**Loss function** quantifies which hypothesis is better by comparing how well each predicts the observed data.

Goal: finding function $h : \mathcal{X} \to \mathcal{Y}$ that approximates the target function $f$ (Generalization)

# Components of supervised learning (function approximation)

**Concept**

- Unknown target function $f : \mathcal{X} \to \mathcal{Y}$
- $\mathcal{X}$: Input space
- $\mathcal{Y}$: Output space

**Training data**

- Samples from the concept $\{(x^{(1)}, y^{(1)}), (x^{(2)}, y^{(2)}), ..., (x^{(N)}, y^{(N)})\}$

# Components of supervised learning (function approximation)

**Concept**

- Unknown target function $f : \mathcal{X} \rightarrow \mathcal{Y}$
- $\mathcal{X}$: Input space
- $\mathcal{Y}$: Output space

**Training data**

- Samples from the concept $\{(x^{(1)}, y^{(1)}), (x^{(2)}, y^{(2)}), ..., (x^{(N)}, y^{(N)})\}$

**Hypotheses space**

- Pick a hypotheses $h : \mathcal{X} \rightarrow \mathcal{Y}$ from hypotheses space $h \in \mathcal{H}$ (e.g., linear functions) that approximates the target function $f$

# Components of supervised learning (function approximation)

**Concept**

- Unknown target function $f : \mathcal{X} \rightarrow \mathcal{Y}$
- $\mathcal{X}$: Input space
- $\mathcal{Y}$: Output space

**Training data**

- Samples from the concept $\{(x^{(1)}, y^{(1)}), (x^{(2)}, y^{(2)}), ..., (x^{(N)}, y^{(N)})\}$

**Hypotheses space**

- Pick a hypotheses $h : \mathcal{X} \rightarrow \mathcal{Y}$ from hypotheses space $h \in \mathcal{H}$ (e.g., linear functions) that approximates the target function $f$

**Learning algorithm**

- We use a learning algorithm to select a hypotheses from hypothesis space that approximates the concept

# Components of supervised learning

Learning model composed of

- A hypothesis set
- A learning algorithm

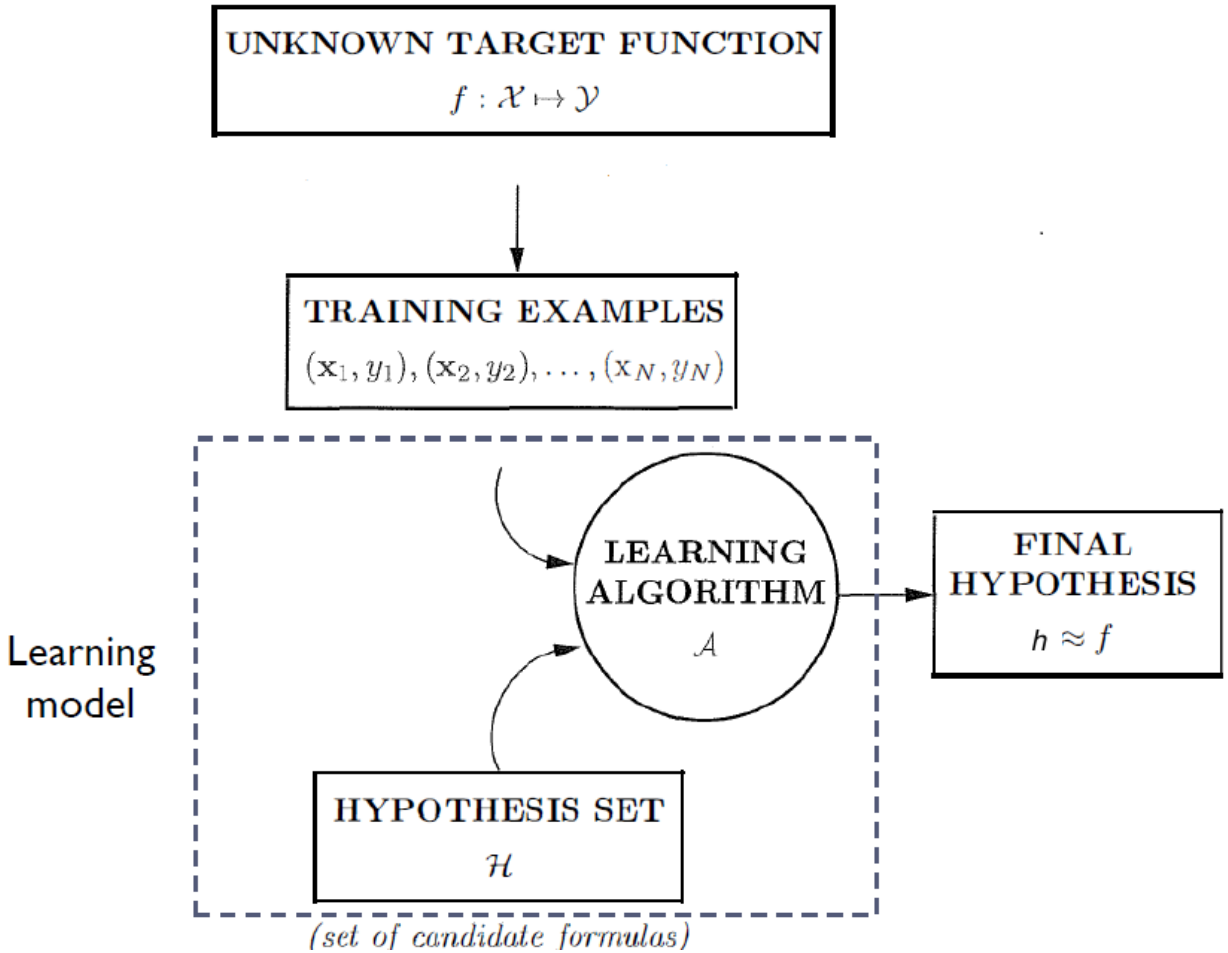



Figure: https://work.caltech.edu/telecourse. html

# Generalization

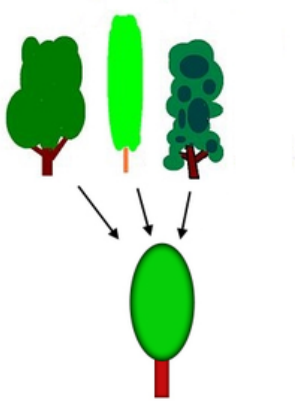
**Hypotheses evaluation**

How well $h$ generalizes to unseen examples.

**Test data**

Samples from the concept $\{(x^{(1)}, y^{(1)}), (x^{(2)}, y^{(2)}), ..., (x^{(N)}, y^{(N)})\}$

Do not exist in the training data



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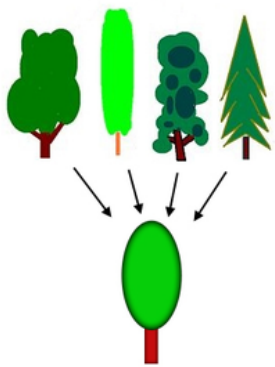


# Independent and identically distributed (i.i.d.)

A collection of random variables is independent and identically distributed if each random variable has the same probability distribution as the others and all are mutually independent.

- $\forall i, x^{(i)} \sim \mathcal{D}$ (Identically Distributed)
- $\forall i \neq j, \mathcal{P}(x^{(i)}, x^{(j)}) = \mathcal{P}(x^{(i)})\mathcal{P}(x^{(j)})$ (Independently Distributed)

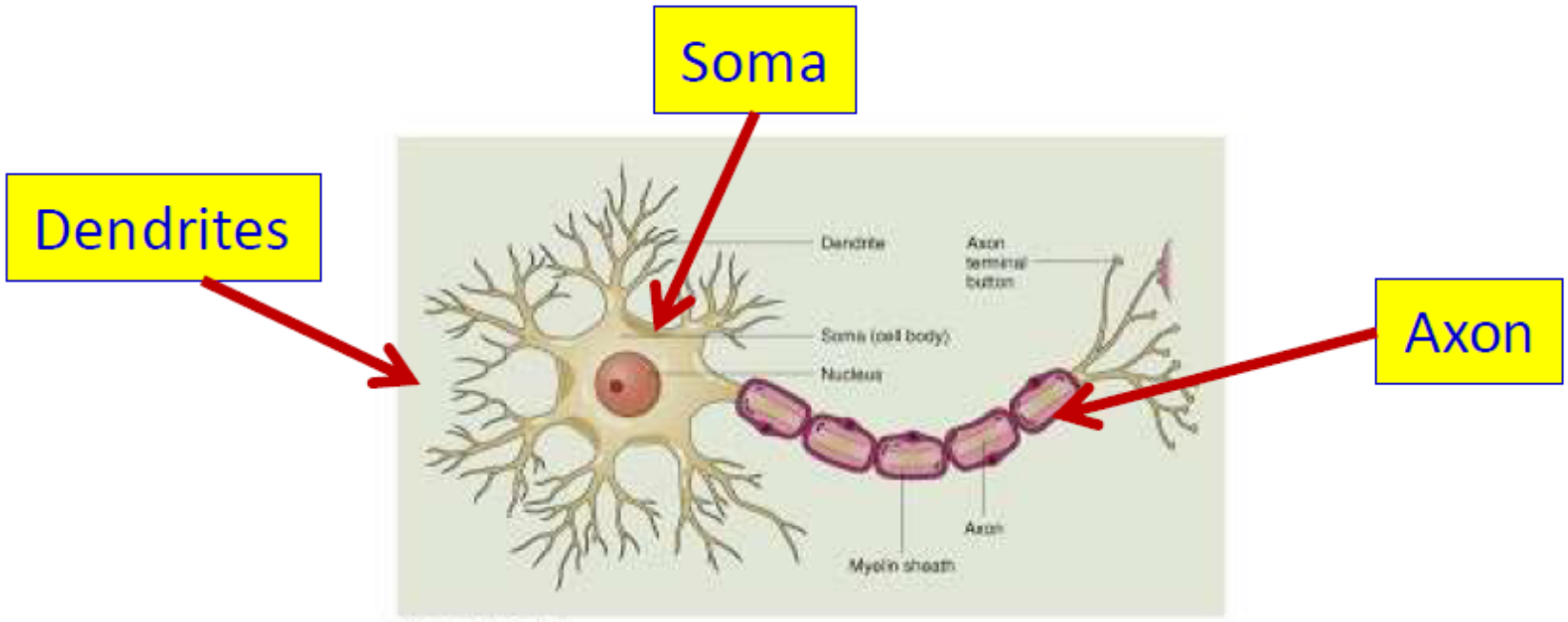
Machine learning algorithms have focused primarily on sets of data points that were assumed to be independent and identically distributed (i.i.d.).

# Neural Networks

# Modeling the brain

**A neuron**

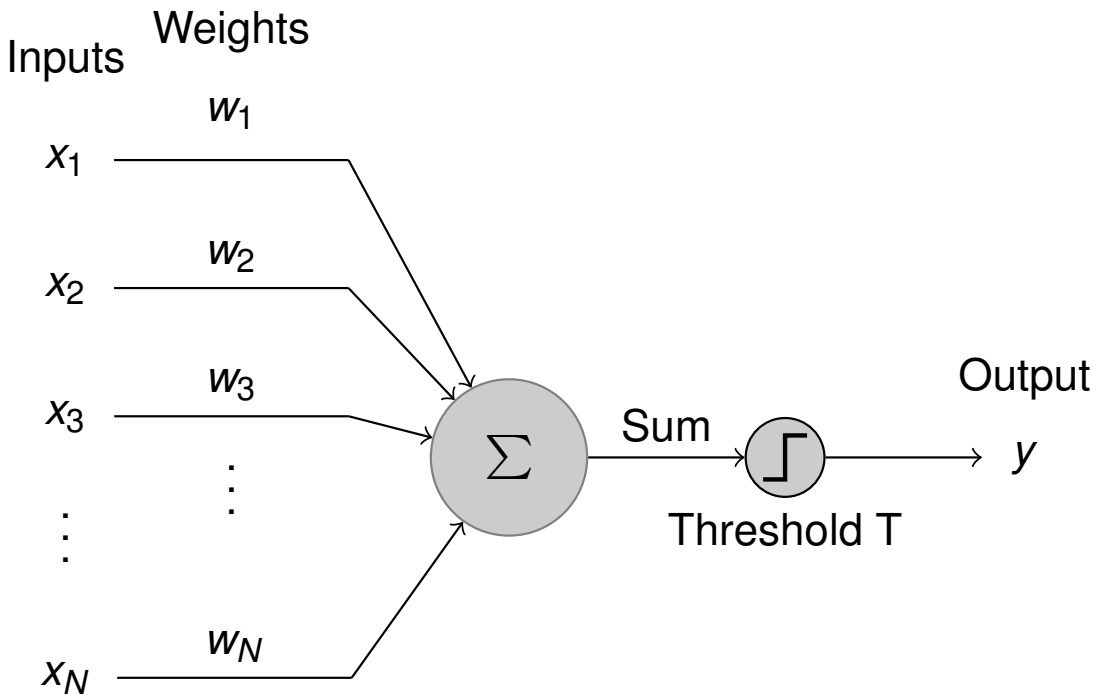
- Signals come in through the dendrites into the Soma
- A signal goes out via the axon to other neurons
  - Only one axon per neuron



# Perceptron

Number of inputs combine linearly

- Threshold logic: Fire if combined input exceeds threshold



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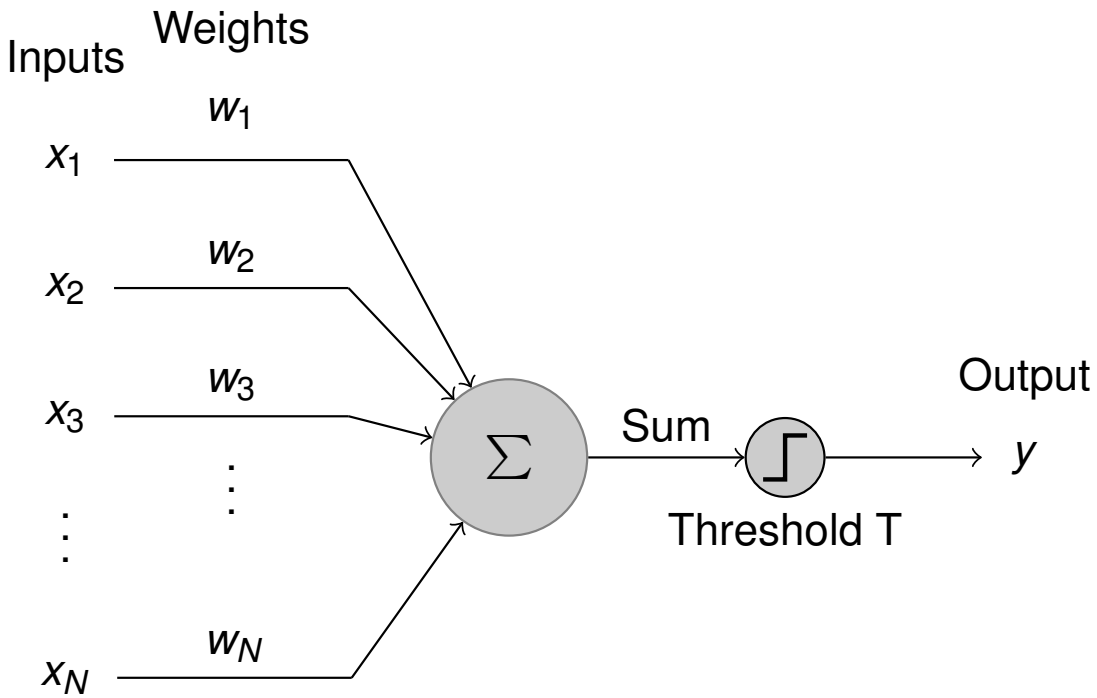
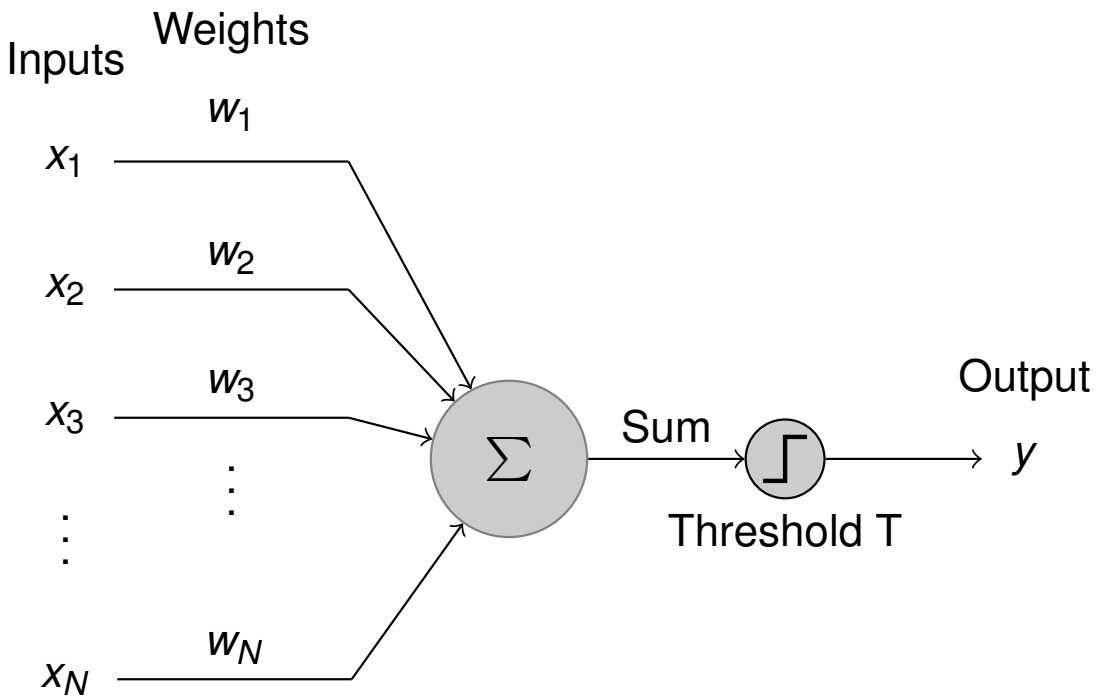



$$y = \begin{cases} 1 & \text{if} \quad \sum_i w_i x_i - T \geq 0 \\ 0 & \text{else} \end{cases}$$

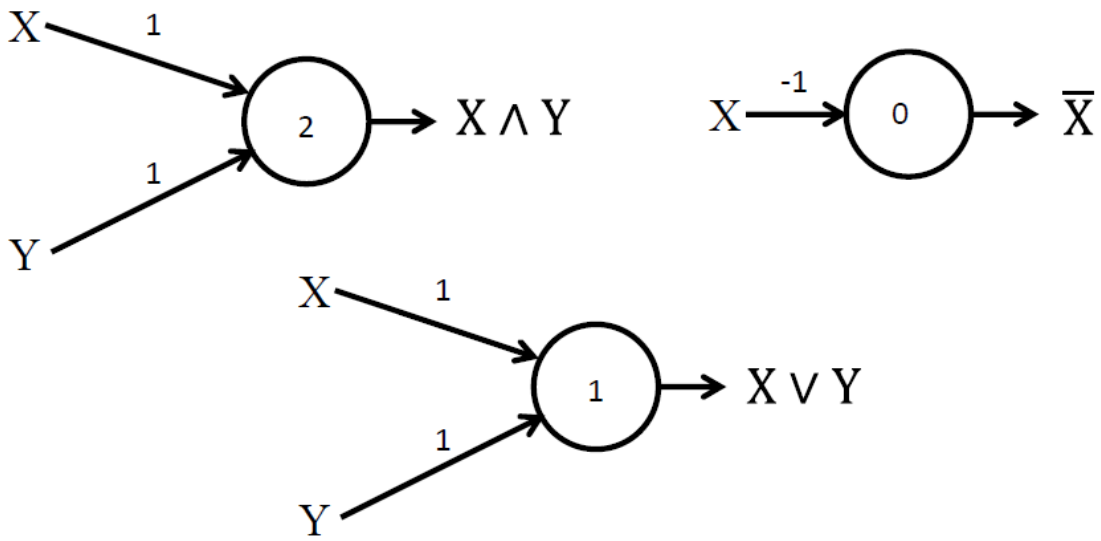
# The universal model

Originally assumed could represent any Boolean circuit and perform any logic

- "The embryo of an electronic computer that [the Navy] expects will be able to walk, talk, see, write, reproduce itself and be conscious of its existence," New York Times (8 July) 1958
- "Frankenstein Monster Designed by Navy That Thinks," Tulsa, Oklahoma Times 1958



# Perceptron

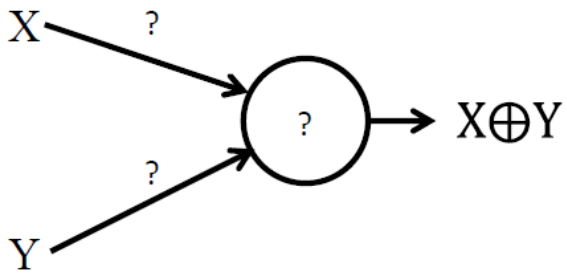



Values shown on edges are weights, numbers in the circles are thresholds ($X, Y \in \{0, 1\}$)

- Easily shown to mimic any Boolean gate
- But ...

# Perceptron

No solution for XOR!
Not universal!

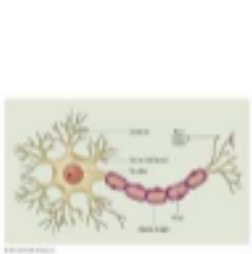


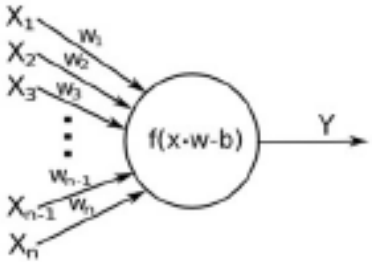

Values shown on edges are weights, numbers in the circles are thresholds ($X, Y \in \{0, 1\}$)

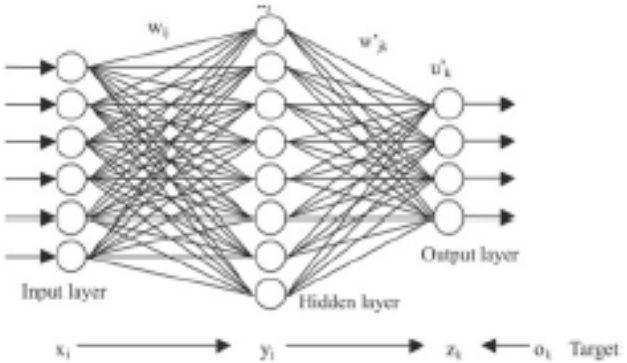
- Easily shown to mimic any Boolean gate
- But ...

# A single neuron is not enough

- Individual elements are weak computational elements
  - Marvin Minsky and Seymour Papert, 1969, Perceptrons: An Introduction to Computational Geometry
- Networked elements are required

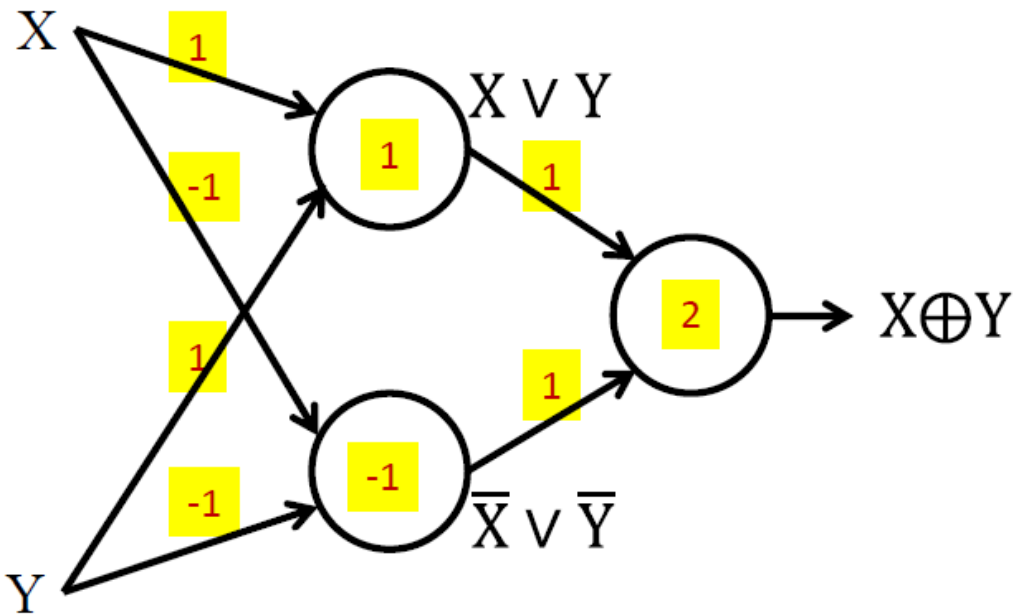




# Multi-layer perceptron!

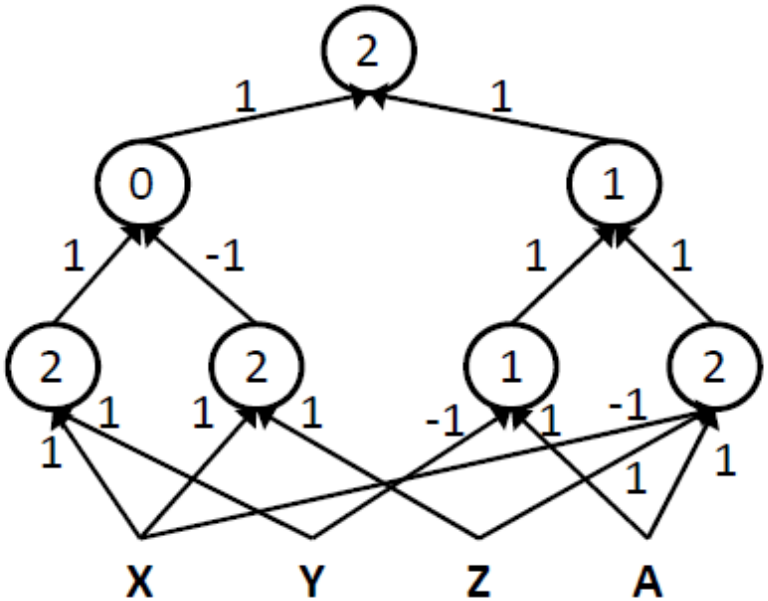
**XOR**



# Multi-layer perceptrons (MLPs)

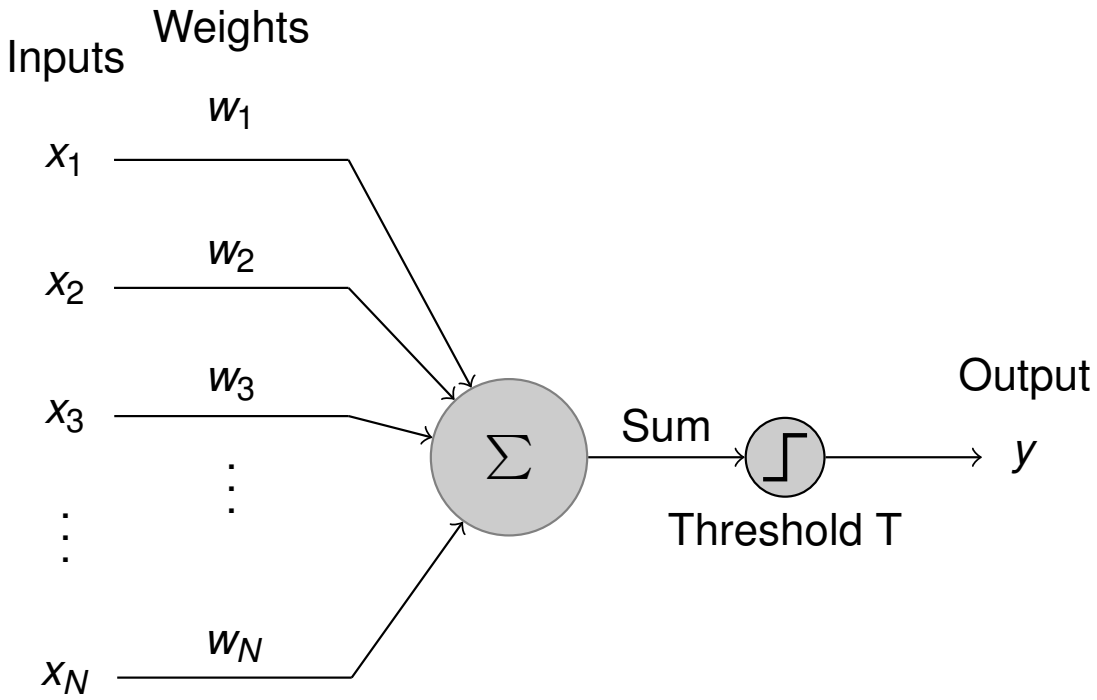
- MLPs can compute *any* Boolean function
  - Any function over any number of inputs and any number of outputs

$$((A\&\bar{X}\&Z)|(A\&\bar{Y}))\&((X\ \&\ Y)|\overline{(X\&Z)})$$



# The perceptron with real inputs

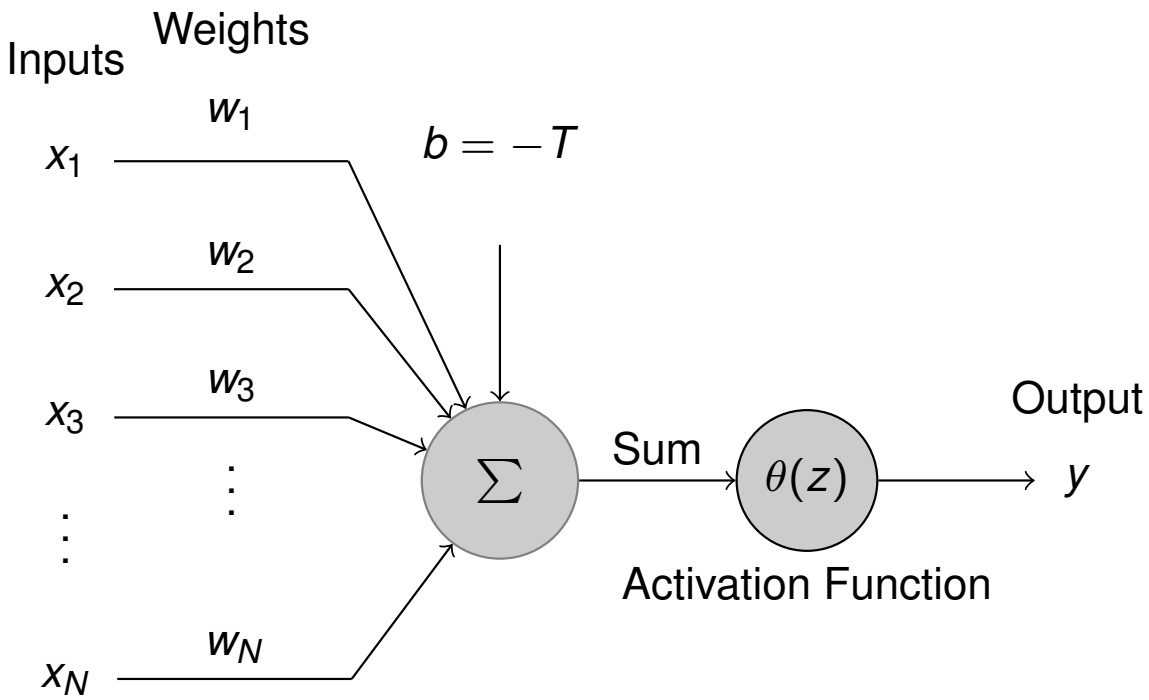
- $x_1, x_2, \ldots, x_n$ are real valued
- $w_1, w_2, \ldots, w_n$ are real valued
- Unit "fires" if weighted input exceeds a threshold




$$y = \begin{cases} 1 & \text{if} \quad \sum_i w_i x_i - T \geq 0 \\ 0 & \text{else} \end{cases}$$

# The perceptron with real inputs

- An alternate view:
  - A threshold "activation" $\theta(z)$ operates on the weighted sum of inputs plus a bias
  - $\theta(z)$ outputs 1 if z is non-negative, 0 otherwise
- Unit "fires" if weighted input exceeds a threshold



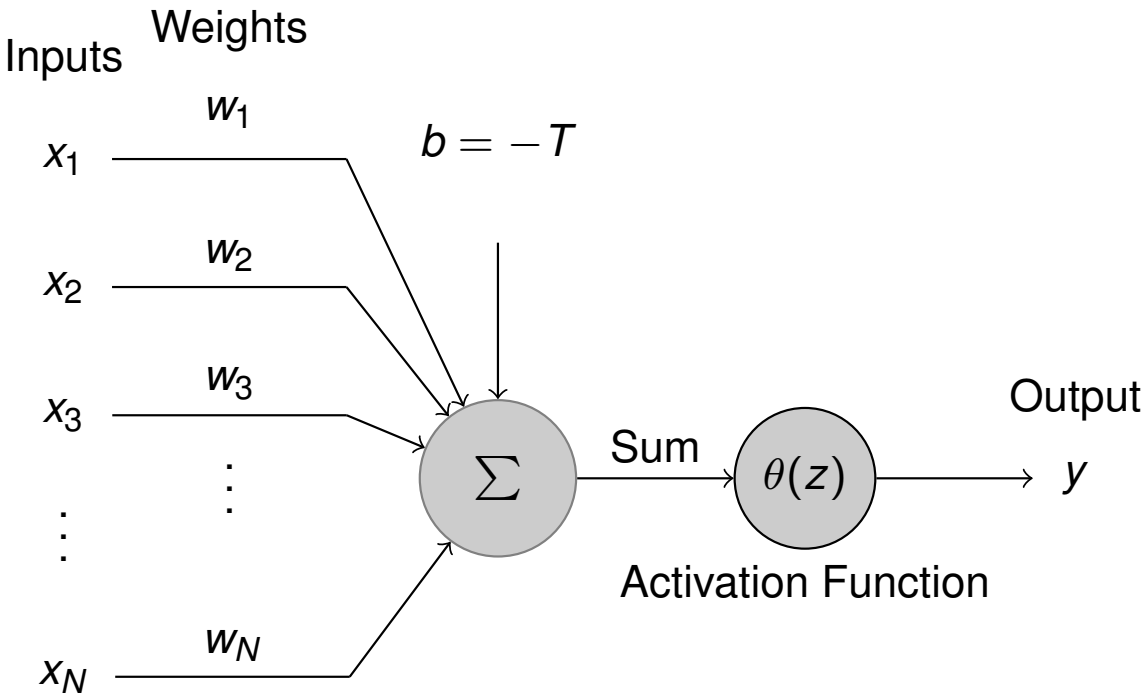

$$z = \sum_i w_i x_i + b$$

$$y = \theta(z) = \begin{cases} 1 & \text{if} \quad z \geq 0 \\ 0 & \text{else} \end{cases}$$

# Perceptron

The bias can also be viewed as the weight of another input component that is always set to 1

- If the bias is not explicitly mentioned, we will implicitly be assuming that every perceptron has an additional input that is always fixed at 1

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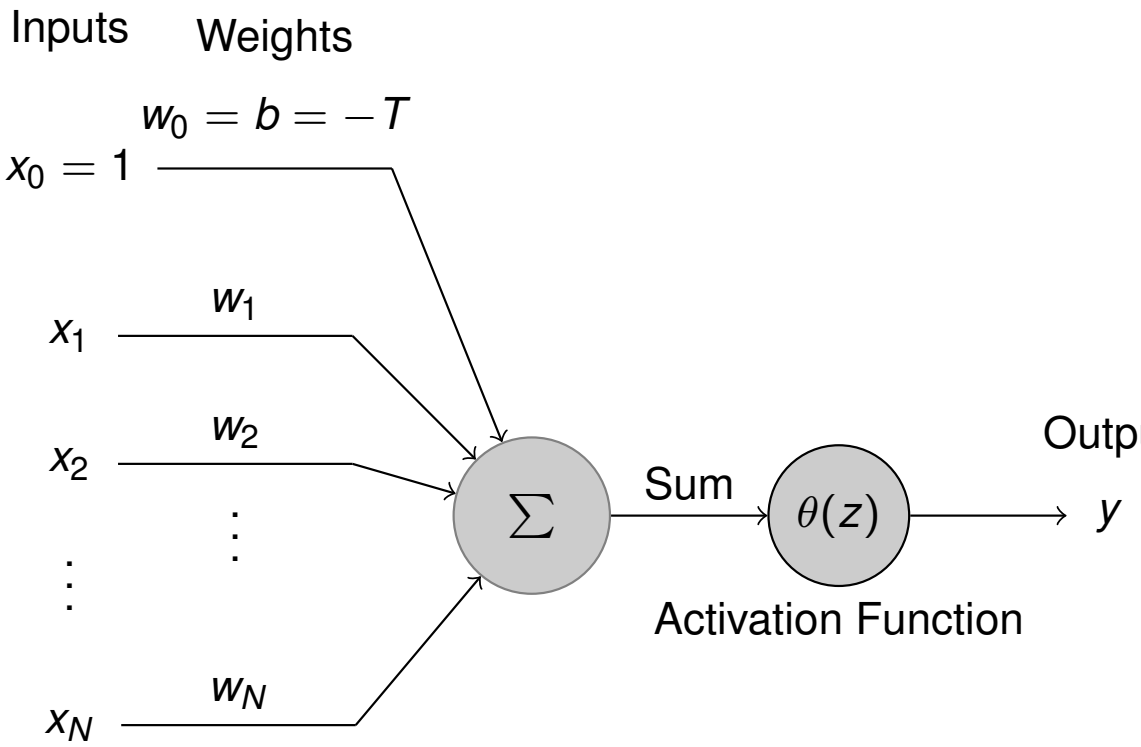
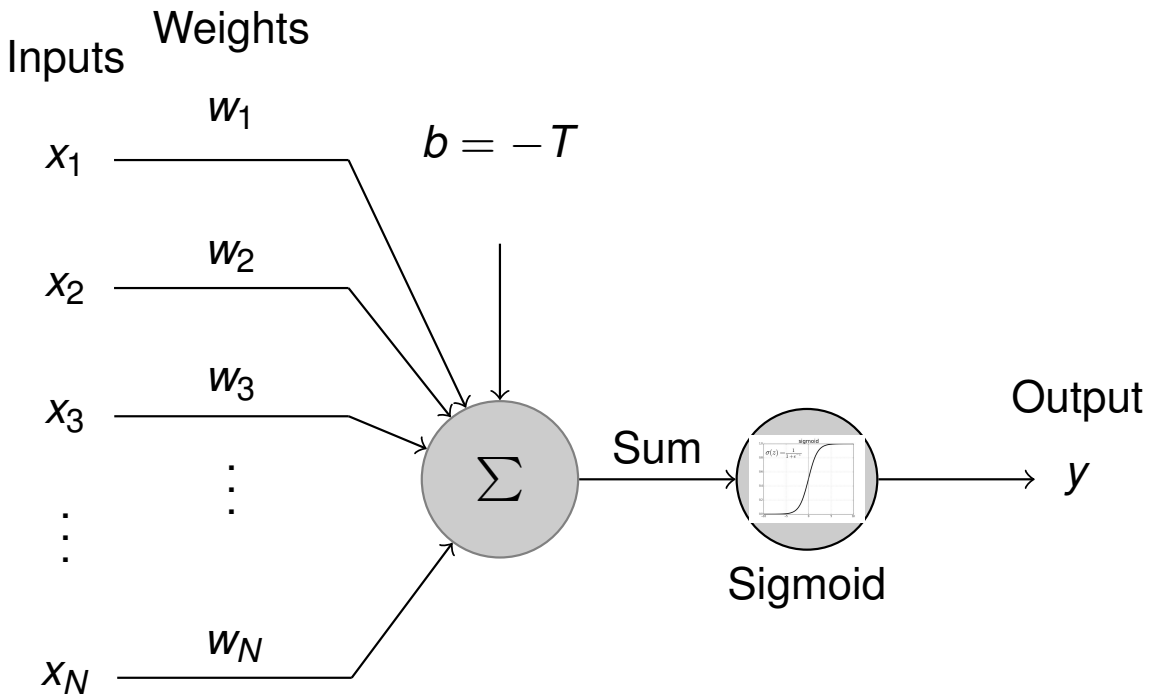



$$z = \sum_{i=1}^{N} w_i x_i + b \text{ or } z = \sum_{i=0}^{N} w_i x_i$$

$$y = \begin{cases} 1 & \text{if} \quad z \geq 0 \\ 0 & \text{else} \end{cases}$$

# A real output

- An alternate view:
  - A threshold "activation" $\theta(z)$ operates on the weighted sum of inputs plus a bias
  - $\theta(z)$ outputs 1 if z is non-negative, 0 otherwise
- The output $y$ can also be real valued
  - Sometimes viewed as the "probability" of firing
- Logistic Regression




$$y = \sigma(\sum_i w_i x_i + b)$$

$$\sigma(z) = \frac{1}{1 + \exp^{-z}}$$

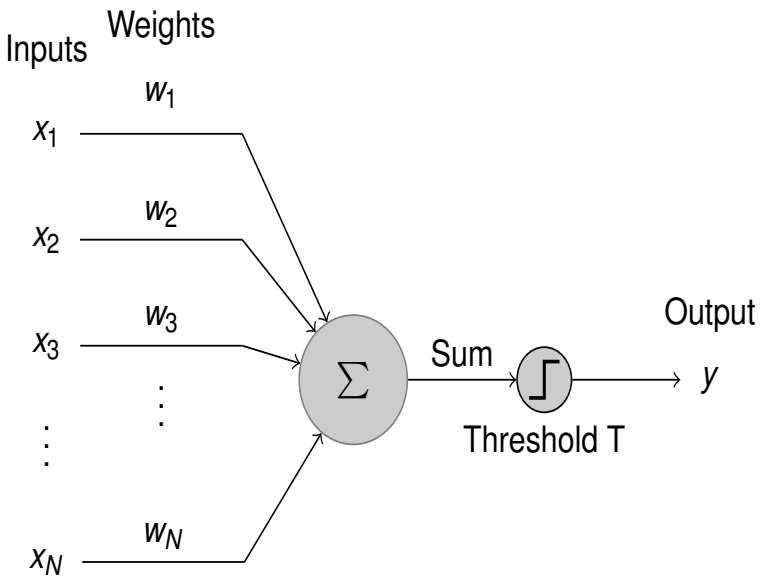
# Vectorization

$$z = \sum_i w_i x_i = \boldsymbol{w}^T \boldsymbol{x} = \begin{bmatrix} w_0 = b & w_1 & w_2 & \dots & w_{N-1} & w_N \end{bmatrix} \begin{bmatrix} 1 \\ x_1 \\ x_2 \\ \vdots \\ x_{N-1} \\ x_N \end{bmatrix}$$

$$\theta(z) = \begin{cases} 1 & \text{if} \quad z \geq 0 \\ 0 & \text{else} \end{cases}$$

# Perceptron

A perceptron is a linear classifier




$$y = \theta(\sum_i w_i x_i - T)$$

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# Perceptron

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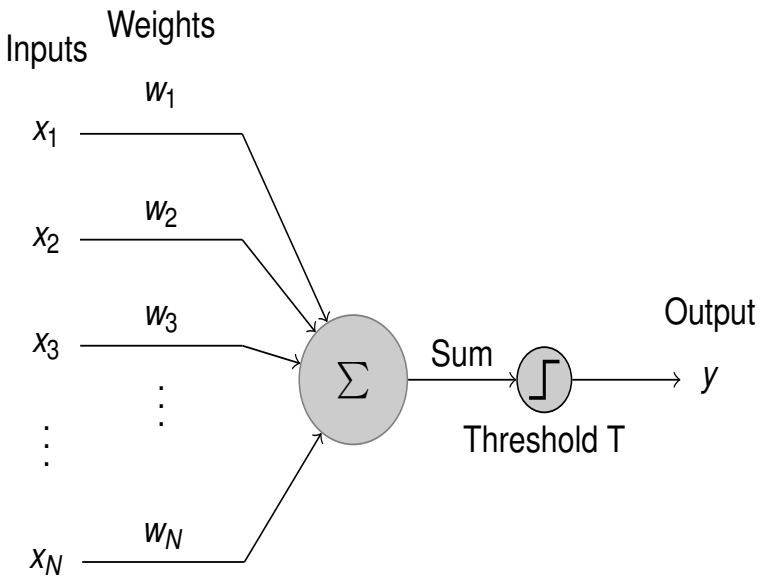


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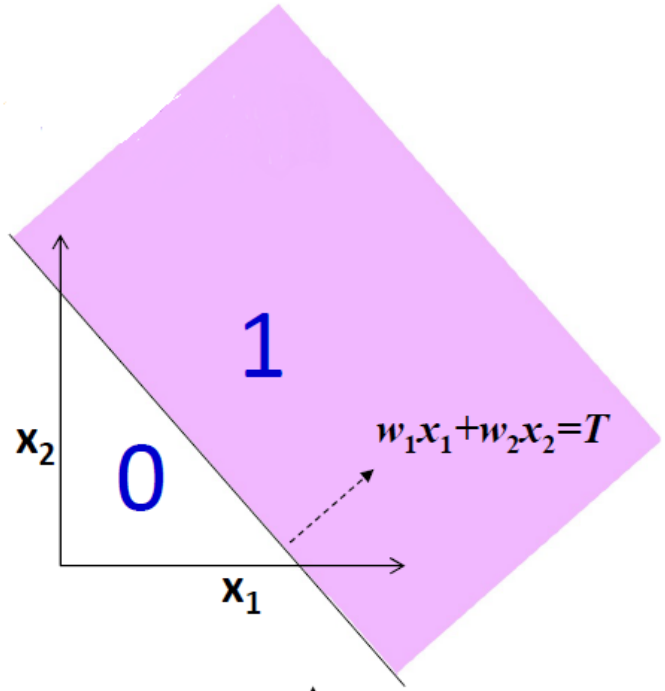
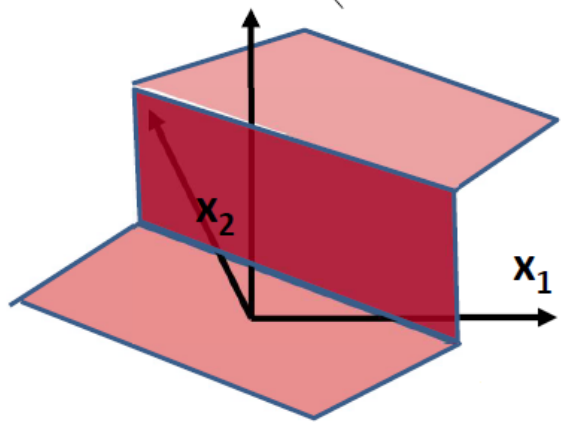


# Linear Discriminant Function

The simplest representation of a linear discriminant function is obtained by taking a linear function of the input vector so that

$$y(\mathbf{x}) = \mathbf{w}^T\mathbf{x} + w_0 \tag{2}$$

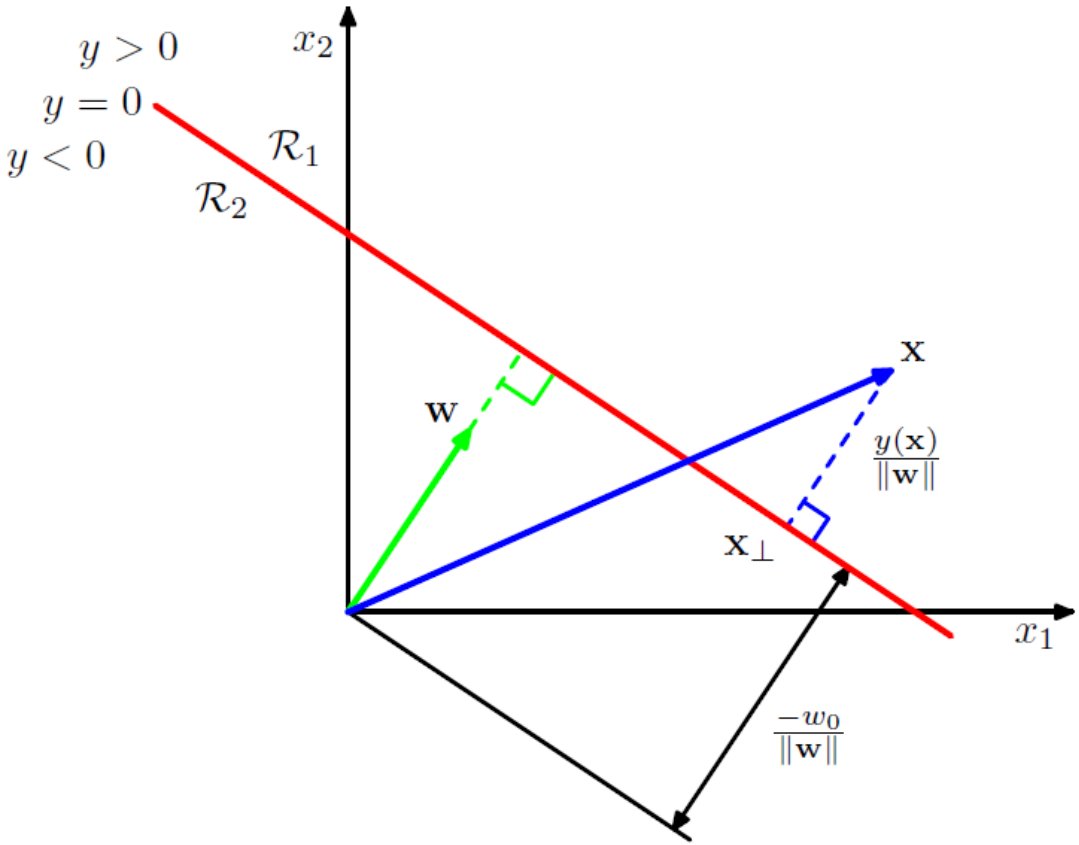
where $\mathbf{w}$ is called a weight vector, and $w_0$ is a bias (not to be confused with bias in the statistical sense).

In perceptron, an input vector $\mathbf{x}$ is assigned to class 1 if $y(\mathbf{x}) \geq 0$ and to class 0 otherwise.

The corresponding decision boundary is therefore defined by the relation $y(\mathbf{x}) \geq 0$, which corresponds to a $(D-1)$-dimensional hyperplane within the $D$-dimensional input space.

# Linear Discriminant Function

Consider two points $\mathbf{x}_A$ and $\mathbf{x}_B$ both of which lie on the decision surface. Because $y(\mathbf{x}_A) = y(\mathbf{x}_B) = 0$, we have $\mathbf{w}^T(\mathbf{x}_A - \mathbf{x}_B) = 0$ and hence the vector $\mathbf{w}$ is orthogonal to every vector lying within the decision surface, and so $\mathbf{w}$ determines the orientation of the decision surface.



# Linear Discriminant Function

Suppose that $r$ is perpendicular distance of the point $\mathbf{x}$ from the decision surface. Consider an arbitrary point $\mathbf{x}$ and let $\mathbf{x}_\perp$ be its orthogonal projection onto the decision surface, so that

$$\mathbf{x} = \mathbf{x}_\perp + r\frac{\mathbf{w}}{\| \mathbf{w} \|} \tag{3}$$

Multiplying both sides of this result by $\mathbf{w}^T$ and adding $w_0$, and making use of $y(\mathbf{x}) = w^T\mathbf{x} + w_0$ and $y(\mathbf{x}_\perp) = w^T\mathbf{x}_\perp + w_0 = 0$, we have

$$w^T\mathbf{x} + w_0 = w^T\mathbf{x}_\perp + w_0 + r\frac{\mathbf{w}^T\mathbf{w}}{\| \mathbf{w} \|}$$

$$y(\mathbf{x}) = r\frac{\| \mathbf{w} \|^2}{\| \mathbf{w} \|} \tag{4}$$

$$r = \frac{y(\mathbf{x})}{\| \mathbf{w} \|}$$

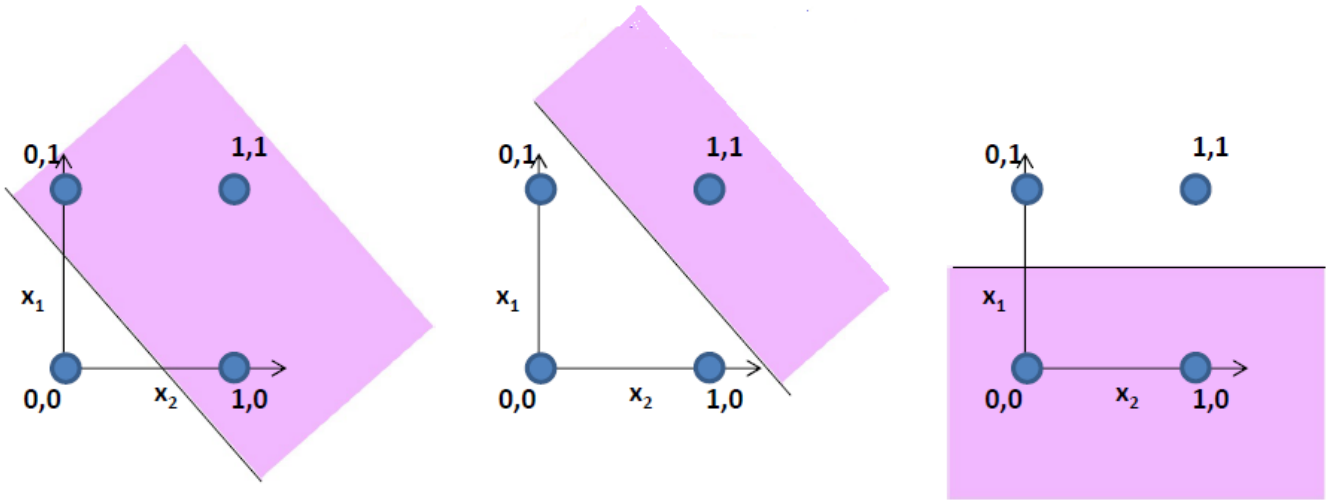
# Linear Discriminant Function

Distance of orgin from hyperplane:
Since we know that $\mathbf{w}$ is orthogonal to the hyperplane, we know that the point $\mathbf{x}'$ on the hyperplane that is closest to the origin can be represented as $\mathbf{x}' = \alpha\mathbf{w}$ for some scalar $\alpha$. Then, since $\mathbf{x}'$ is on the hyperplane, we know that $\mathbf{w}^T\mathbf{x}' + w_0 = 0 \Rightarrow \alpha\mathbf{w}^T\mathbf{w} + w_0 = 0 \Rightarrow \alpha = \frac{-w_0}{||\mathbf{w}||^2}$. The the distance from $\mathbf{x}'$ to the origin is just $||\mathbf{x}'|| = ||\alpha\mathbf{w}|| = \alpha * ||\mathbf{w}|| = \frac{-w_0}{||\mathbf{w}||^2}||\mathbf{w}|| = \frac{-w_0}{||\mathbf{w}||}$. This assumes that $w_0$ is negative.

# Boolean functions with a real perceptron

Boolean perceptrons are also linear classifiers

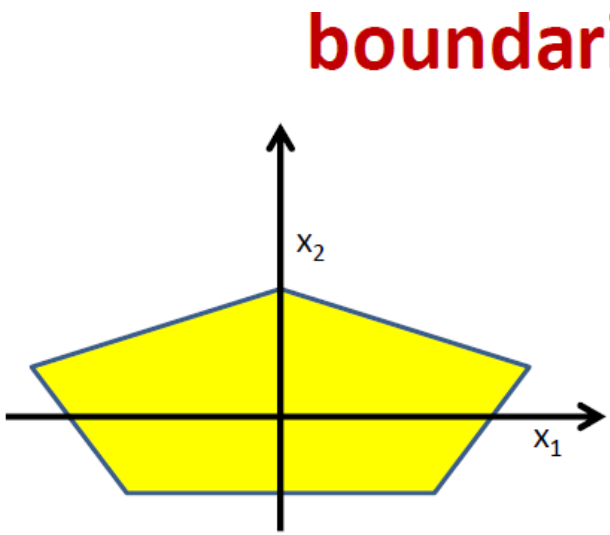
- Purple regions have output 1 in the figures
- What are these functions?
- Why can we not compose an XOR?



# A convex region

Build a network of units with a single output that fires if the input is in the coloured area

- Neurons can now be composed into “networks” to compute arbitrary classification “boundaries”



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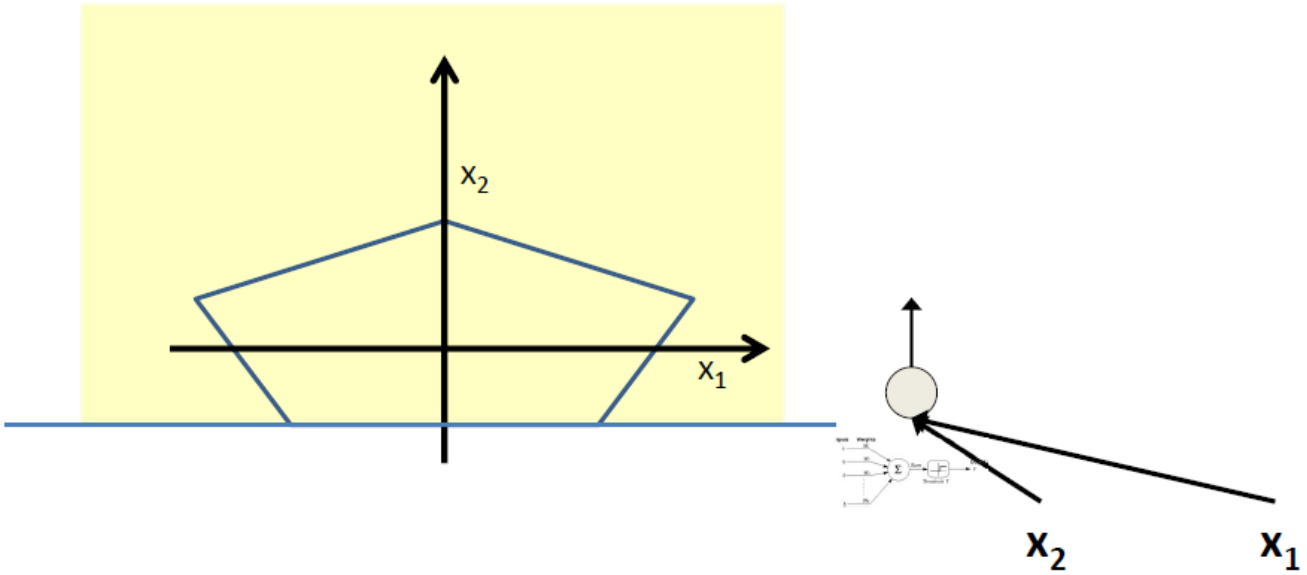

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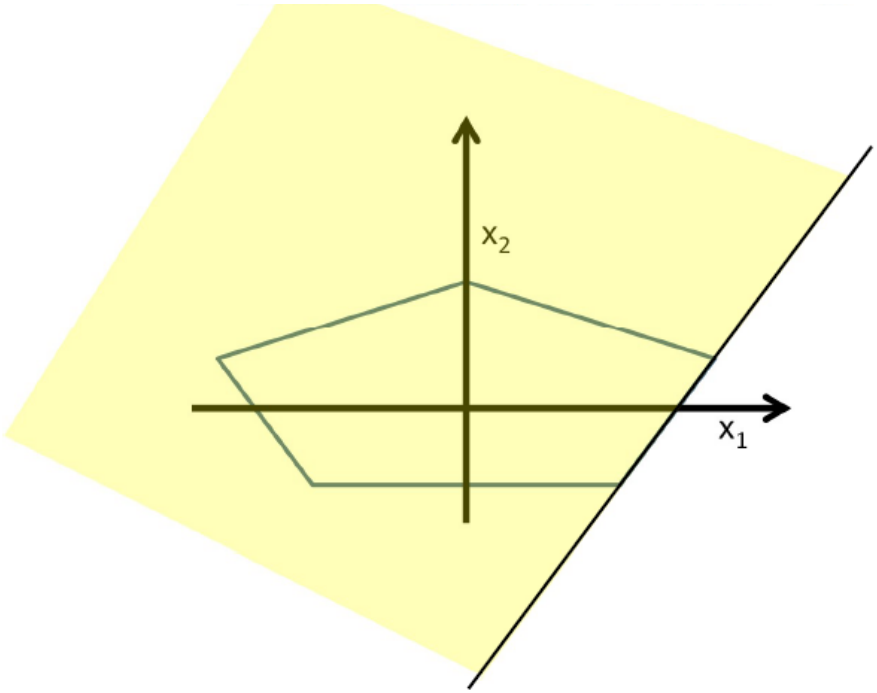


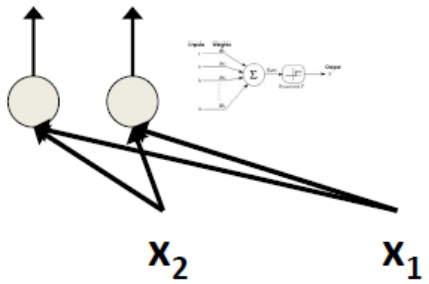

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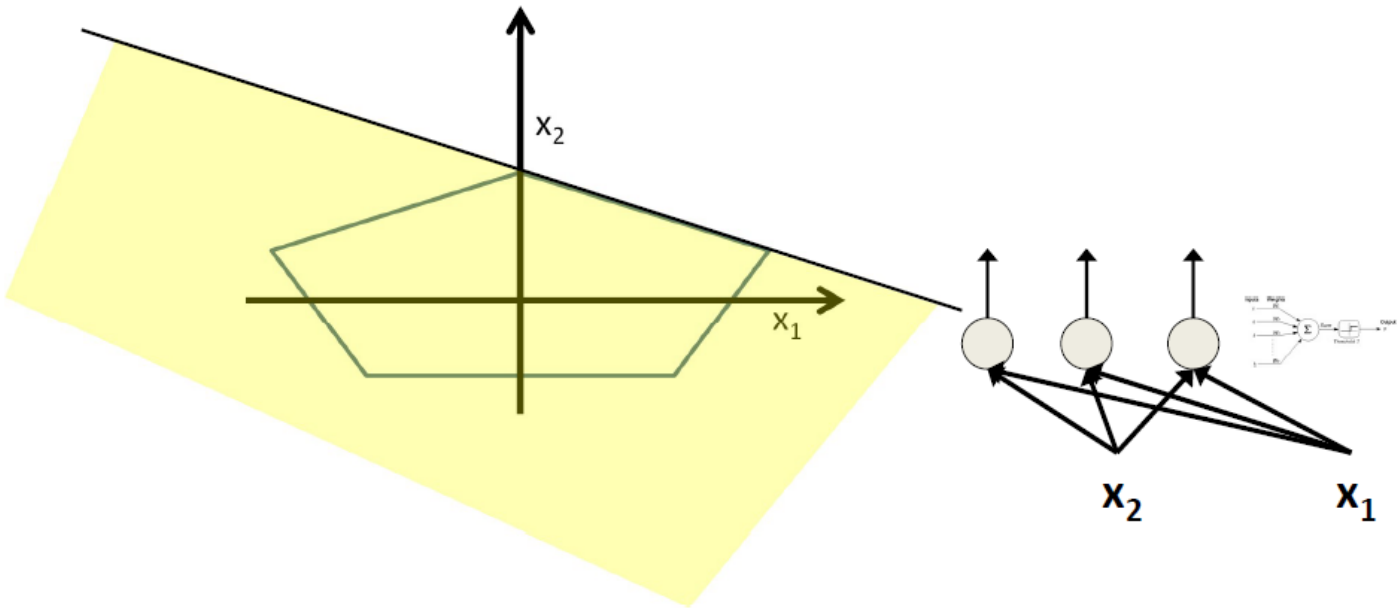

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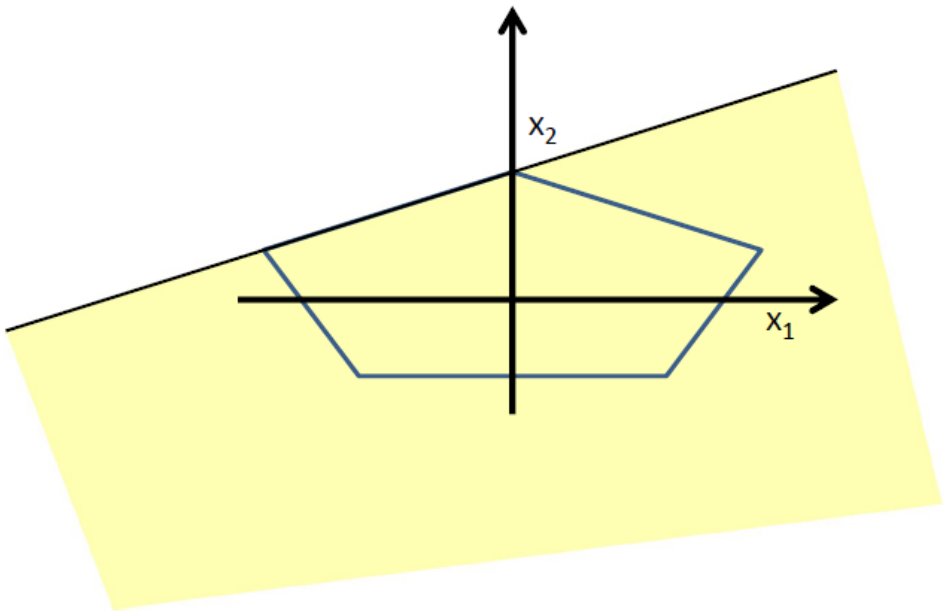


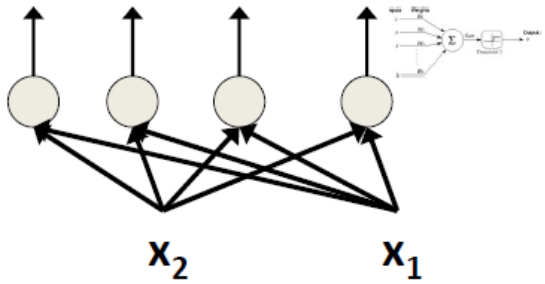

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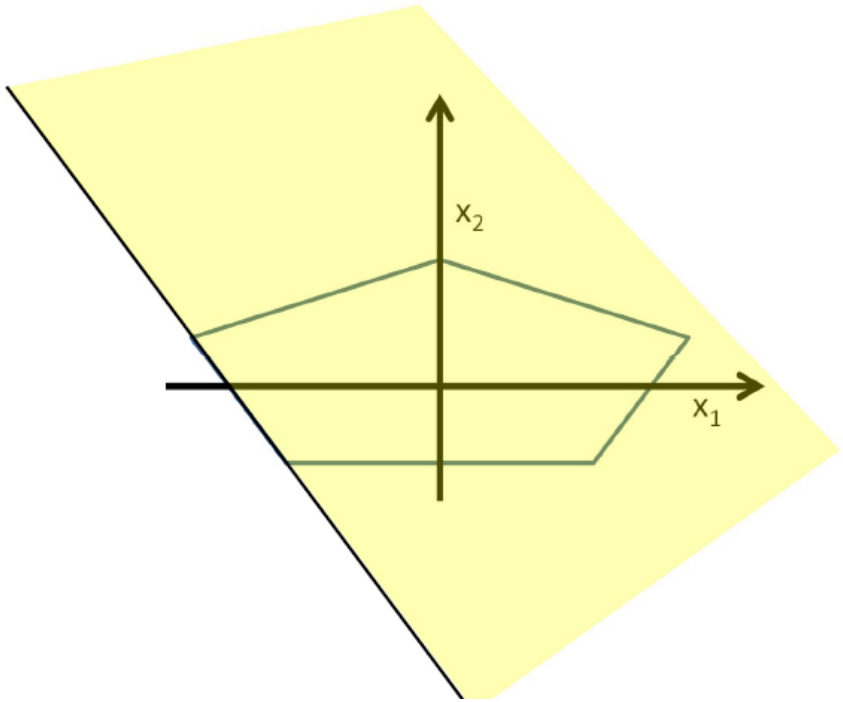


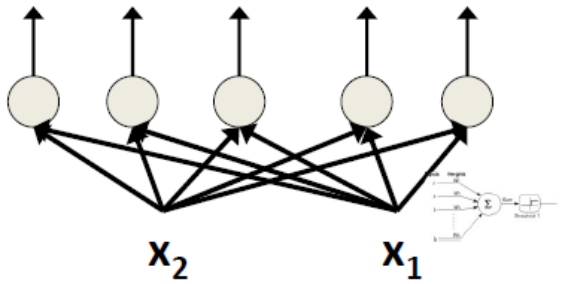

# A convex region

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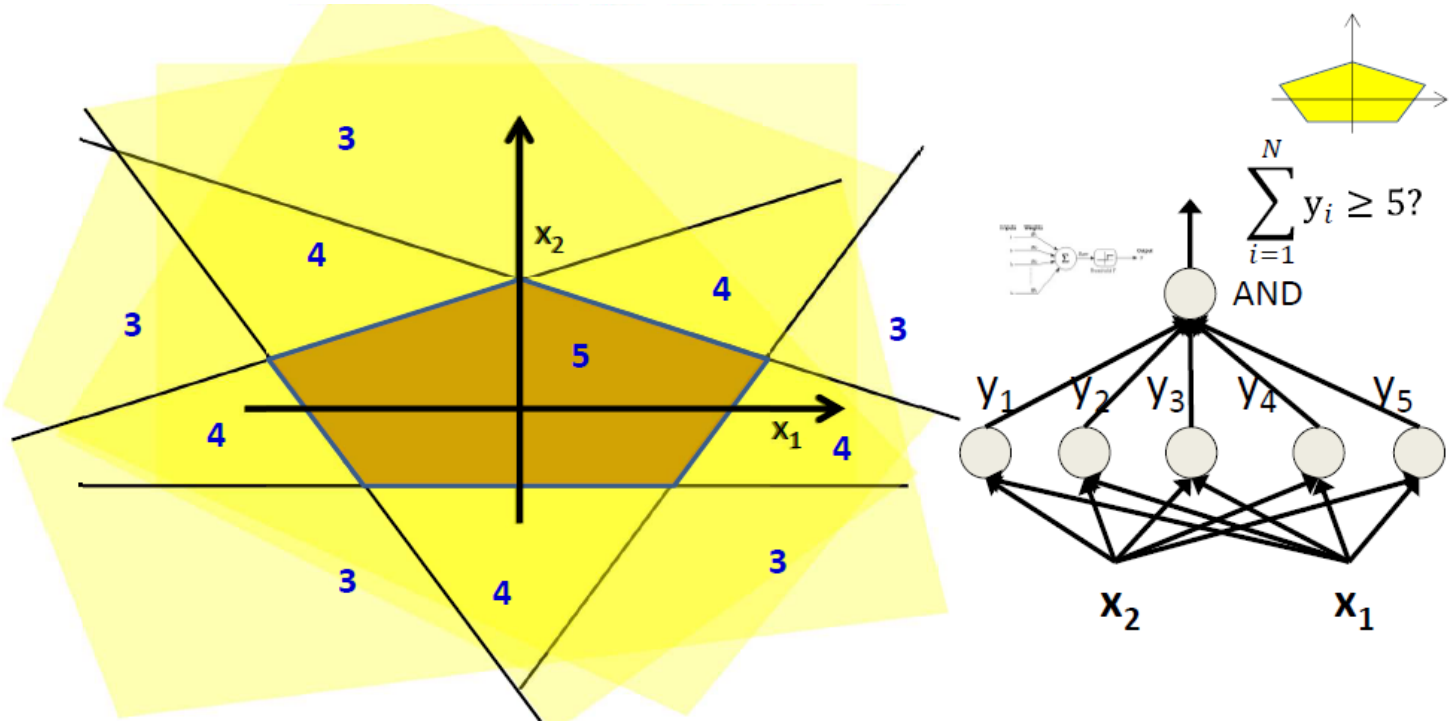

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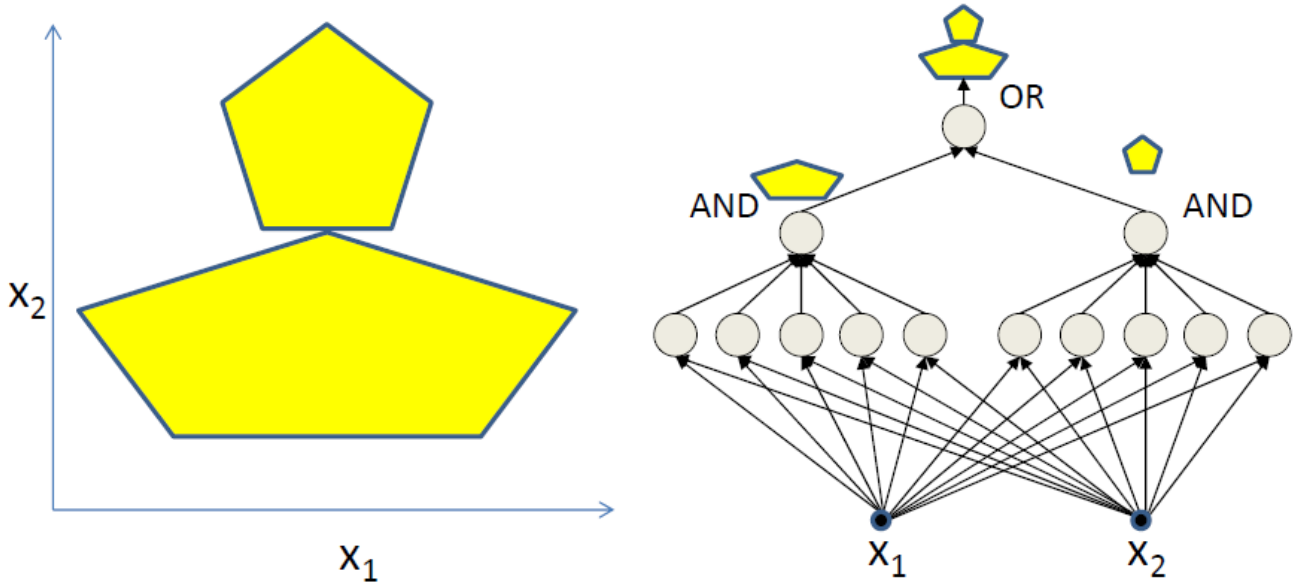
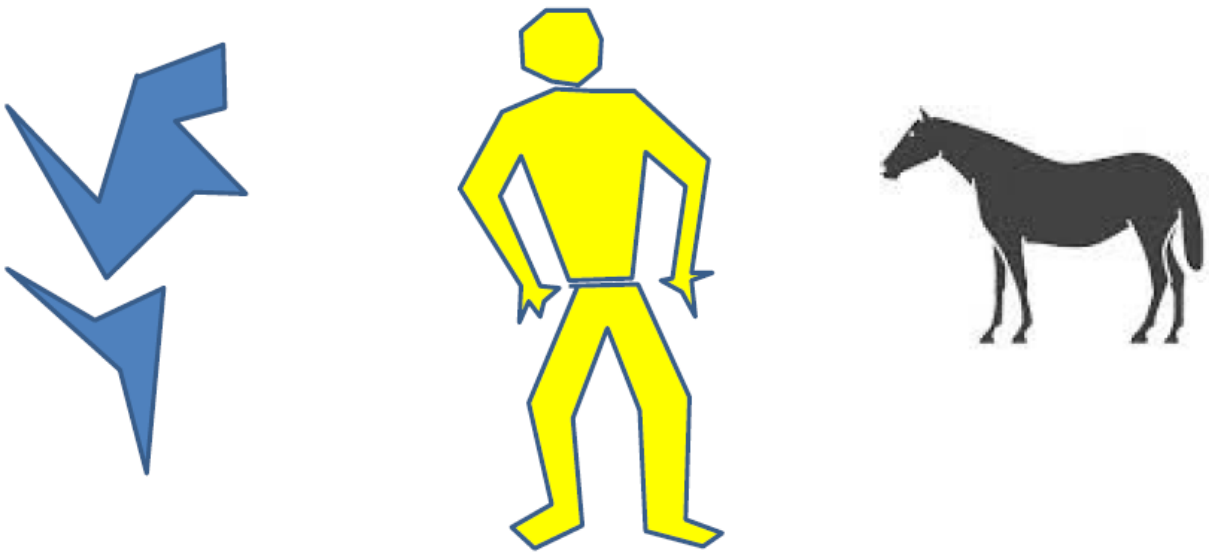


# Complex decision boundaries

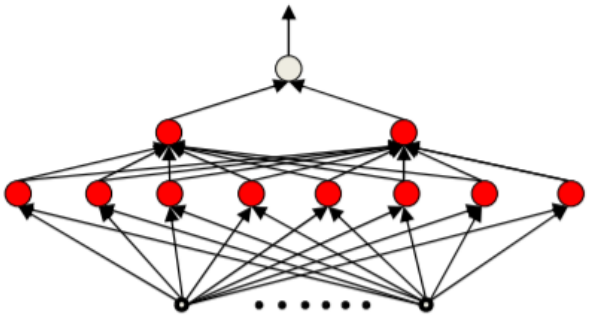
Can compose very complex decision boundaries

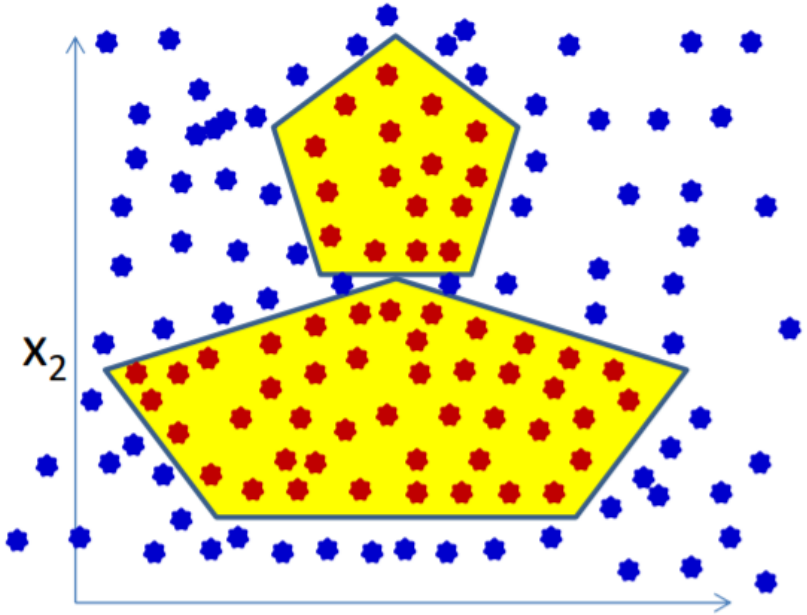


A visual proof that neural nets can compute any function

# A real problem

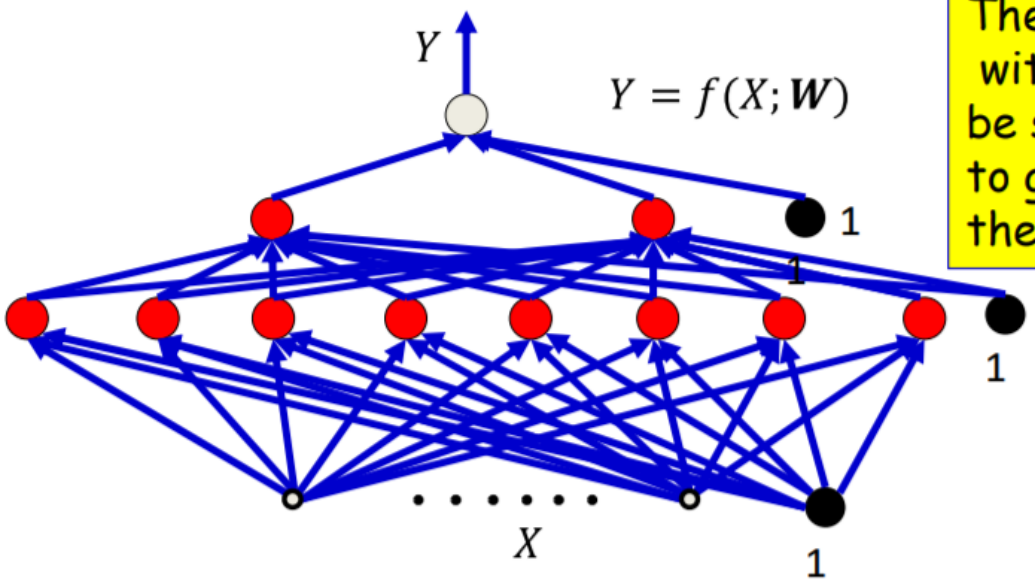
- Learn an MLP for this function
  - 1 in the yellow regions, 0 outside
- Using just the samples
- We know this can be perfectly represented using an MLP





# What we learn: The parameters of the network

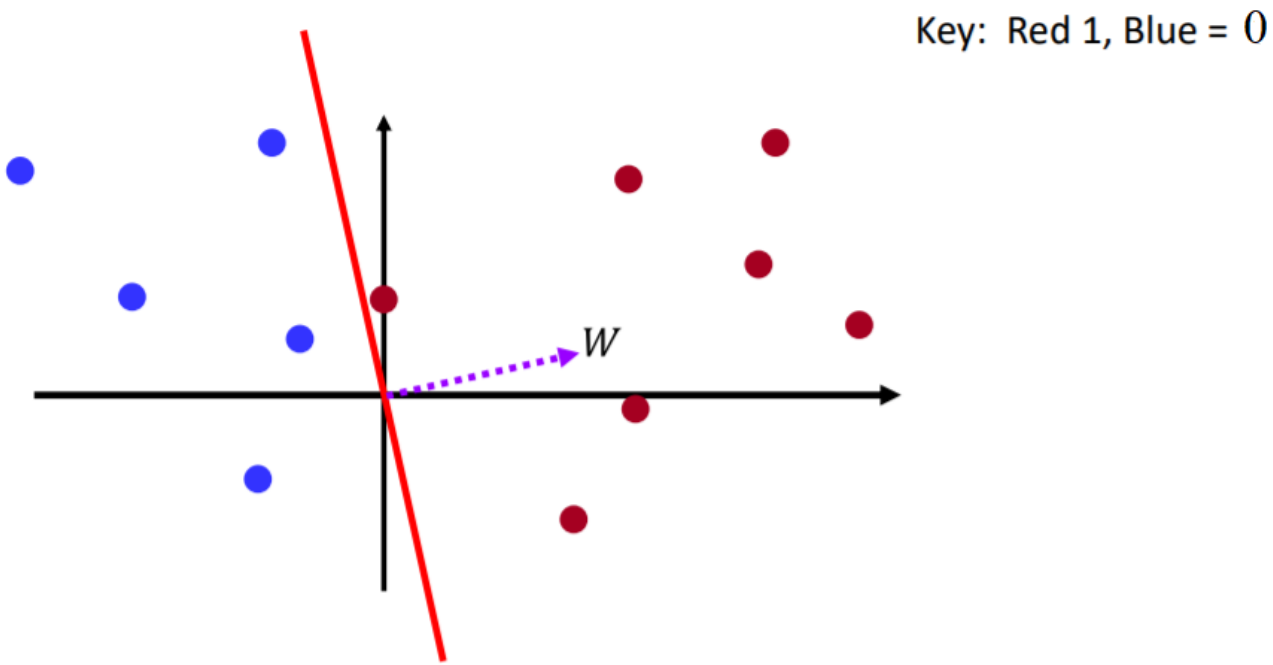
- **Given:** the architecture of the network
- **The parameters of the network:** The weights and biases
  - The weights associated with the blue arrows in the picture
- **Learning the network:** Determining the values of these parameters such that the network computes the desired function




The network is a function f() with parameters W which must be set to the appropriate values to get the desired behavior from the net

# The Perceptron Problem

- Find the hyperplane $\boldsymbol{w}^T\boldsymbol{x} = 0$ that perfectly separates the two groups of points
  - $\boldsymbol{w}^T\boldsymbol{x} = 0$ is the hyperplane comprising all $\boldsymbol{x}$'s orthogonal to vector $\boldsymbol{w}$
  - Learning the perceptron $=$ finding the weight vector $\boldsymbol{w}$ for the separating hyperplane
  - $\boldsymbol{w}$ points in the direction of the positive class

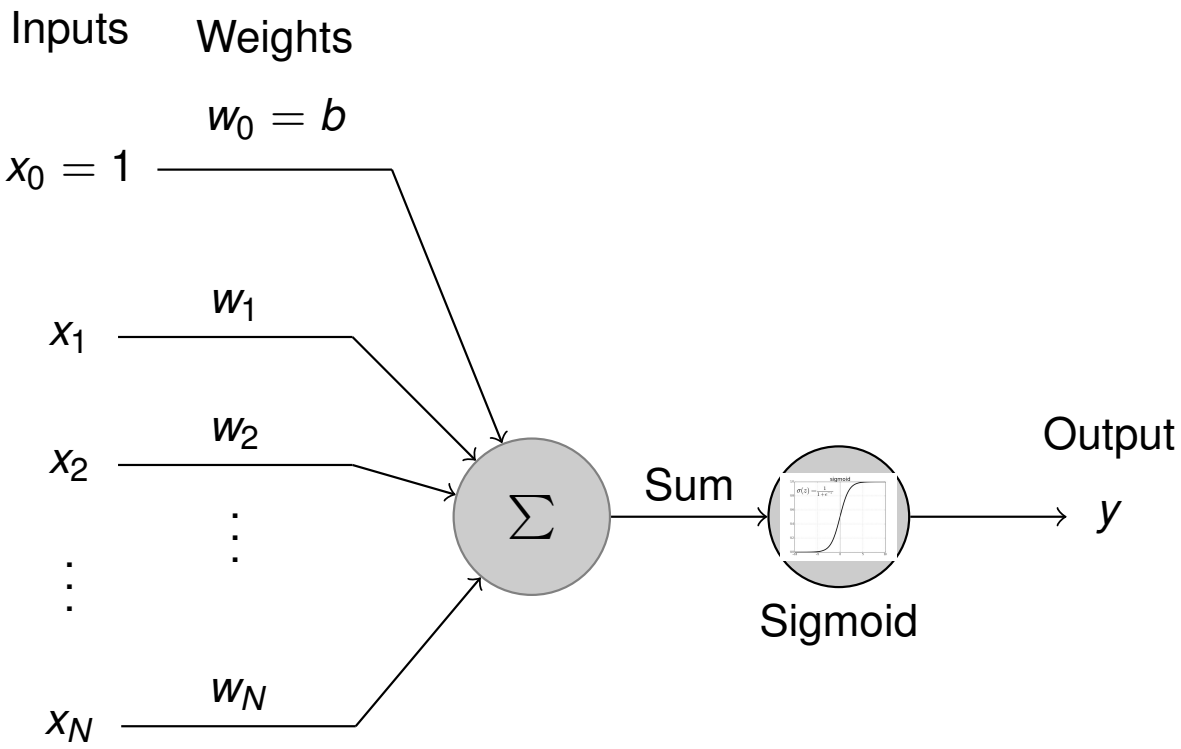


# Logistic Regression

# Logistic regression

It is the perceptron with a sigmoid activation

- It actually computes the probability that the input belongs to class 1



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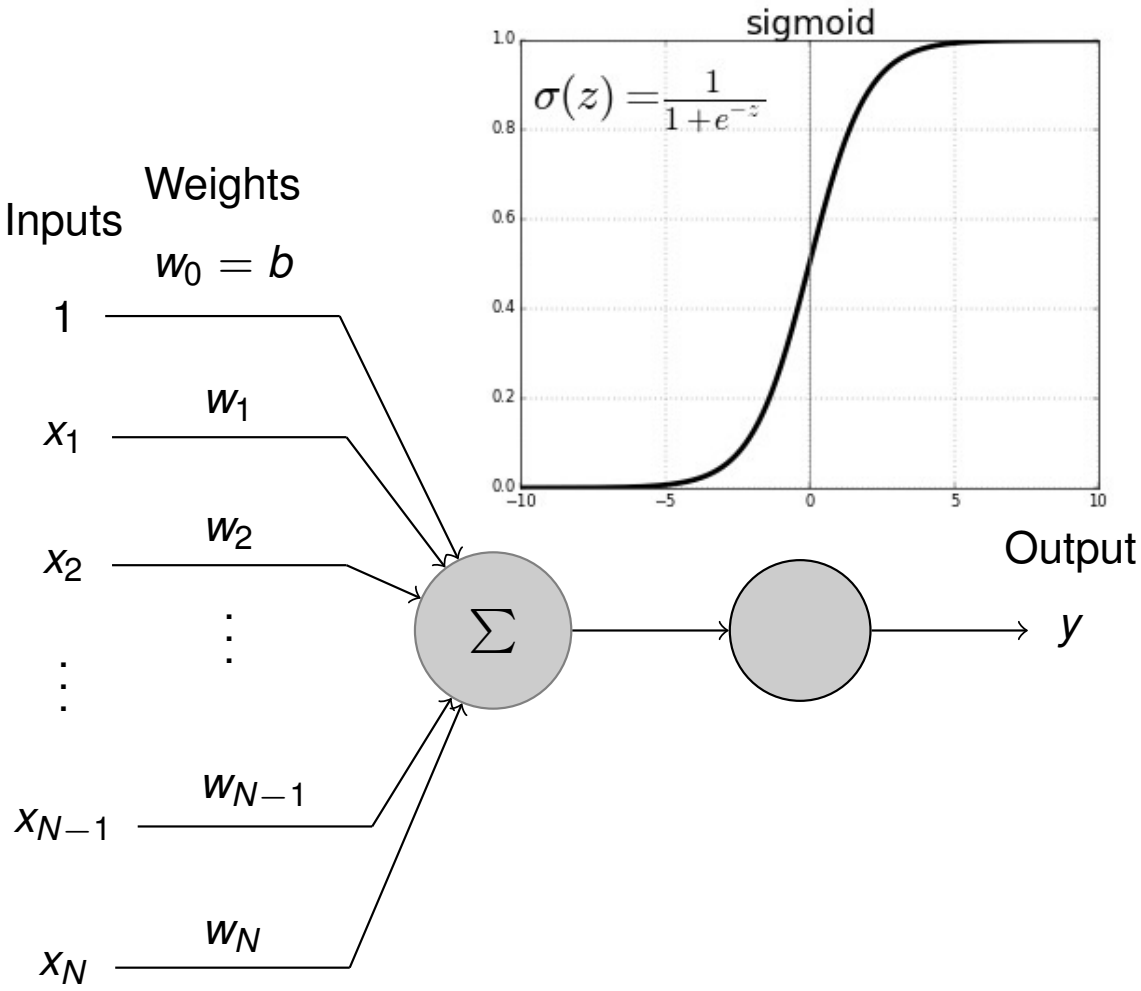


$$z = \sum_i w_i x_i$$

$$p(y = 1|x) = \sigma(z) = \frac{1}{1 + \exp(-z)}$$

$$y = \begin{cases} 1 & \text{if} \quad \sigma(z) \geq \frac{1}{2} \\ 0 & \text{if} \quad \sigma(z) < \frac{1}{2} \end{cases}$$

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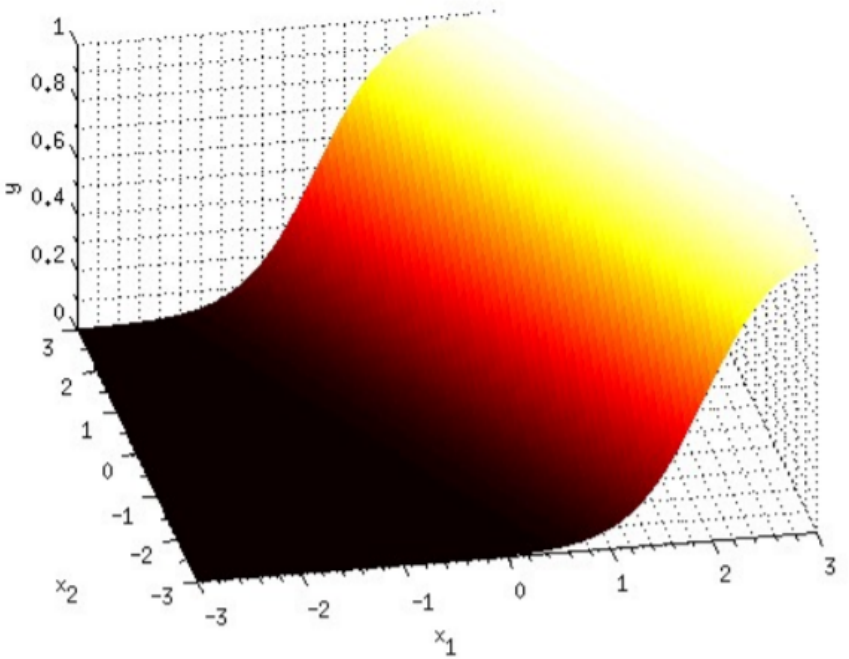
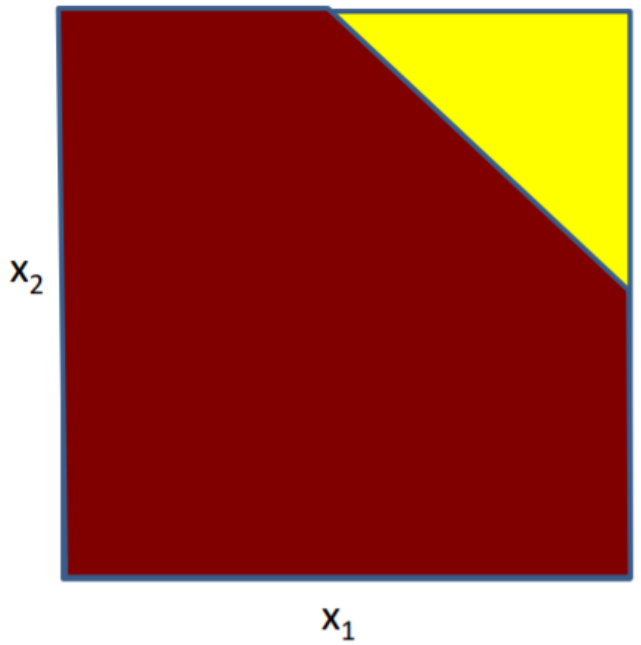



When X is a 2-D variable

Decision: y > 0.5?




$$P(Y = 1|X) = \frac{1}{1 + \exp\left(-\sum_i w_i x_i - b\right)}$$

# Vectorization

$$z = \sum_i w_i x_i = \boldsymbol{w}^T \boldsymbol{x} = \begin{bmatrix} w_0 = b & w_1 & w_2 & \dots & w_{N-1} & w_N \end{bmatrix} \begin{bmatrix} 1 \\ x_1 \\ x_2 \\ \vdots \\ x_{N-1} \\ x_N \end{bmatrix}$$

$$f(\boldsymbol{x}, \boldsymbol{w}) = \sigma(\boldsymbol{w}^T \boldsymbol{x}) = \frac{1}{1 + \exp(-\boldsymbol{w}^T \boldsymbol{x})}$$

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- **Learning**
  - Estimate the parameters to minimize the empirical loss $L$

$$\boldsymbol{w}^* = \underset{\boldsymbol{w}}{\operatorname{argmin}}\ L(f(X, \boldsymbol{w}), \boldsymbol{y})$$

# Cross entropy

If we have two separate probability distributions $P(x)$ and $Q(x)$ over the same random variable $x$ , we can measure how different these two distributions are using the Kullback-Leibler (KL) divergence:

$$D_{KL}(P||Q) = \mathbb{E}_{x\sim P}[\log \frac{P(x)}{Q(x)}] = \mathbb{E}_{x\sim P}[\log P(x) - \log Q(x)]$$

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- KL divergence is non-negative and measures the difference between two distributions, it is often conceptualized as measuring some sort of distance between these distributions. However, it is not a true distance measure because it is not symmetric

# Cross entropy

- Minimizing loss function

$$\underset{Q(x)}{\operatorname{argmin}} D_{KL}(P||Q) = \sum_i p_i(x) \log p_i(x) - \sum_i p_i(x) \log q_i(x)$$

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**Example**

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$$CrossEntropy(P(x), Q(x)) = -1 \times \log(1 - 0.7) - 0 \times \log 0.7 = 1.2$$

# Logistic regression loss function

- Logistic Regression

$$P(y = 1|\boldsymbol{x}^{(i)}; \boldsymbol{w}) = f(\boldsymbol{x}^{(i)}, \boldsymbol{w})$$
$$P(y = 0|\boldsymbol{x}^{(i)}; \boldsymbol{w}) = 1 - f(\boldsymbol{x}^{(i)}, \boldsymbol{w})$$
$$y^{(i)} \in \{0, 1\}$$

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- Cross entropy as the loss function

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**How do we find the best $w$?**

# References


- Pattern Recognition and Machine Learning, Ch.1 & Ch.4
- Deep Learning, Ch.5