Neural Networks

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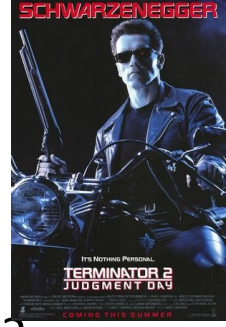
Outline

- **Overview of neural networks**
- Perceptron model
- Neural network
- Training the neural networks
  - Backpropagation (BP) algorithm

Terminator 2 (1991)



- John Connor: Can you learn stuff you haven't been programmed with so you could be... you know, more human? And not such a dork all the time?
- The Terminator: My CPU is a neural net processor; a learning computer. But Skynet pre-sets the switch to read-only when we're sent out alone.
- Sarah Connor: Doesn't want you doing too much thinking, huh?
- The Terminator: No.

Switch: weights

……

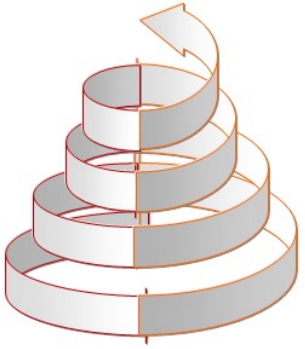
- The Terminator: The Skynet Funding Bill is passed. The system goes on-line August 4th, 1997. Human decisions are removed from strategic defense. Skynet begins to learn at a geometric rate. It becomes self-aware at 2:14 a.m. Eastern time, August 29th. In a panic, they try to pull the plug.
- Sarah Connor: Skynet fights back.
- The Terminator: Yes. It launches its missiles against the targets in Russia.
- John Connor: Why attack Russia? Aren't they our friends now?
- The Terminator: Because Skynet knows the Russian counter-attack will eliminate its enemies over here.

http://www.imdb.com/title/tt0103064/quotes

人工神经网络简史

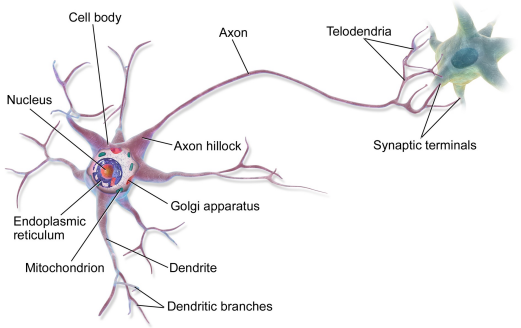
- 1943:美国心理学家McCulloch和数学家Pitts提出神经元数学模型(M-P)
- 1949:心理学家Hebb提出了改变神经元间连接强度的Hebb规则
- 1957:计算机科学家Rosenblatt用硬件完成了最早的神经网网络模型，称之为感知器(Perceptron)，模拟生物的感知和学习能力。
- 1969:Minskey和Papert发表了《Perceptron》一一书指出了Perceptron无科学价值而言，连XOR逻辑分类都做不到，只能作线性划分。
- 1982:加州大学物理学家Hopfield提出模拟人类记忆的递归神经网络模型，并用电路实现。
- 1985:Hinton和Terry Sejnowski)提出玻尔兹曼机(Boltzman机)模型， 表达随机过程形成结构的过程。
- 1986:Rumelhart, Hinton等提出了反向传播算法(BP)，掀起十年年高潮
- 1988:蔡少棠提出了了细胞神经网络模型
- 1990s:神经网络再次衰落

完成了螺旋上升之肯定－否定-
再肯定－再否定－出现突破



Neurons in Biology

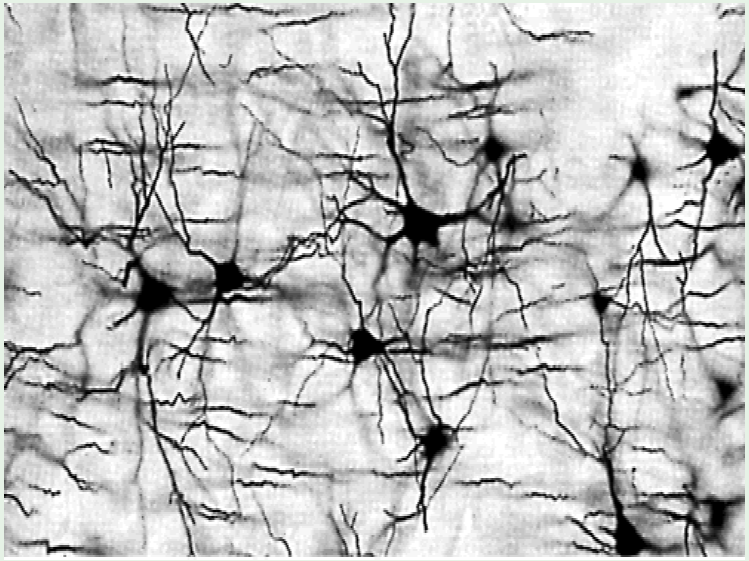
- The human brain has 100,000,000,000 neurons
- On average, each neuron is connected to 1000 other neurons
- Impulses arriving simultaneously are added together
- Sufficiently strong impulses lead to the generation of an electrical discharge (an action potential, a 'nerve impulse').
- The action potential then forms the input to the next neuron in the network.

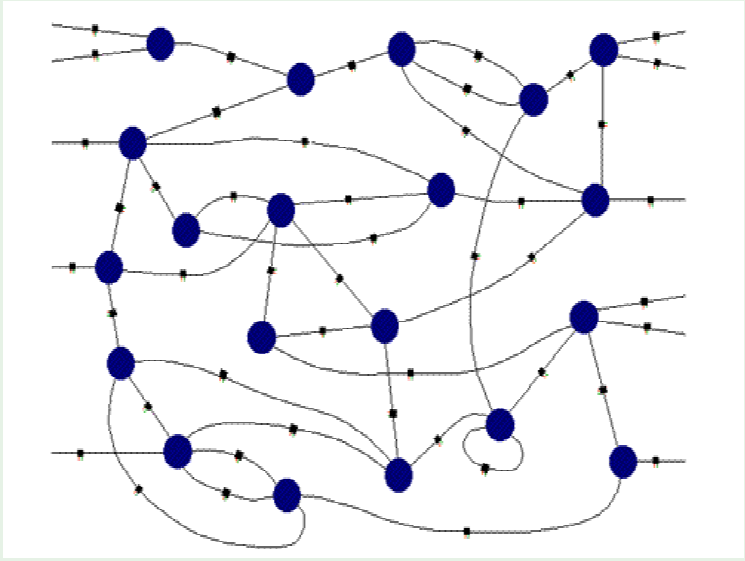


http://www.bris.ac.uk/synaptic/basics/basics-1.html

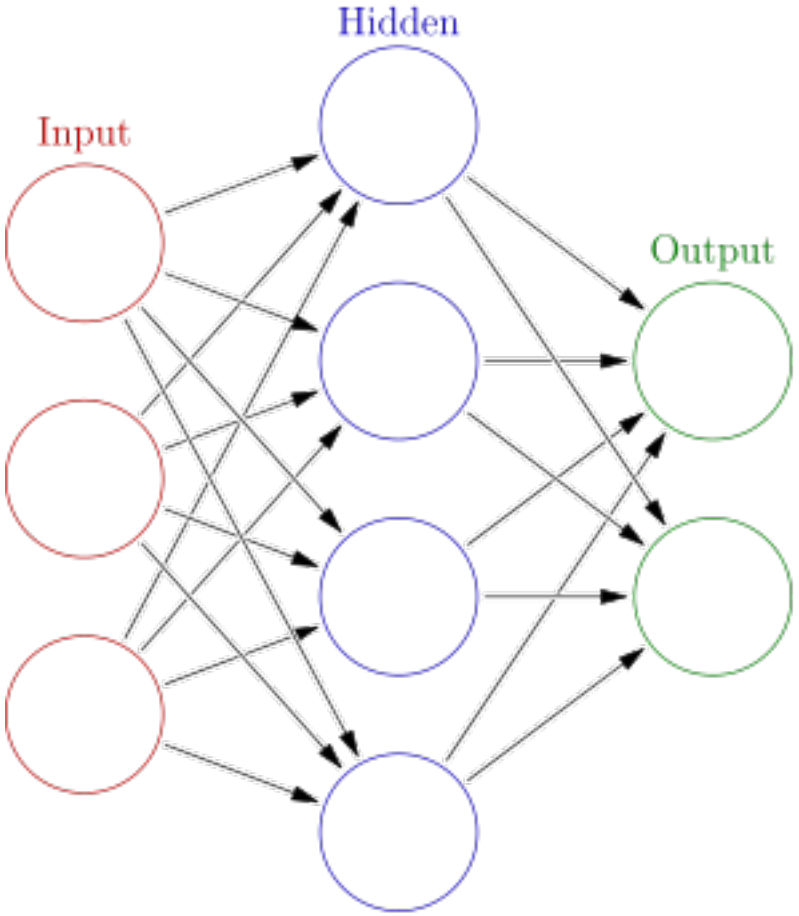
Biological inspiration

biological function $\longrightarrow$ biological structure



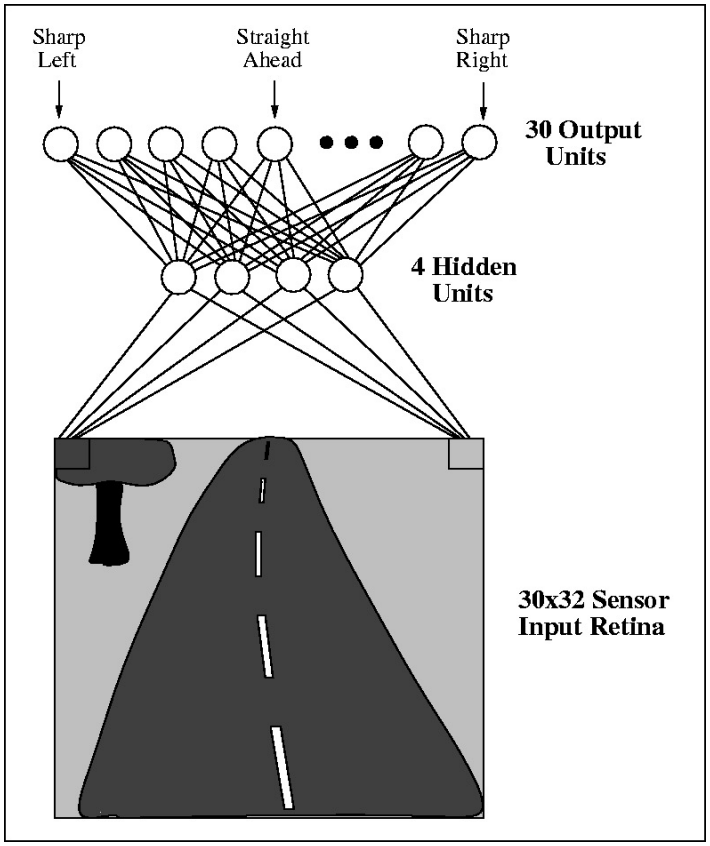


Neural Networks in Machine Learning



Applications

- ALVINN (Autonomous Land Vehicle In a Neural Network)



1990s

http://ftp.utcluj.ro/pub/docs/imaging/Autonomous_driving/Articole%20sortate/CThorpe/ALVINN%20Project%20Home%20Page.htm

The main aim of neural networks

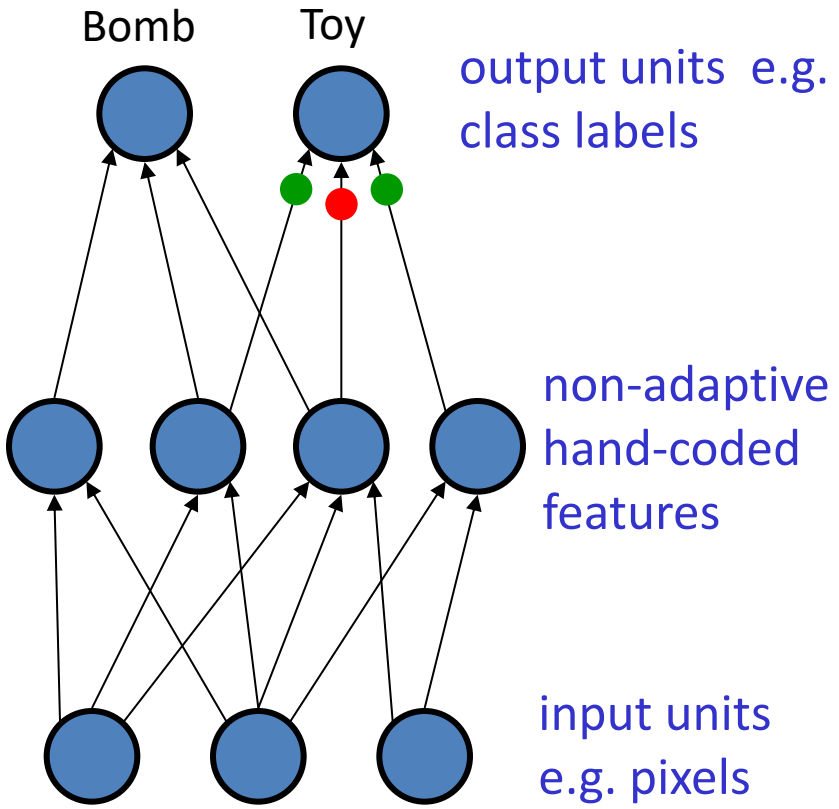
- People are much better than computers at recognizing patterns. How do they do it?
  - Neurons in the perceptual system represent features of the sensory input.
  - The brain learns to extract many layers of features. Features in one layer represent combinations of simpler features in the layer below.

- Can we train computers to extract many layers of features by mimicking the way the brain does it?
  - Nobody knows how the brain does it, so this requires both engineering insights and scientific discoveries.

From G. E. Hinton

First generation neural networks

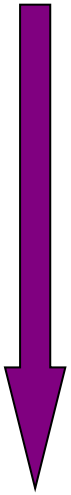
- Perceptrons (~1960) used a layer of hand-coded features and tried to recognize objects by learning how to weight these features.
  - There was a neat learning algorithm for adjusting the weights.
  - But perceptrons are fundamentally limited in what they can learn to do.



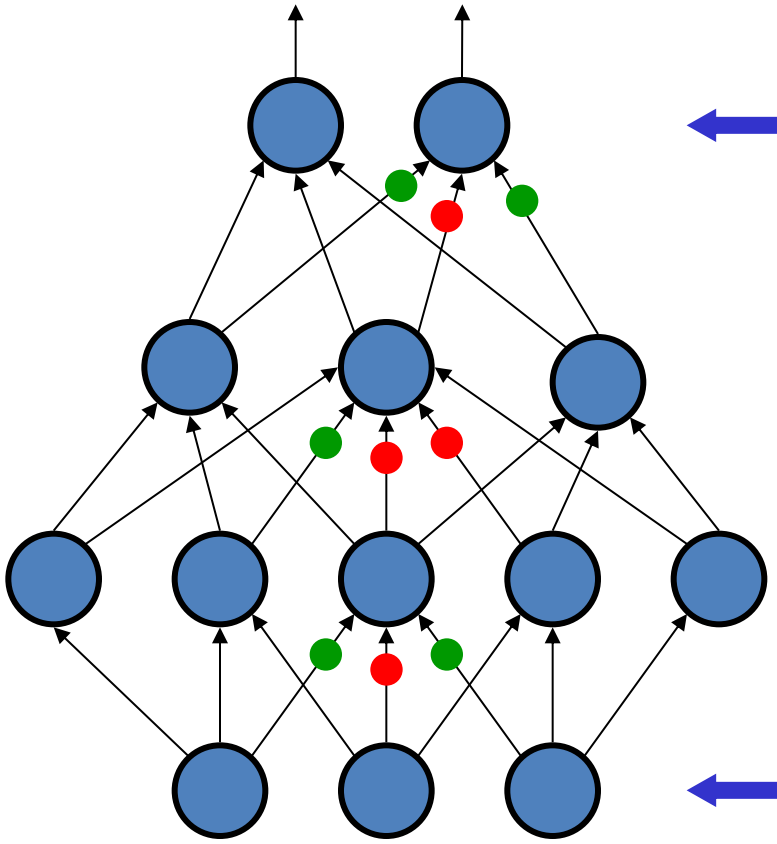
Sketch of a typical perceptron from the 1960's

Second generation neural networks (~1985)

Back-propagate error signal to get derivatives for learning



Compare outputs with correct answer to get error signal



outputs

hidden layers

input vector

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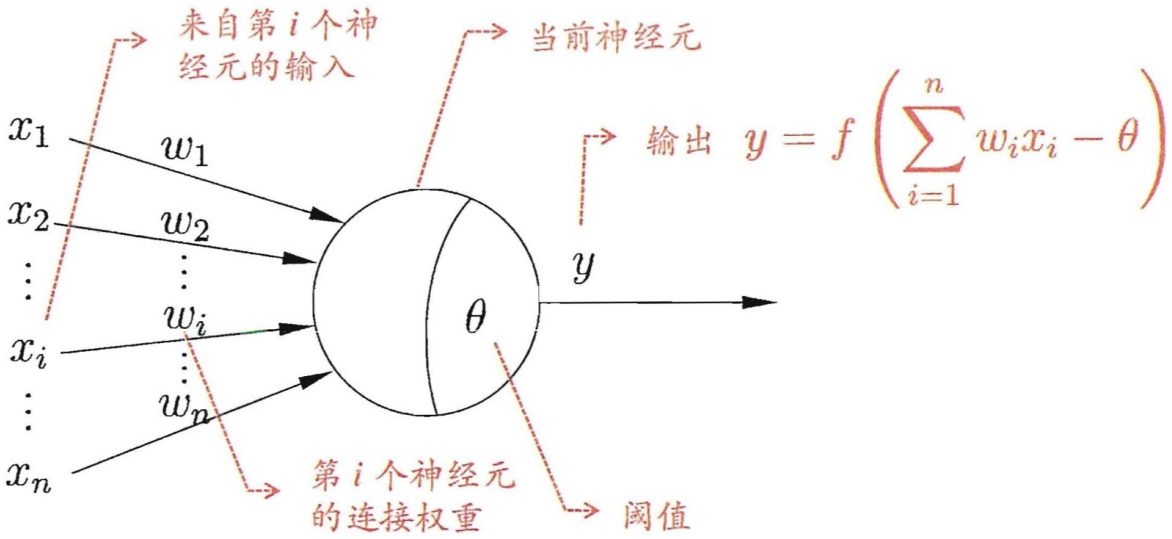
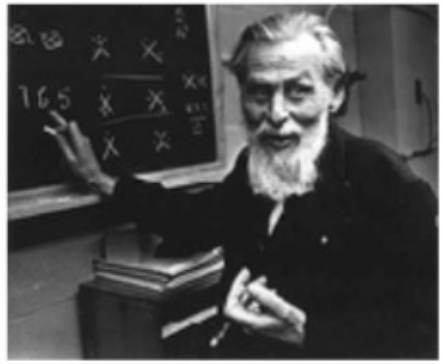
M-P neuron model



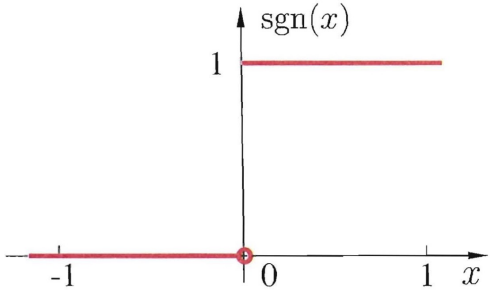
M-P 神经元模型（图片源自：周志华 - 机器学习）



Warren Sturgis McCulloch
(1898-1969)

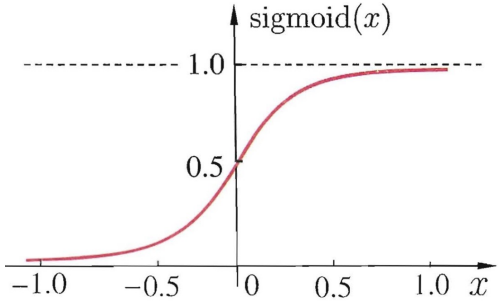
Walter Harry Pitts
(1923-1969)

Step function



$$\mathrm{sgn}(x) = \begin{cases} 1, & x \geqslant 0; \\ 0, & x < 0. \end{cases}$$

Sigmoid function

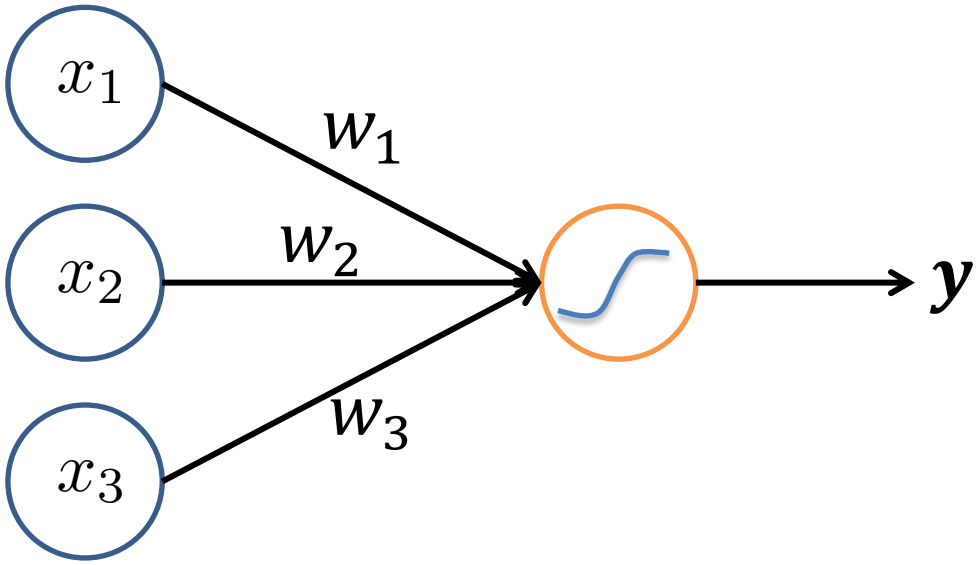


$$\mathrm{sigmoid}(x) = \frac{1}{1+e^{-x}}$$

W S McCulloch, W Pitts. A logical calculus of the ideas immanent in nervous activity. Bulletin of Mathematical Biophysics. Vol.5:115-133, Dec. 1943.

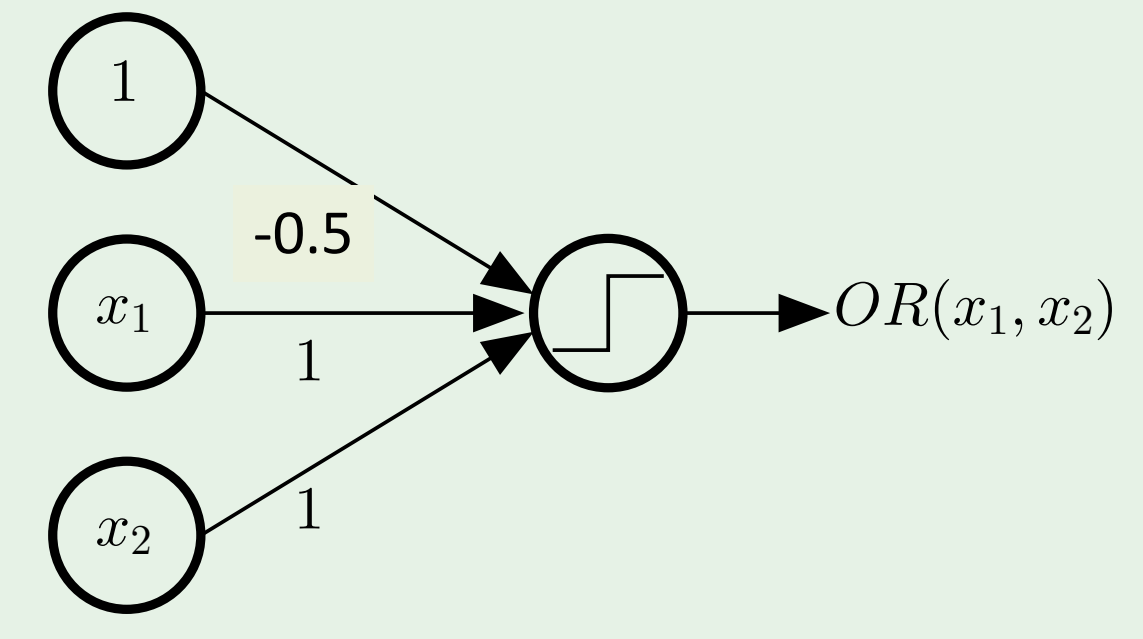
Perceptron

- Input layer + M-P neuron (output)

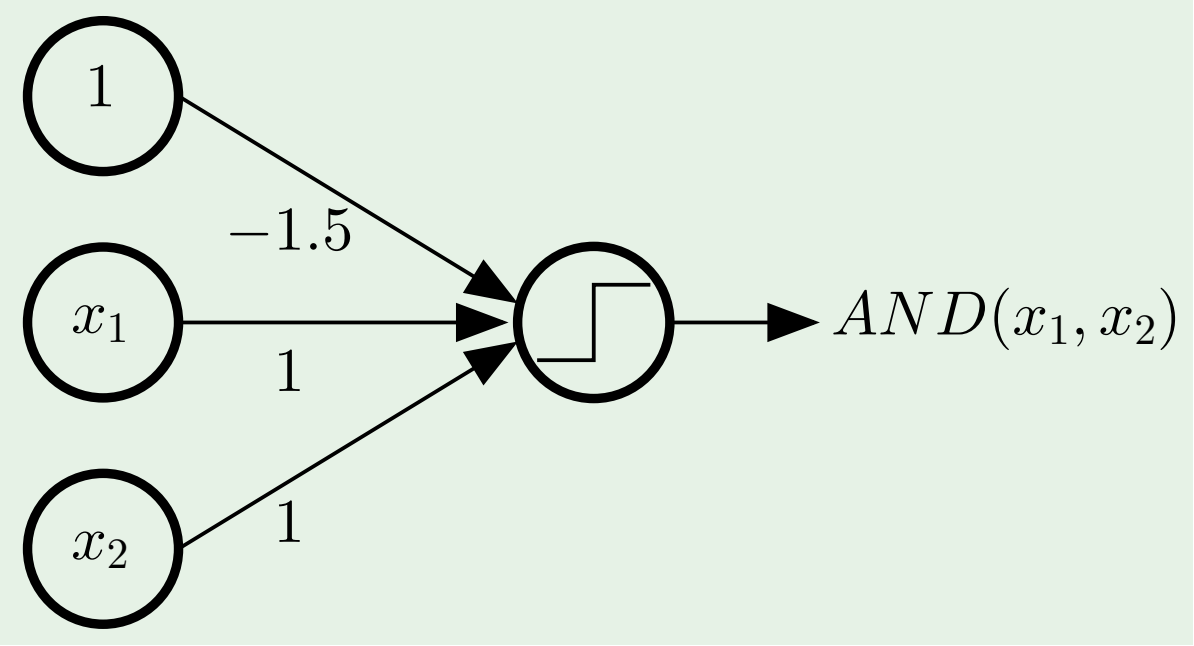


What can it do?

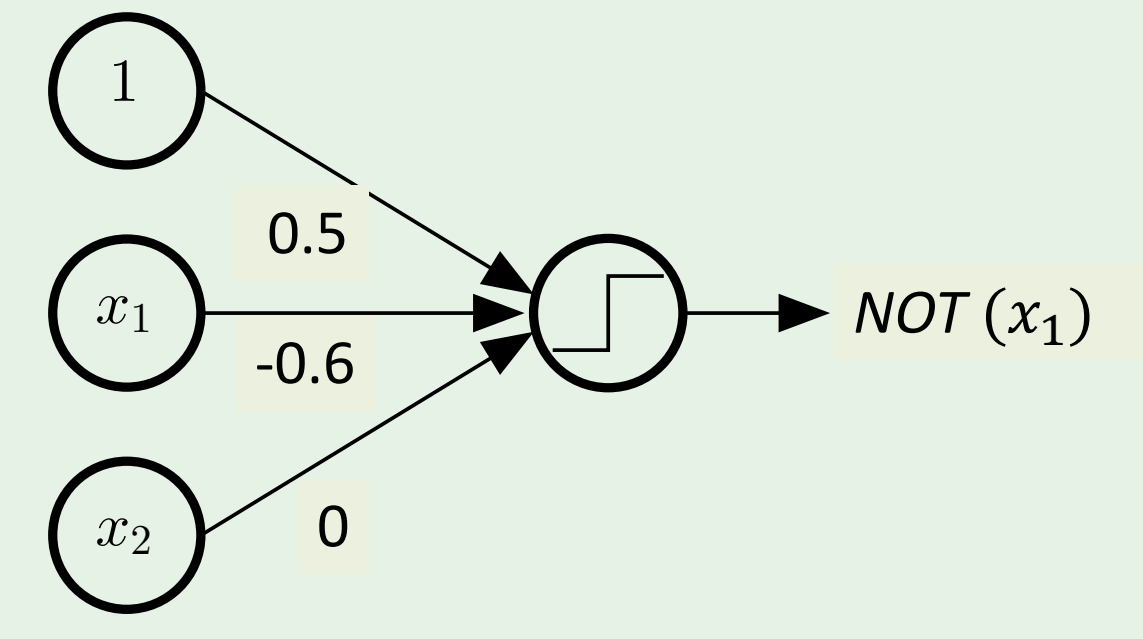
OR by perceptron



AND by perceptron

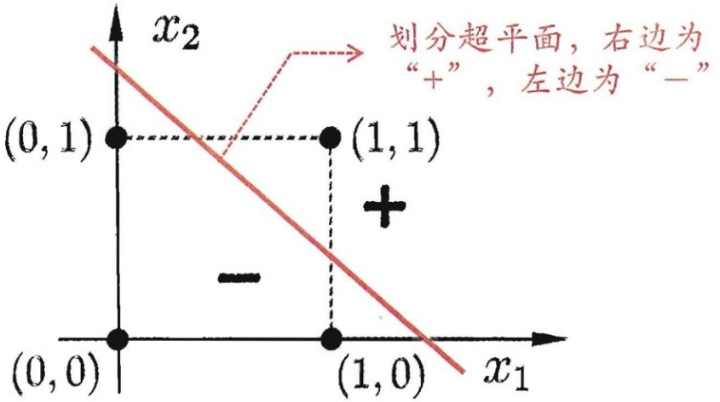


NOT by perceptron

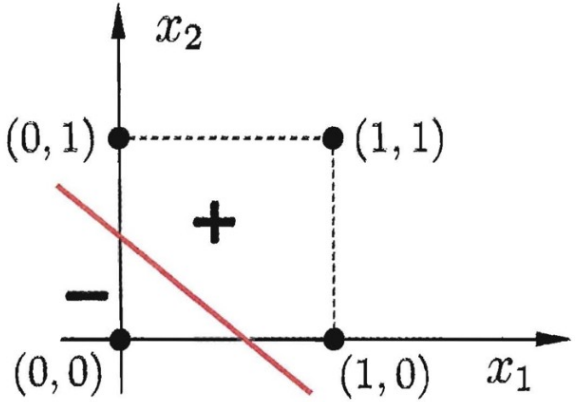


A single perceptron could not implement XOR

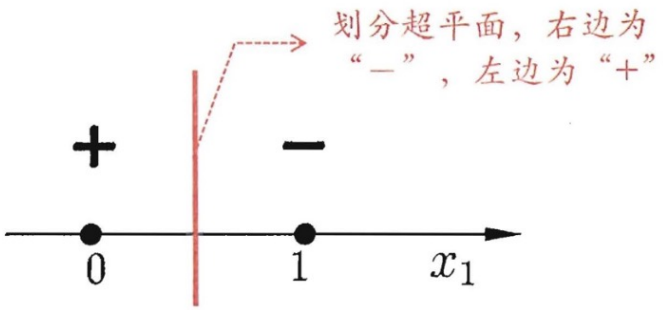
$$y(\mathbf{x}) = \text{sign}(\mathbf{w}^T\mathbf{x} + w_0)$$ Linear classifier



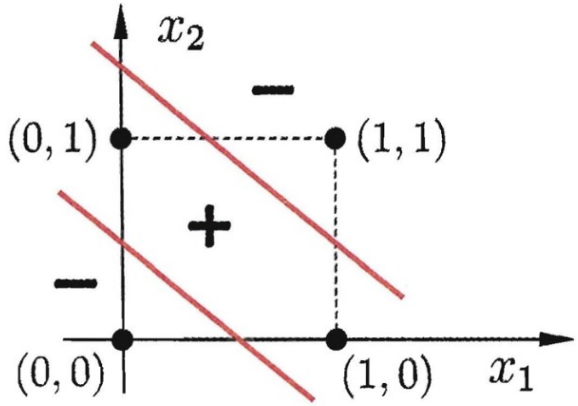
(a) “与”问题 $(x_1 \wedge x_2)$



(b) “或”问题 $(x_1 \vee x_2)$

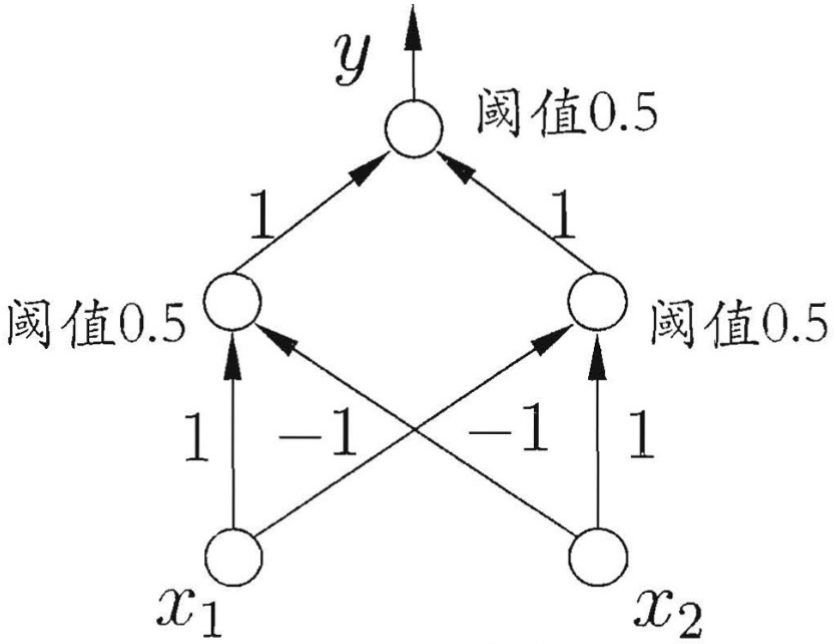


(c) “非”问题 $(\neg x_1)$

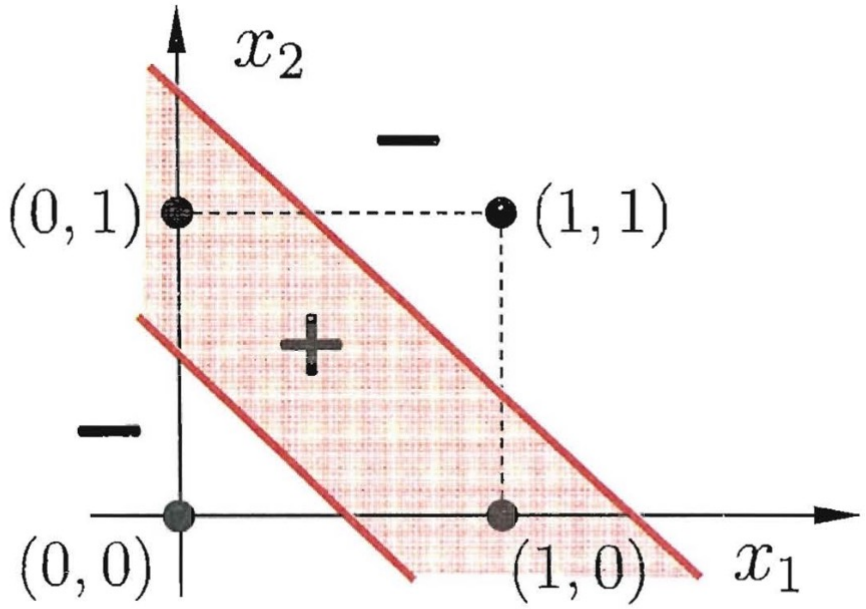


(d) “异或”问题 $(x_1 \oplus x_2)$

A two-layer perceptron for XOR

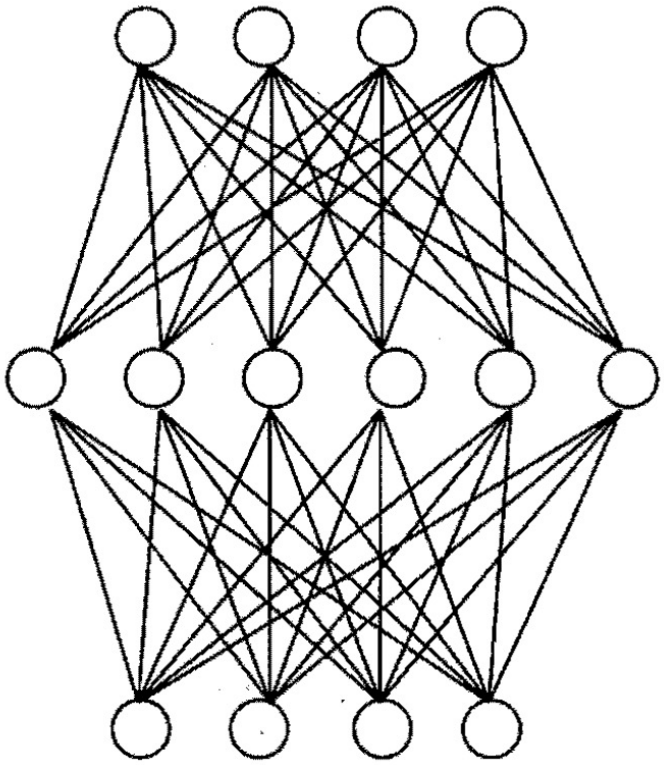


(a) 网络结构

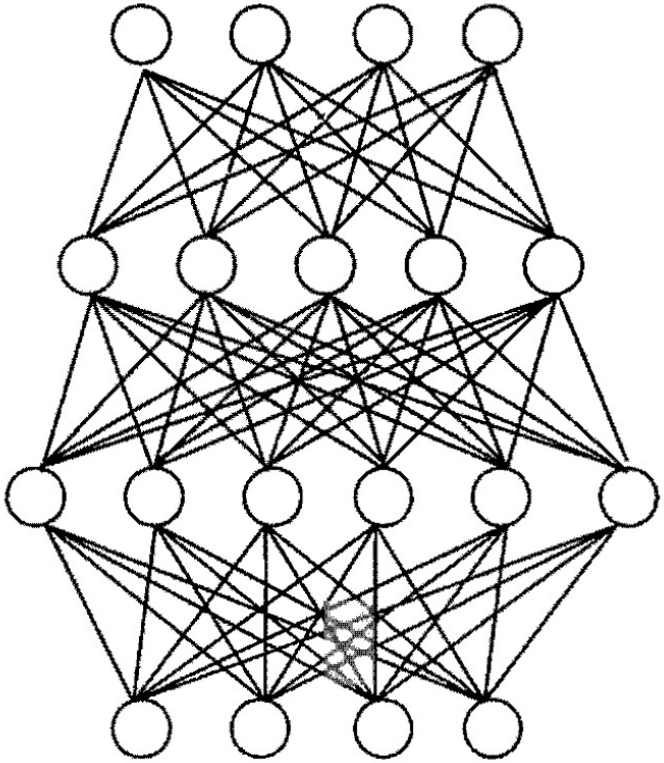


(b) 分类区域

Multilayer network



(a) 单隐层前馈网络



(b) 双隐层前馈网络

Perceptron learning

$$w_i \leftarrow w_i + \Delta w_i \ ,$$

$$\Delta w_i = \eta(y - \hat{y})x_i \ ,$$

Perceptron convergence theorem: if there exists an exact solution (which means the training data is linearly separable), then the perceptron learning algorithm is guaranteed to find an exact solution in a finite number of steps.

In practice, the number of steps required to achieve convergence could be substantial. Until convergence is achieved, we are not able to distinguish between a nonseparable problem and one that is simply slow to converge.

The perceptron algorithm does not converge when the data are not linearly separable.

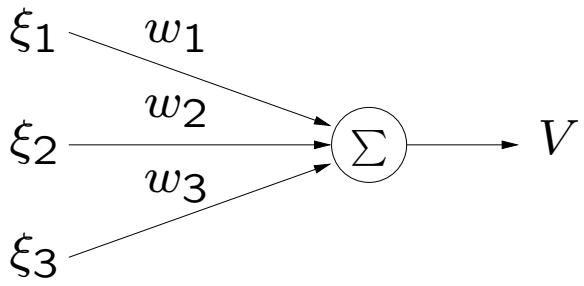
Recall:

The Hebbian Neuron

A computational system which implements Hebbian learning.

Let's assume a linear unit; experiment shows this is largely sufficient:

$$V = \sum_j w_j \xi_j = \bar{w}^T \bar{\xi} \tag{2}$$



Plain Hebbian learning:

$$\Delta \bar{w} = \eta \, V \, \bar{\xi} \tag{3}$$

A adaptive learning rule

Algorithm: Perceptron Learning Algorithm

$P \leftarrow inputs \quad with \quad label \quad 1;$

$N \leftarrow inputs \quad with \quad label \quad 0;$

Initialize $\mathbf{w}$ randomly;

while !*convergence* **do**

  Pick random $\mathbf{x} \in P \cup N$;

  if $\mathbf{x} \in P \quad and \quad \mathbf{w}.\mathbf{x} < 0$ **then**

    $\mathbf{w} = \mathbf{w} + \mathbf{x}$;

  end

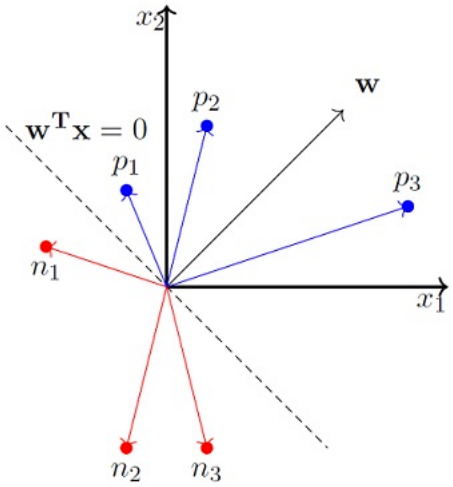
  if $\mathbf{x} \in N \quad and \quad \mathbf{w}.\mathbf{x} \geq 0$ **then**

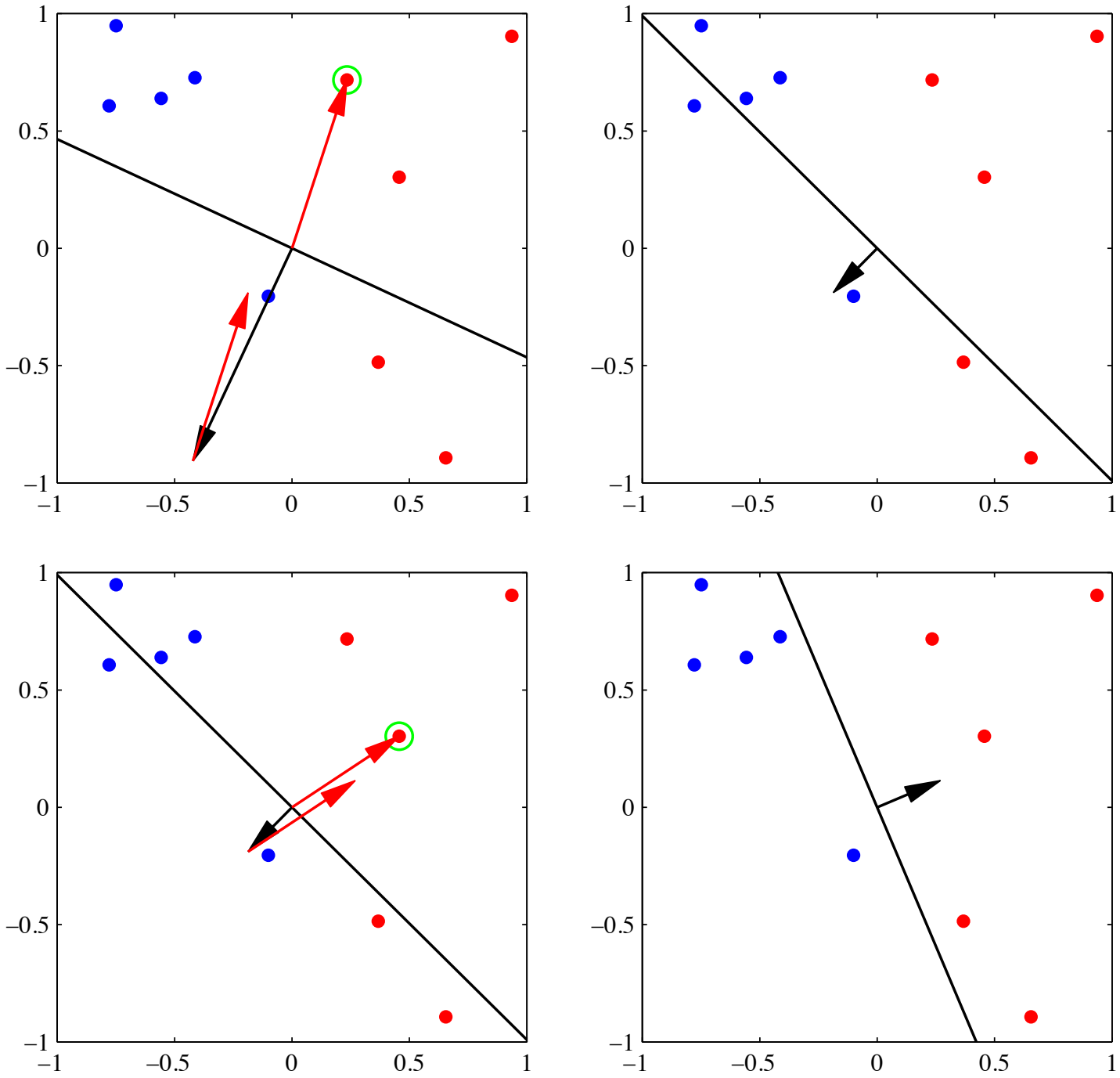
    $\mathbf{w} = \mathbf{w} - \mathbf{x}$;

  end

end

//the algorithm converges when all the inputs are classified correctly





PRML

The Perceptron algorithm

More general form of a linear classifier

$$y(\mathbf{x}) = \text{sign}\left(\mathbf{w}^T \boldsymbol{\phi}(\mathbf{x})\right)$$

where $\boldsymbol{\phi}(\mathbf{x})$ is the feature vector of $\mathbf{x}$ (recall the basis functions in linear regression), and typically includes a bias component $\phi_0(\mathbf{x}) = 1$.

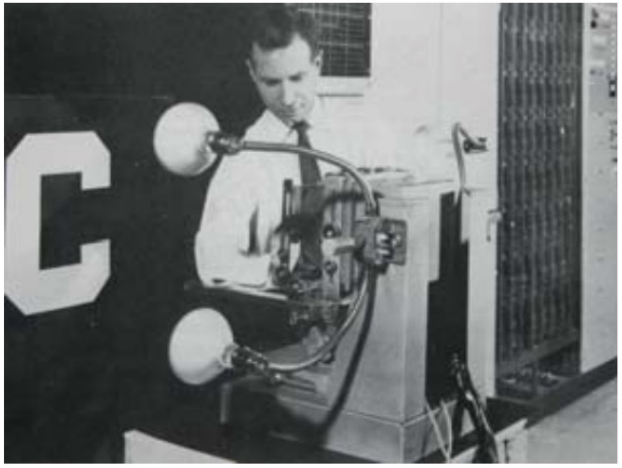
Given a set of samples $\{\mathbf{x}_n, t_n\}_{n=1}^N,\ \mathbf{x}_n \in \mathbb{R}^D,\ t_n \in \{-1, 1\}$, our goal is to find the optimal parameter $\mathbf{w}$ to minimize the training error

$$E_p(\mathbf{w}) = -\sum_{n \in \mathcal{M}} \mathbf{w}^T \boldsymbol{\phi}_n t_n$$

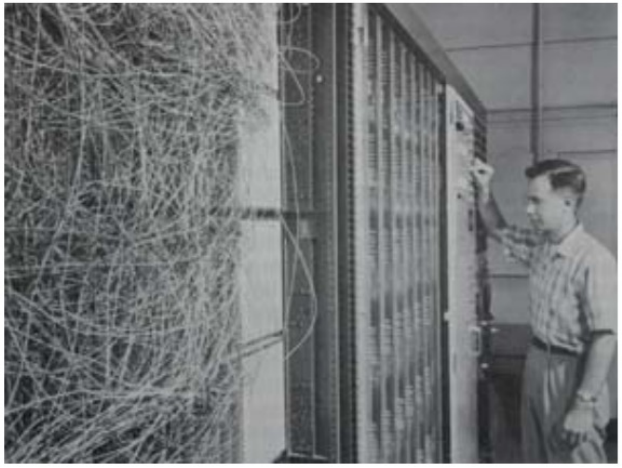
where $\boldsymbol{\phi}_n = \boldsymbol{\phi}(\mathbf{x}_n)$ and $\mathcal{M}$ denotes the set of all misclassified patterns.

Perceptron in Action

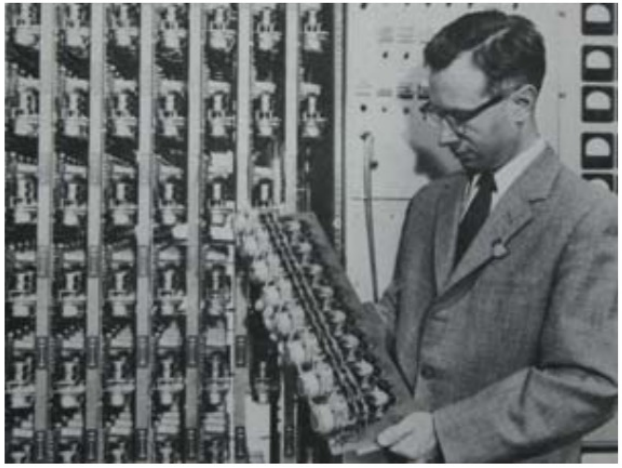
Frank Rosenblatt



Input: a simple camera system (400 pixel image)



Patch board: different configurations of input features



Racks of adaptive weights: Each weight was implemented using a rotary variable resistor, driven by an electric motor thereby allowing the value of the weight to be adjusted automatically by the learning algorithm.

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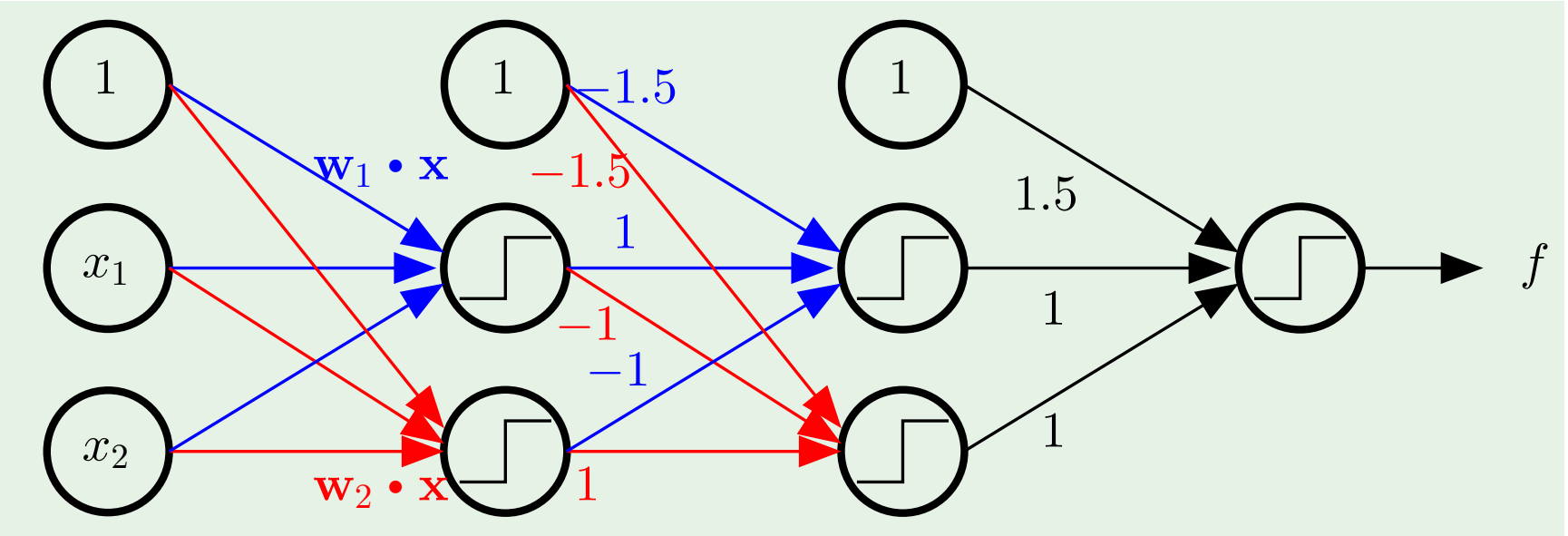
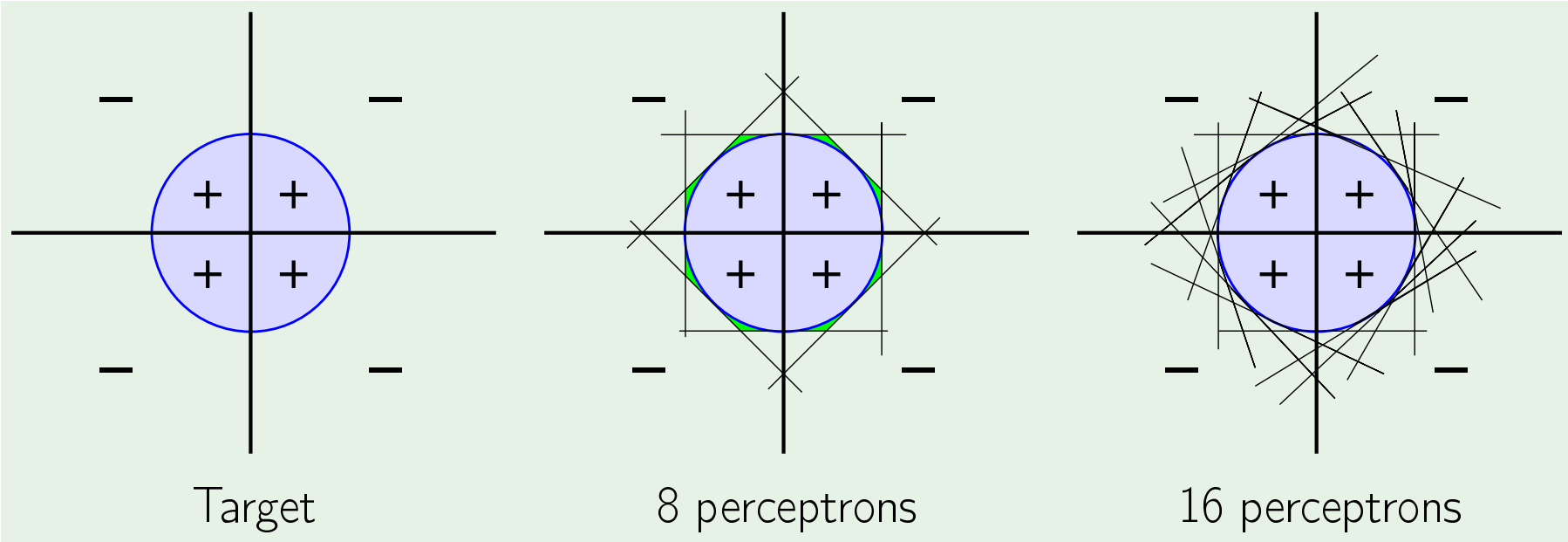
The multilayer perceptron



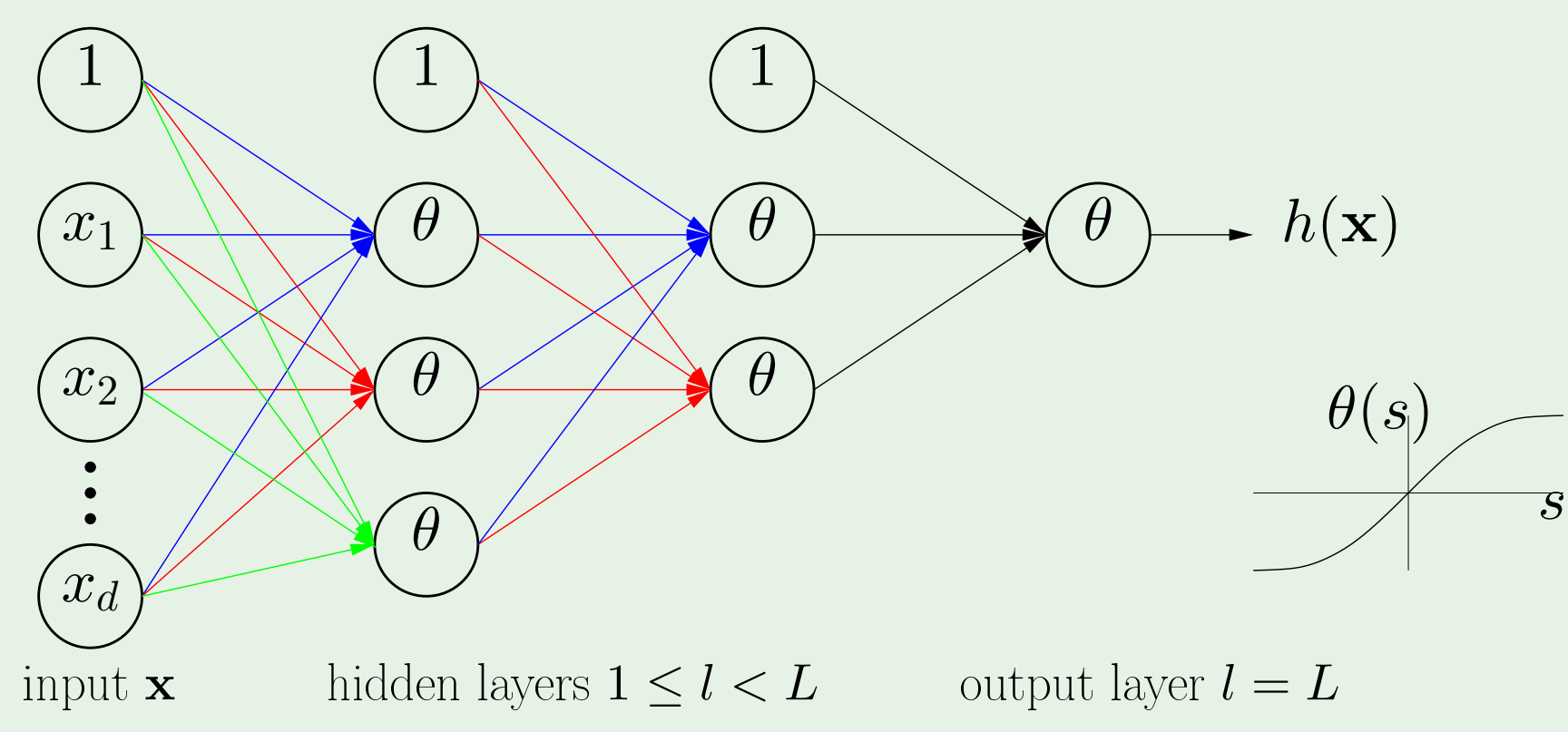
3 layers, feedforward

The multilayer perceptron is powerful



But not good for generalization and optimization

Neural networks



Functions by neural networks

Neural network is defined by recursively constructing a nonlinear function over linear combination of inputs.

For input $\mathbf{x} = (x_1, \cdots, x_D) \in \mathbb{R}^D$, we construct M linear combinations

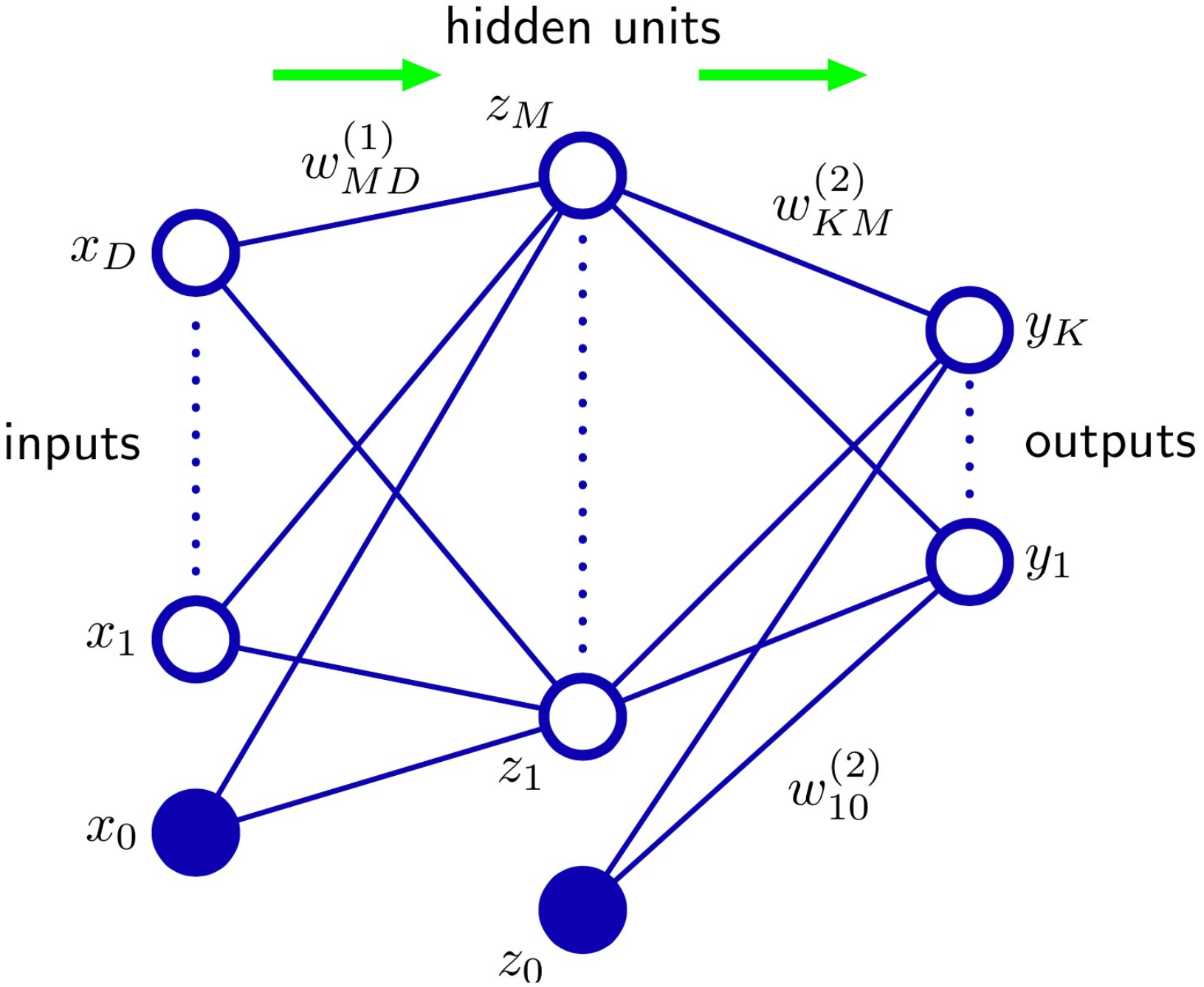
$$a_j = \sum_{i=1}^{D} w_{ji}^{(1)} x_i + w_{j0}^{(1)}, \quad j = 1, \cdots, M$$

where the superscript (1) indicates the corresponding parameters are in the first layer of the network. $w_{ji}^{(1)}$ are *weights* and $w_{j0}^{(0)}$ are biases. a_j are known as *activations*.

Each activation is then transformed using a differentiable, nonlinear *activation function* $h(\cdot)$ to give

$$z_j = h(a_j), \quad j = 1, \cdots, M$$

which are called *hidden units*. The nonlinear functions $h(\cdot)$ are often sigmoid functions such as logistic and tanh.


hidden units
z_M
$w^{(1)}_{MD}$
$w^{(2)}_{KM}$
x_D
y_K
inputs
outputs
y_1
x_1
z_1
$w^{(2)}_{10}$
x_0
z_0

PRML

Recursive Nature

- Activations of hidden units:

$$a_j = \sum_{i=1}^{D} w_{ji}^{(1)} x_i + w_{j0}^{(1)} \qquad j = 1, ..., M$$

- Each activation is transformed using a differentiable, nonlinear activation function

$$z_j = h(a_j) \qquad j = 1, ..., M$$

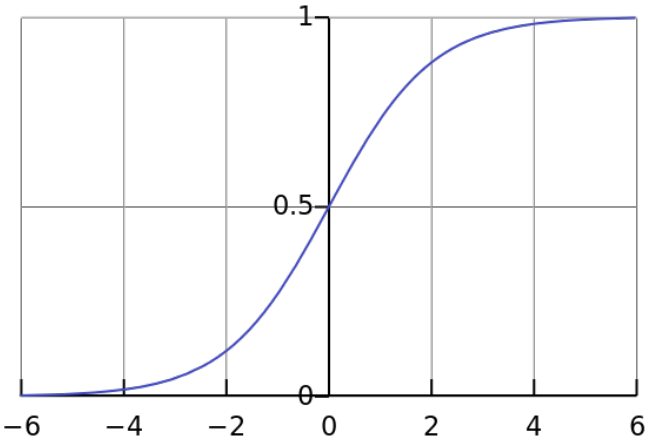
- The hidden units can be linearly combined to give output unit activation

$$a_k = \sum_{j=1}^{M} w_{kj}^{(2)} z_j + w_{k0}^{(2)} \qquad k = 1, ..., K$$

- Output layer

- Sigmoid function

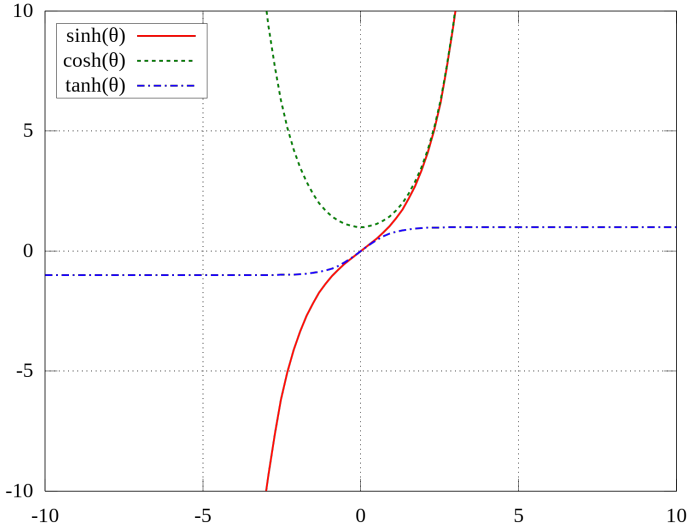
$$\sigma(t) = \frac{1}{1 + e^{-t}}$$

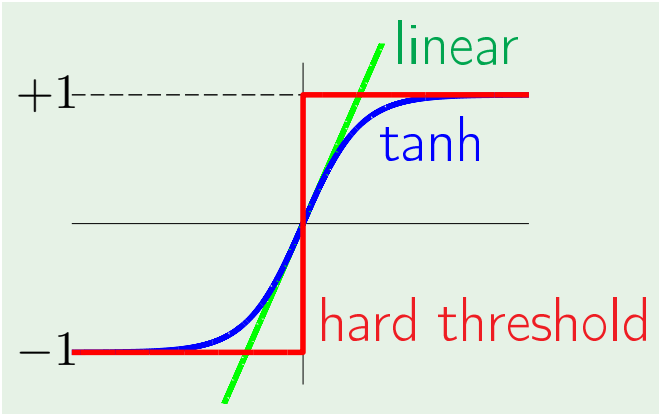


- tanh function

$$\tanh x = \frac{\sinh x}{\cosh x} = \frac{e^x - e^{-x}}{e^x + e^{-x}} =$$

$$= \frac{e^{2x} - 1}{e^{2x} + 1} = \frac{1 - e^{-2x}}{1 + e^{-2x}}$$





Output layer for classification

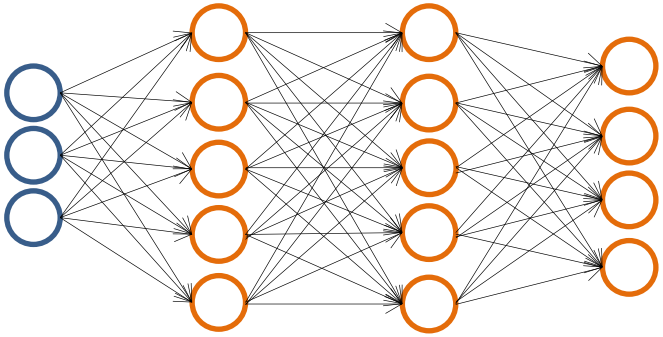
Multi-class classification

Pedestrian

Car

Motorcycle

Truck



$h_\Theta(x) \in \mathbb{R}^4$

Want $h_\Theta(x) \approx \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \end{bmatrix}$, $h_\Theta(x) \approx \begin{bmatrix} 0 \\ 1 \\ 0 \\ 0 \end{bmatrix}$, $h_\Theta(x) \approx \begin{bmatrix} 0 \\ 0 \\ 1 \\ 0 \end{bmatrix}$, etc.

when pedestrian when car when motorcycle

Forms of network output

- The output unit activations are transformed to the network output y_k
  - Regression problems: $y_k = a_k$
  - Multiple binary classification problems, each output unit activation can be logistic sigmoid function: $y_k = \sigma(a_k)$
  - Multi-class problems, soft max function:

$$\sigma(\mathbf{z})_j = \frac{e^{\mathbf{z}_j}}{\sum_{k=1}^{K} e^{\mathbf{z}_k}}$$

Overall neural network function

- Overall network function (using sigmoidal activation function)

$$y_k(\mathbf{x}, \mathbf{w}) = \sigma\left(\sum_{k=1}^{M} w_{kj}^{(2)} h\left(\sum_{i=1}^{D} w_{ji}^{(1)} x_i + w_{j0}^{(1)}\right) + w_{k0}^{(2)}\right)$$

  where weight parameters are grouped into **w**

- Neural network is a function that maps **x** to **y**, controlled by adjustable **w**.

Function with a dummy variable

- We can introduce a dummy variable x_0=1 to simply the notation
- The first layer activation:

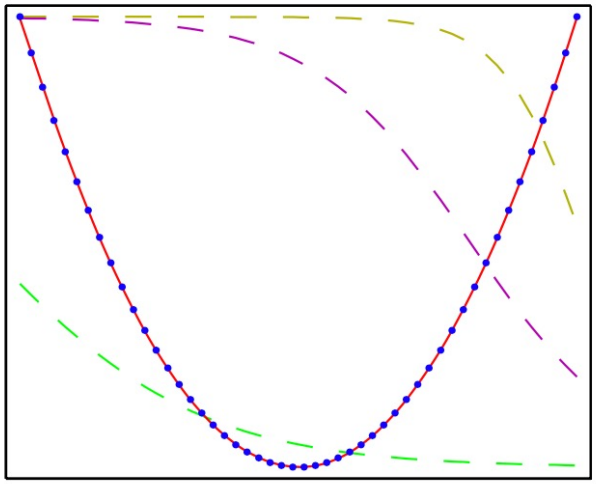
$$a_j = \sum_{i=0}^{M} w_{ji}^{(1)} x_j$$

- Neural network function

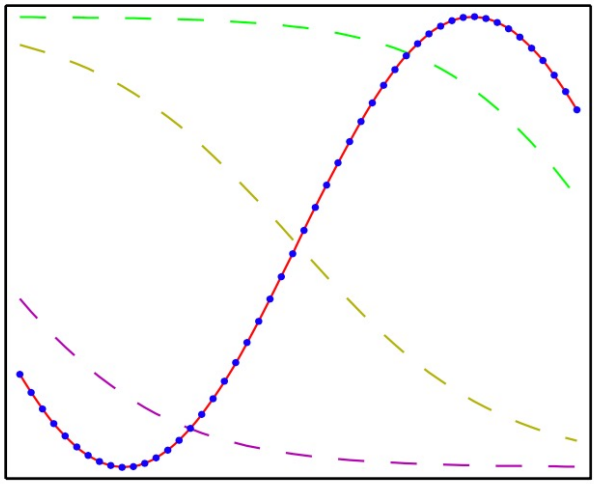
$$y_k(\mathbf{x}, \mathbf{w}) = \sigma\left(\sum_{k=1}^{M} w_{kj}^{(2)} h\left(\sum_{i=1}^{D} w_{ji}^{(1)} x_i\right)\right)$$

A Reassuring Theorem

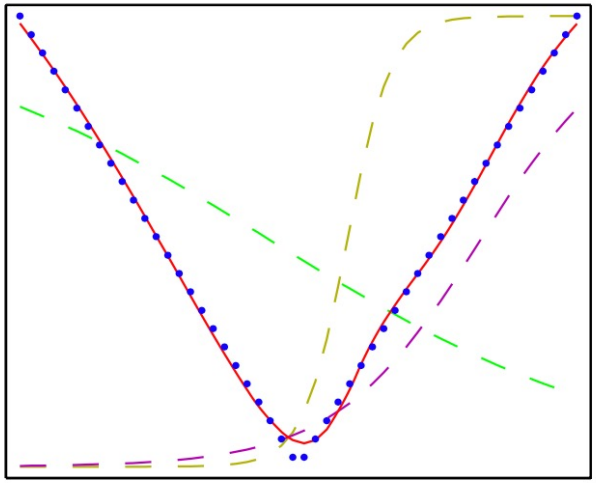
- *A two-layer network with linear outputs can uniformly approximate any continuous function on a compact input domain to arbitrary accuracy provided that the network has a sufficiently large number of hidden units*



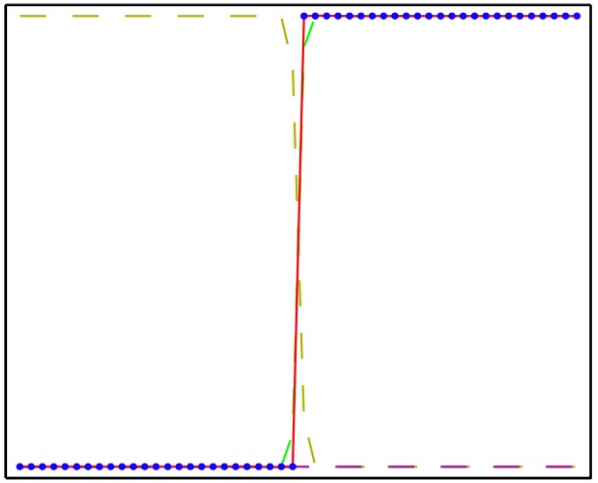
(a) $f(x) = x^2$



(b) $f(x) = \sin(x)$



(c) $f(x) = |x|$



(d) $f(x) = H(x)$ where $H(x)$ is the Heaviside step function

50 training points

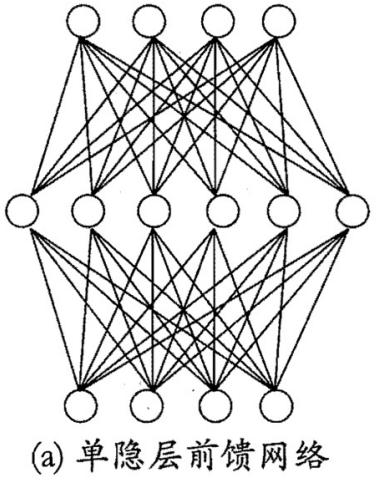
These data points are then used to train a two-layer network having 3 hidden units with 'tanh' activation functions and linear output units. The resulting network functions are shown by the red curves, and the outputs of the three hidden units are shown by the three dashed curves.

Question

- Why not using linear function as the activation function of the neural network?

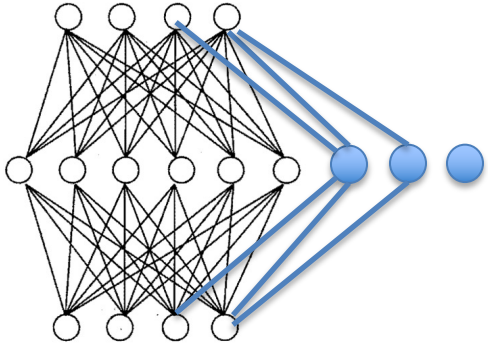
Question

- Discuss the two possible operations, i.e., extending the depth or the width

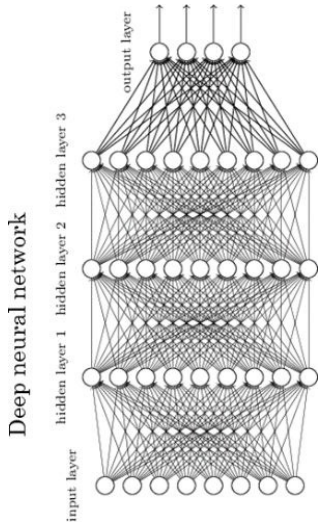


(a) 单隐层前馈网络

wide



deep



Thank you!