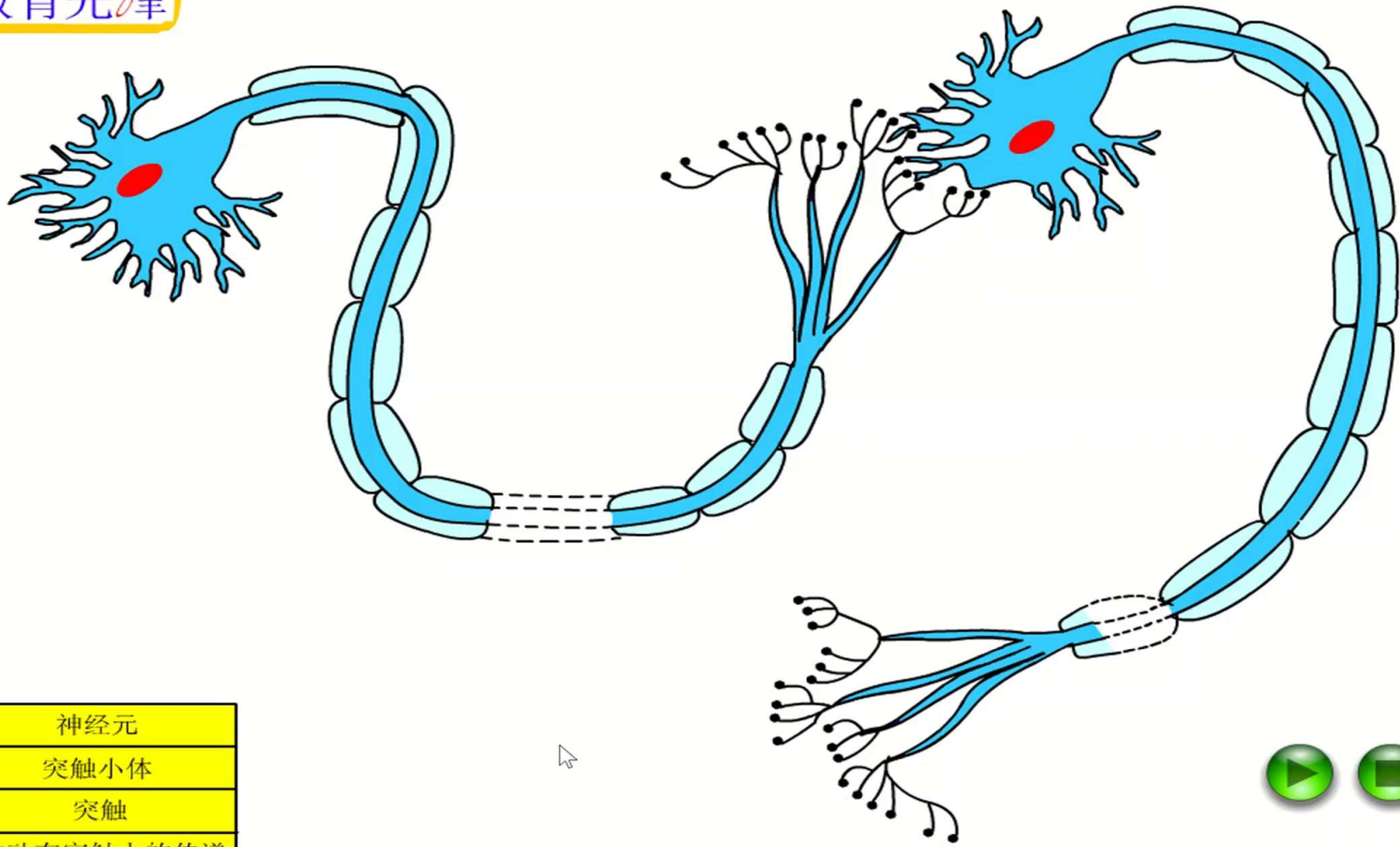
Neural Network

Outline

- Modeling one neuron
- Activation functions
- Fully connected feed-forward network
- How to train a multi-layer network
- Representational power of NN

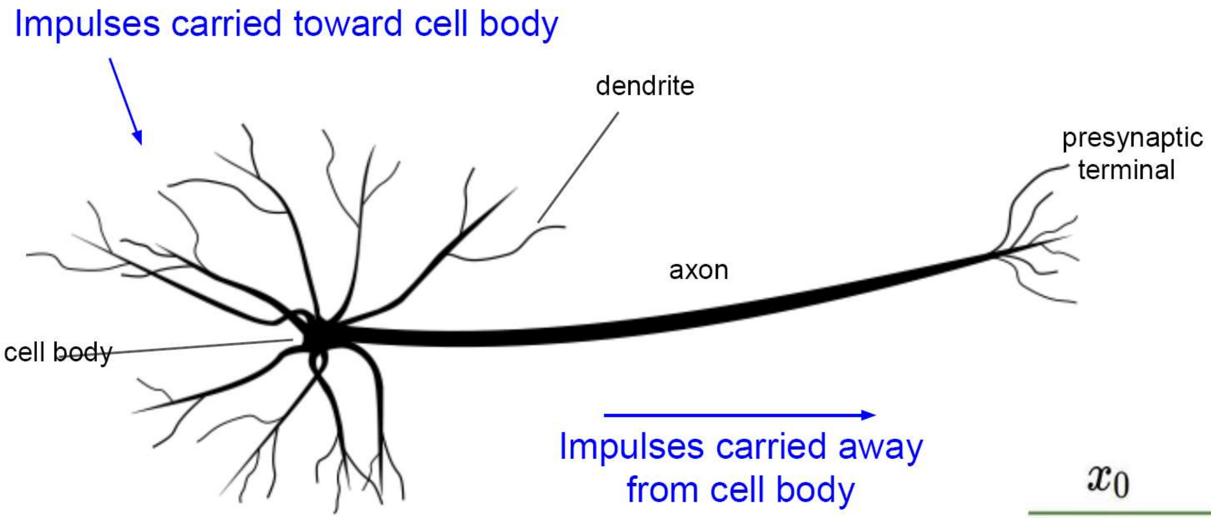
Biology

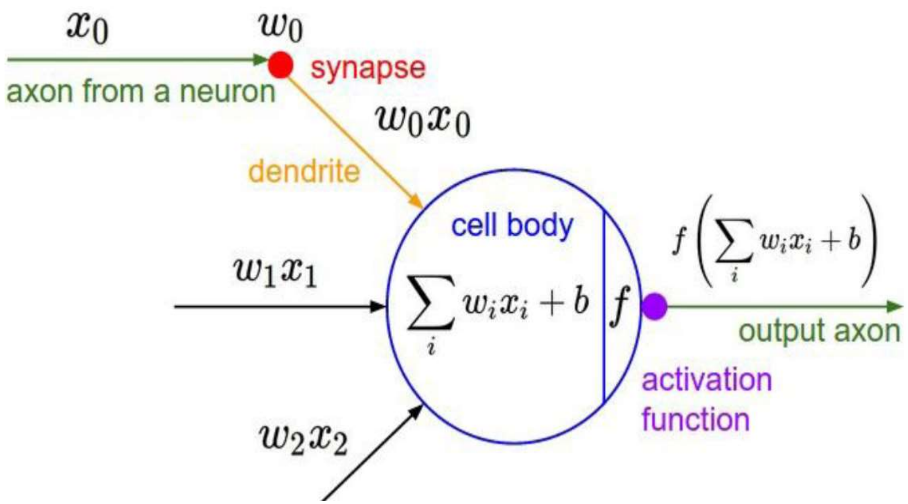
- Neurons respond slowly
  - 10^{-3} s compared to 10^{-9} s for electrical circuits
- The brain uses massively parallel computation
  - $\approx 10^{11}$ neurons in the brain
  - $\approx 10^{4}$ connections per neuron



神经元
突触小体
突触
冲动在突触上的传递

Modeling one neuron





Single neuron as a linear classifier

- With an appropriate loss function on the neuron’s output, a single neuron can be turned into a linear classifier.
- A single neuron can be used to implement a binary classifier (e.g. binary Softmax or binary SVM classifiers).

Single neuron as a linear classifier

- **Binary Softmax classifier**
  - Interpreting:
    - $\sigma(\sum_i w_i x_i + b)$ to be the probability of one of the classes $P(y_i = 1 \mid x_i; w)$
    - The probability of the other class to be $P(y_i = 0 \mid x_i; w) = 1 - P(y_i = 1 \mid x_i; w)$
  - With this interpretation, we can formulate the cross-entropy loss, and optimizing it would lead to a **binary Softmax classifier** (also known as logistic regression)
- Alternatively, we could attach a max-margin hinge loss to the output of the neuron and train it to become a **binary Support Vector Machine**.

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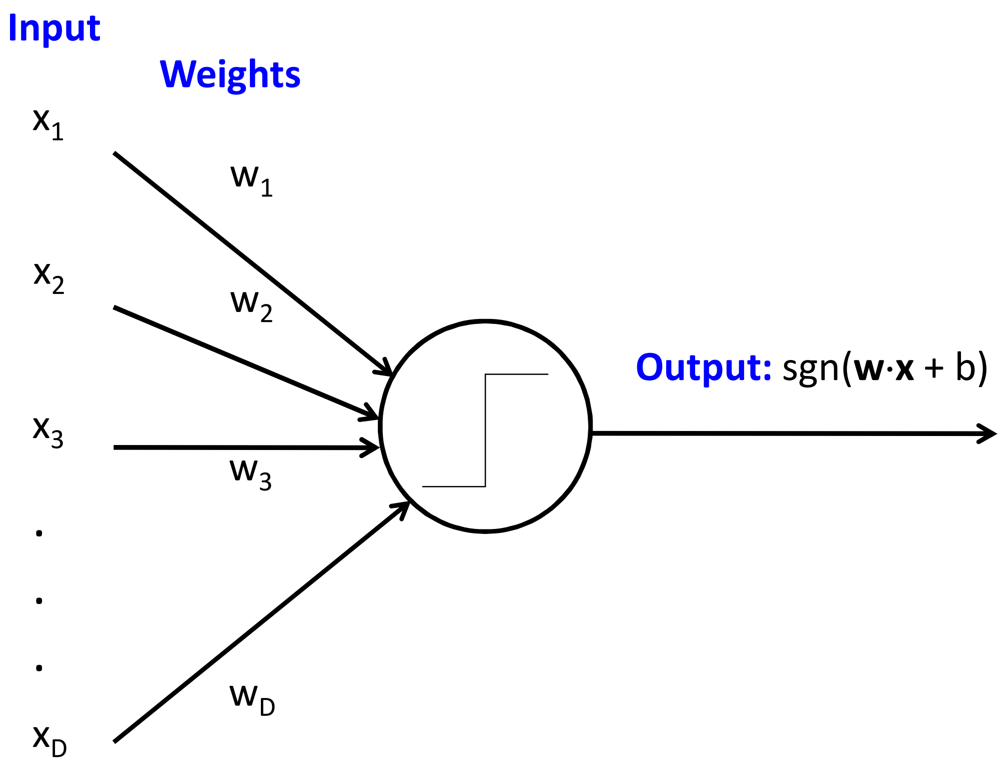
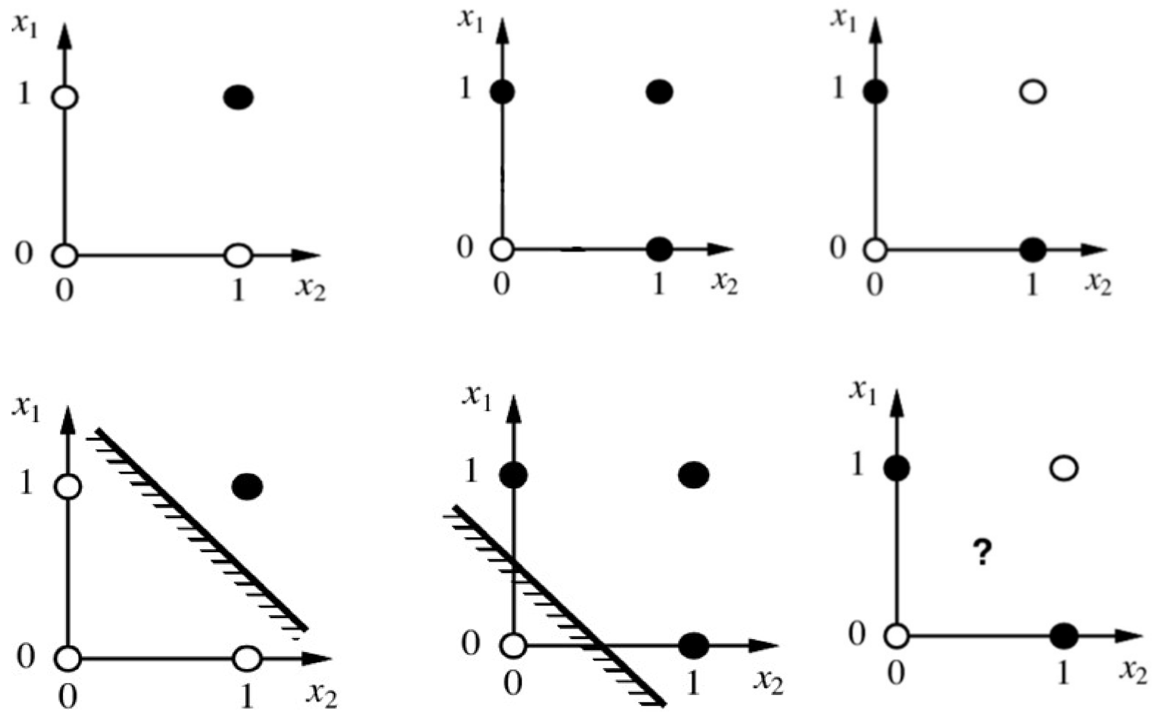
Activation Functions

- Neural networks are used to implement complex functions, and non-linear Activation Functions enable them to approximate arbitrarily complex functions.
- Without the non-linearity introduced by the Activation Function：
  - a neuron is equivalent to a linear classifier
  - a multi-layer neural network is equivalent to a single layer neural network

Perceptron



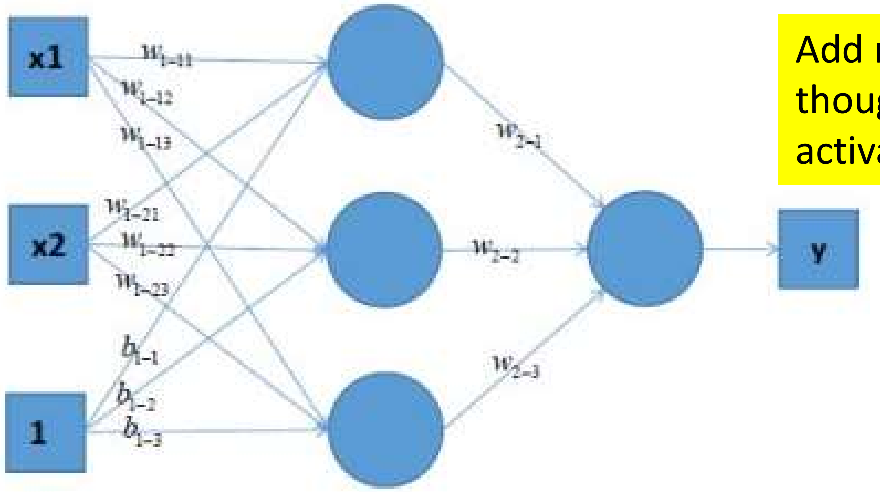
Linear separability



x_1 **and** x_2 x_1 **or** x_2 x_1 **xor** x_2

Multilayer Perceptron （MLP）

- A MLP with a single hidden layer



Add nonlinearity though activation functions!

$$y = w_{2-1}(w_{1-11}x_1 + w_{1-21}x_2 + b_{1-1}) + w_{2-2}(w_{1-12}x_1 + w_{1-22}x_2 + b_{1-2}) + w_{2-3}(w_{1-13}x_1 + w_{1-23}x_2 + b_{1-3})$$

$$\Downarrow$$

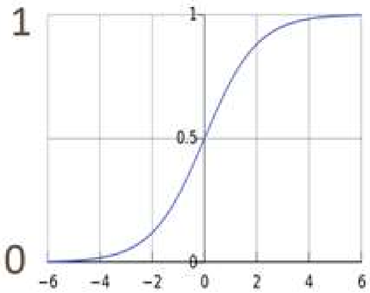
$$y = x_1(w_{2-1}w_{1-11} + w_{2-2}w_{1-12} + w_{2-3}w_{1-13}) + x_2(w_{2-1}w_{1-21} + w_{2-2}w_{1-22} + w_{2-3}w_{1-23}) + w_{2-1}b_{1-1} + w_{2-2}b_{1-2} + w_{2-3}b_{1-3}$$

Still a linear classifier

Some Activation Functions

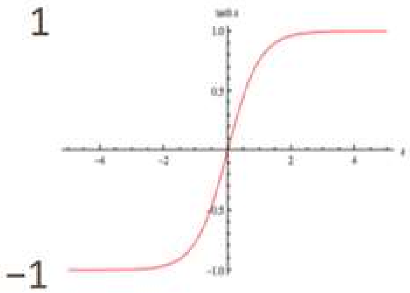
logistic ("sigmoid")

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



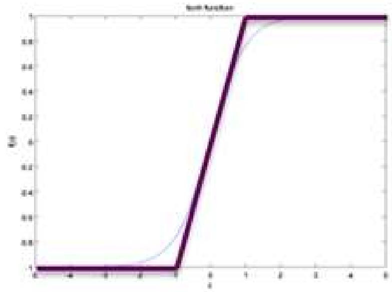
tanh

$$\tanh(z) = \frac{e^z - e^{-z}}{e^z + e^{-z}}$$



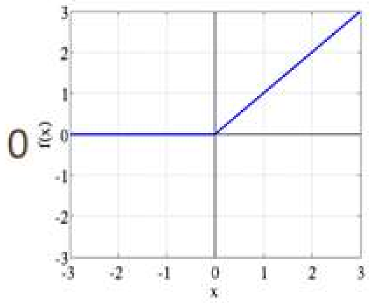
hard tanh

$$\text{HardTanh}(x) = \begin{cases} -1 & \text{if } x < -1 \\ x & \text{if } -1 <= x <= 1 \\ 1 & \text{if } x > 1 \end{cases}$$

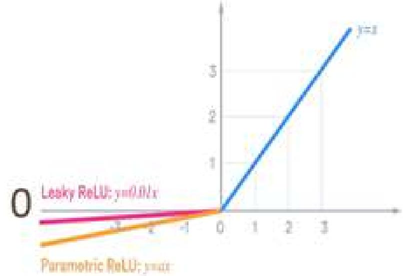


(Rectified Linear Unit) ReLU

$$\text{ReLU}(z) = \max(z, 0)$$



Leaky ReLU / Parametric ReLU



tanh is just a rescaled and shifted sigmoid (2 × as steep, [−1,1]):

$$\tanh(z) = 2\text{logistic}(2z) - 1$$

Logistic and tanh are still used (e.g., logistic to get a probability)

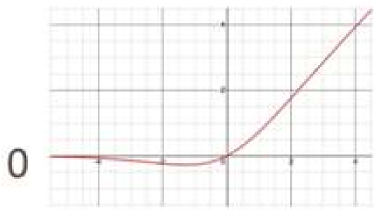
However, now, for deep networks, the first thing to try is ReLU: it trains quickly and performs well due to good gradient backflow.

ReLU has a negative "dead zone" that recent proposals mitigate

GELU is frequently used with Transformers (BERT, RoBERTa, etc.)

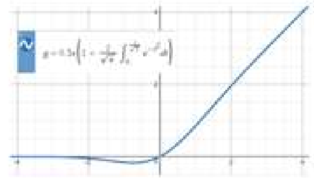
Swish arXiv:1710.05941

$$\text{swish}(x) = x \cdot \text{logistic}(\beta x)$$



GELU arXiv:1606.08415

$$\begin{aligned} \text{GELU}(x) &= x \cdot P(X \le x), X \sim N(0,1) \\ &\approx x \cdot \text{logistic}(1.702x) \end{aligned}$$



Activation Functions：

- **Maxout :** $\max(w_1^T x + b_1, w_2^T x + b_2)$
  - Does not have the basic form of dot product -> nonlinearity
  - Generalizes ReLU and Leaky ReLU
  - Linear Regime! Does not saturate! Does not die!
  - Problem:
    - doubles the number of parameters/neuron

Activation Functions:

- **Swish : $f(x)= x * \sigma(\beta x) = x/(1+\exp(- \beta x))$**
- **Swish can be loosely viewed as a smooth function which nonlinearly interpolates between the linear function and the ReLU function. The degree of interpolation can be controlled by the model if β is set as a trainable parameter.**
  - If $\beta = 0$, Swish becomes the scaled linear function $f(x) = x/2$.
  - If $\beta = 1$, Swish is equivalent to the Sigmoid-weighted Linear Unit (SiL) of Elfwing et al. (2017) that was proposed for reinforcement learning.
  - As $\beta \to \infty$, the sigmoid component approaches a 0-1 function, Swish becomes like the ReLU function.

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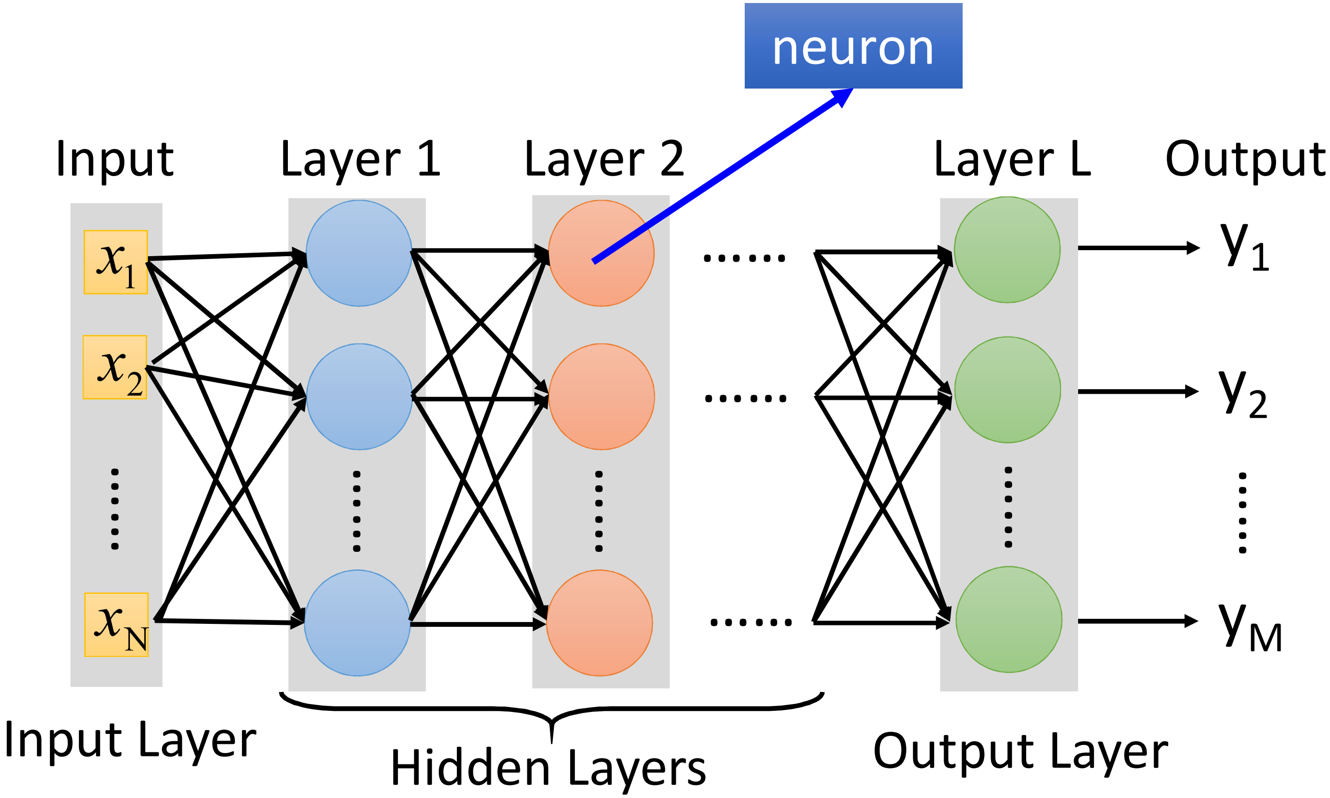
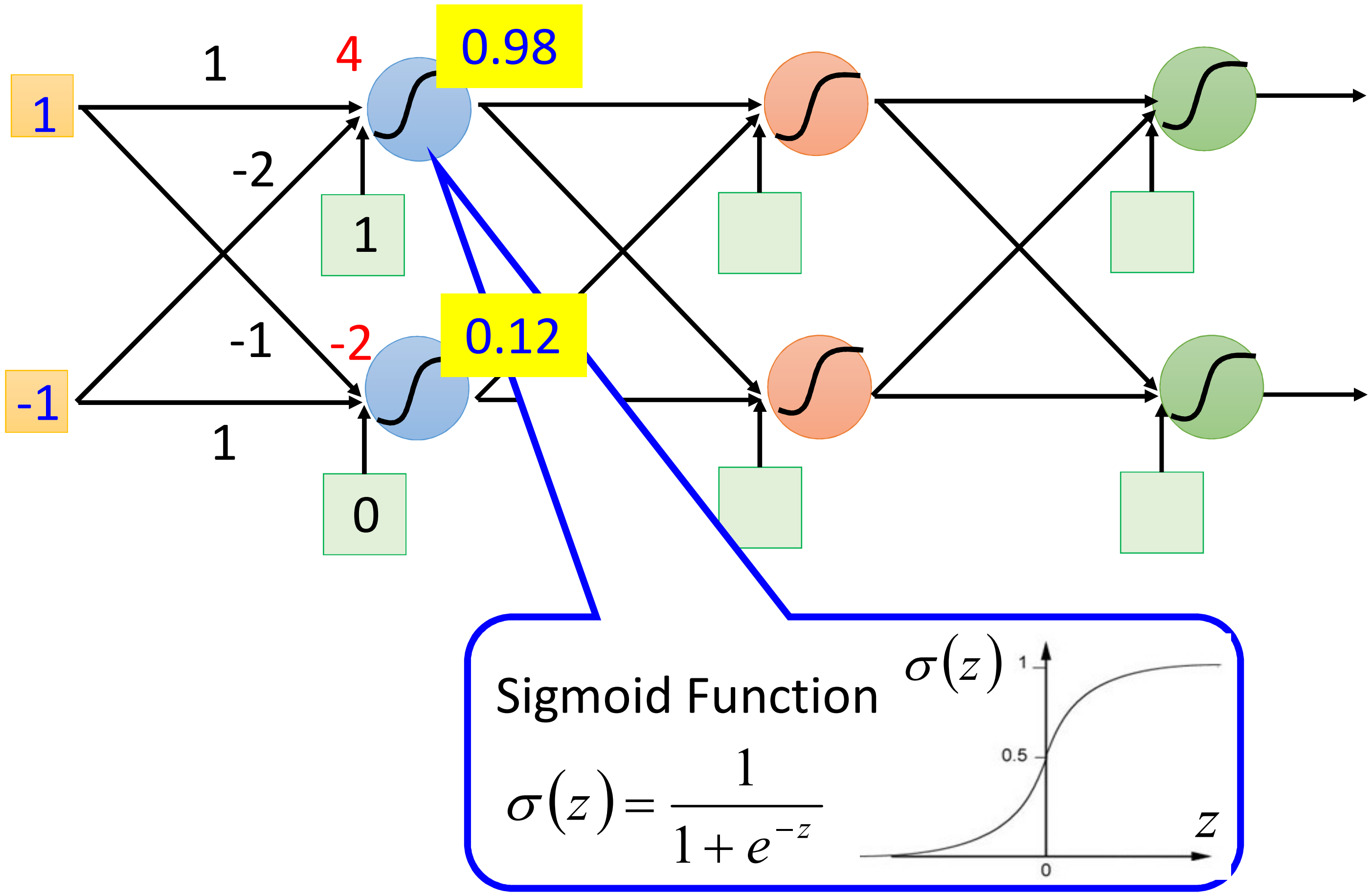
Fully connected Feedforward Network

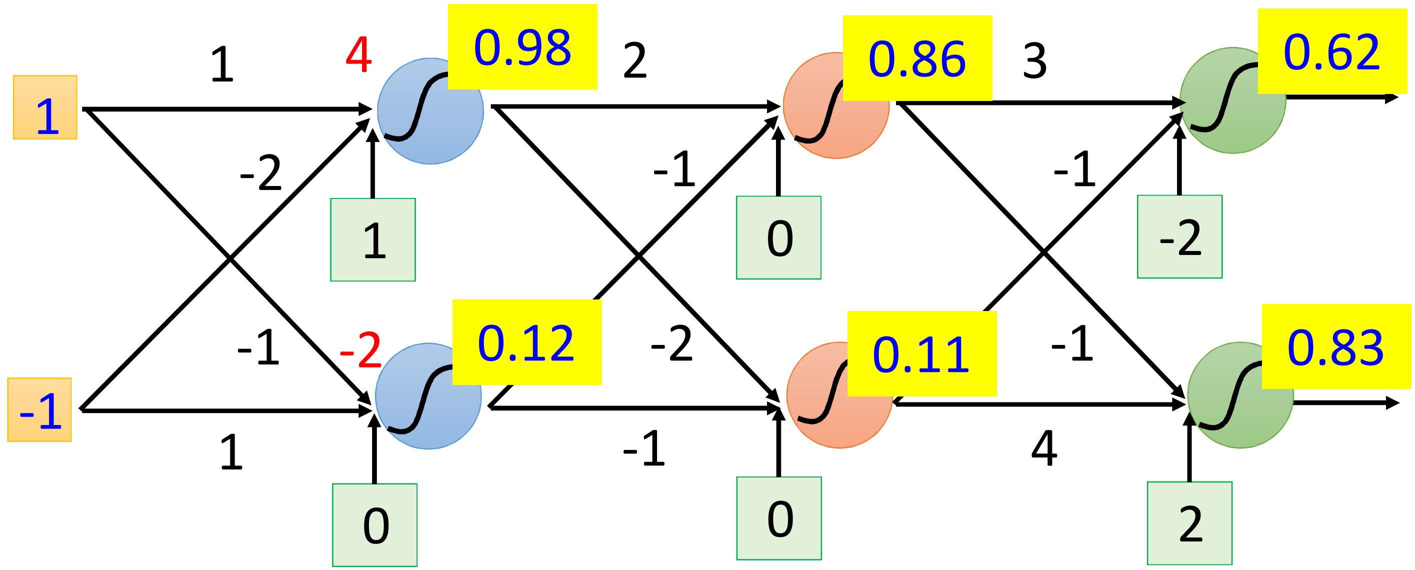


- ➢ Neurons between two adjacent layers are fully pairwise connected
- ➢ But neurons within a single layer share no connections

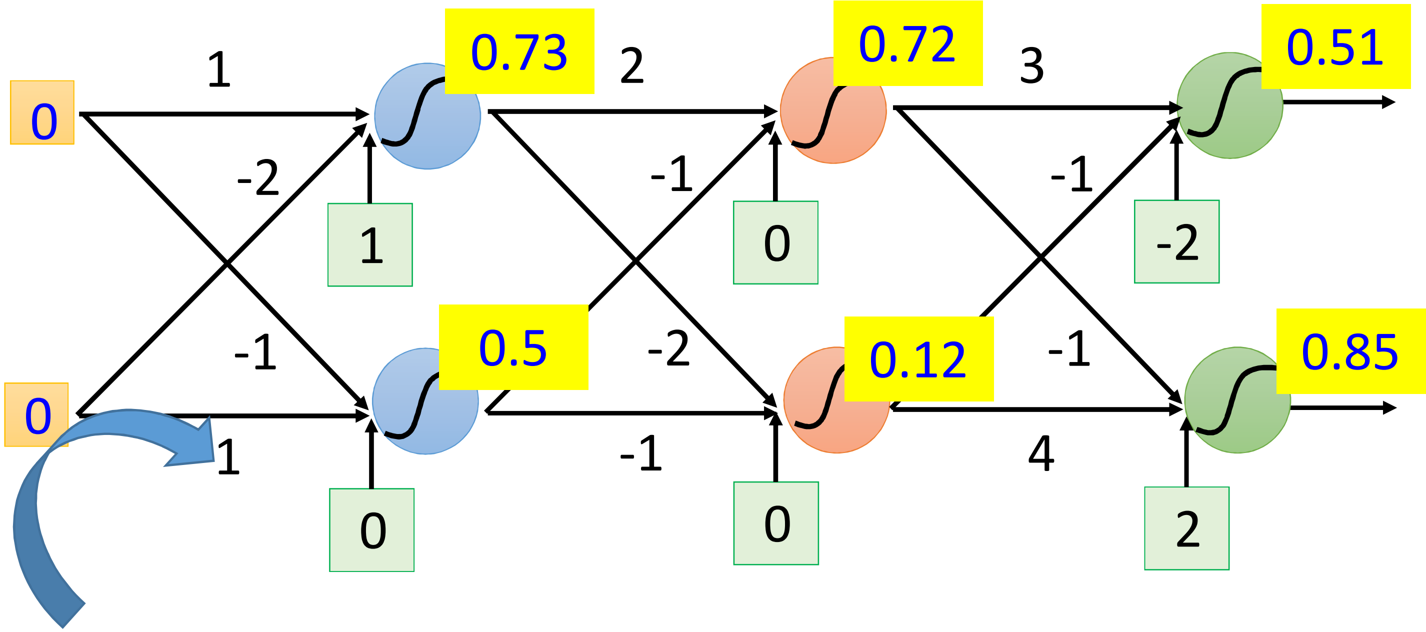
Fully connected Feedforward Network



Fully connected Feedforward Network



Fully connected Feedforward Network



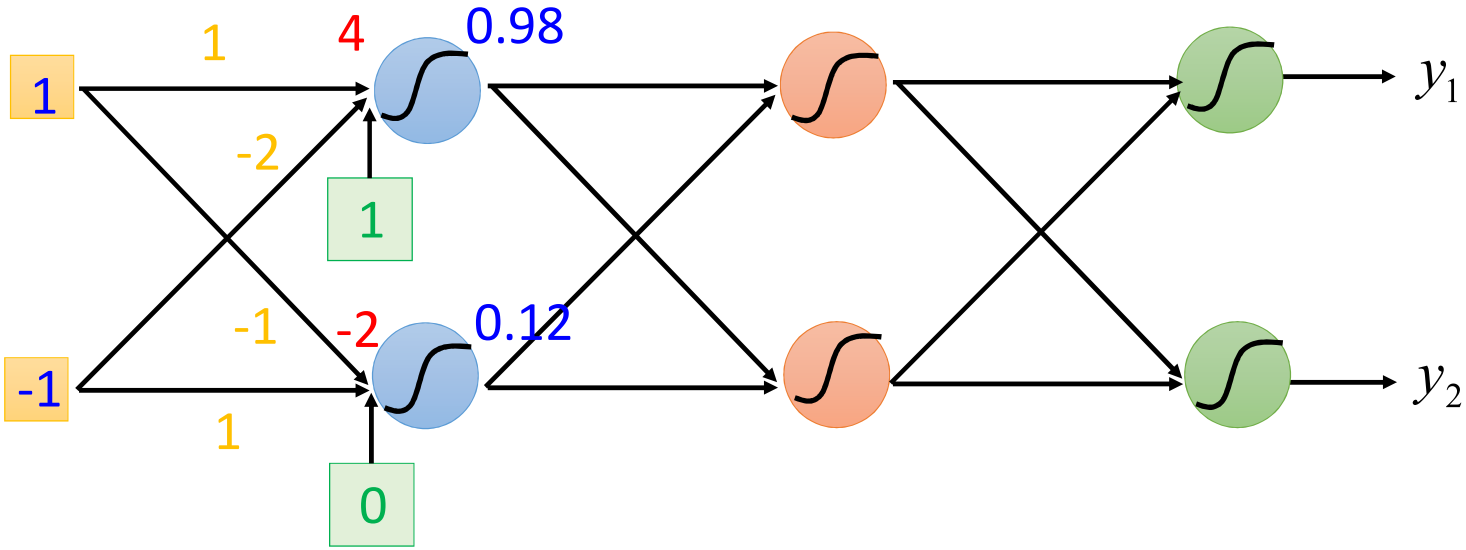
This is a function.

Input vector, output vector

$$f\left(\begin{bmatrix}1\\-1\end{bmatrix}\right)=\begin{bmatrix}0.62\\0.83\end{bmatrix} \quad f\left(\begin{bmatrix}0\\0\end{bmatrix}\right)=\begin{bmatrix}0.51\\0.85\end{bmatrix}$$

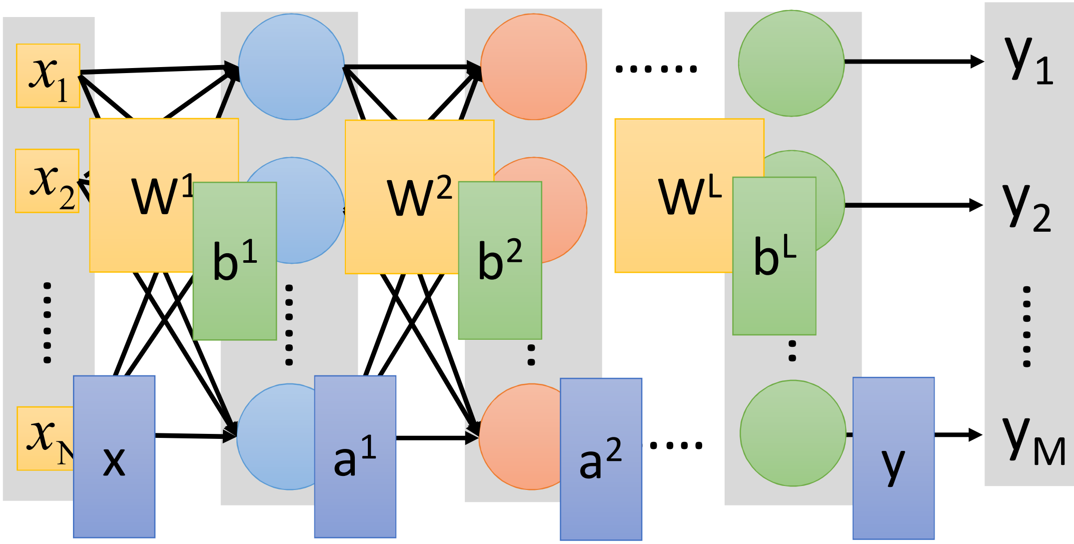
Given network structure, we define ***a function set***

Matrix Operation



$$\sigma\Big(\underbrace{\begin{bmatrix}1 & -2\\ -1 & 1\end{bmatrix}\begin{bmatrix}1\\ -1\end{bmatrix}+\begin{bmatrix}1\\ 0\end{bmatrix}}_{\begin{bmatrix}4\\ -2\end{bmatrix}}\Big)=\begin{bmatrix}0.98\\ 0.12\end{bmatrix}$$

Neural Network

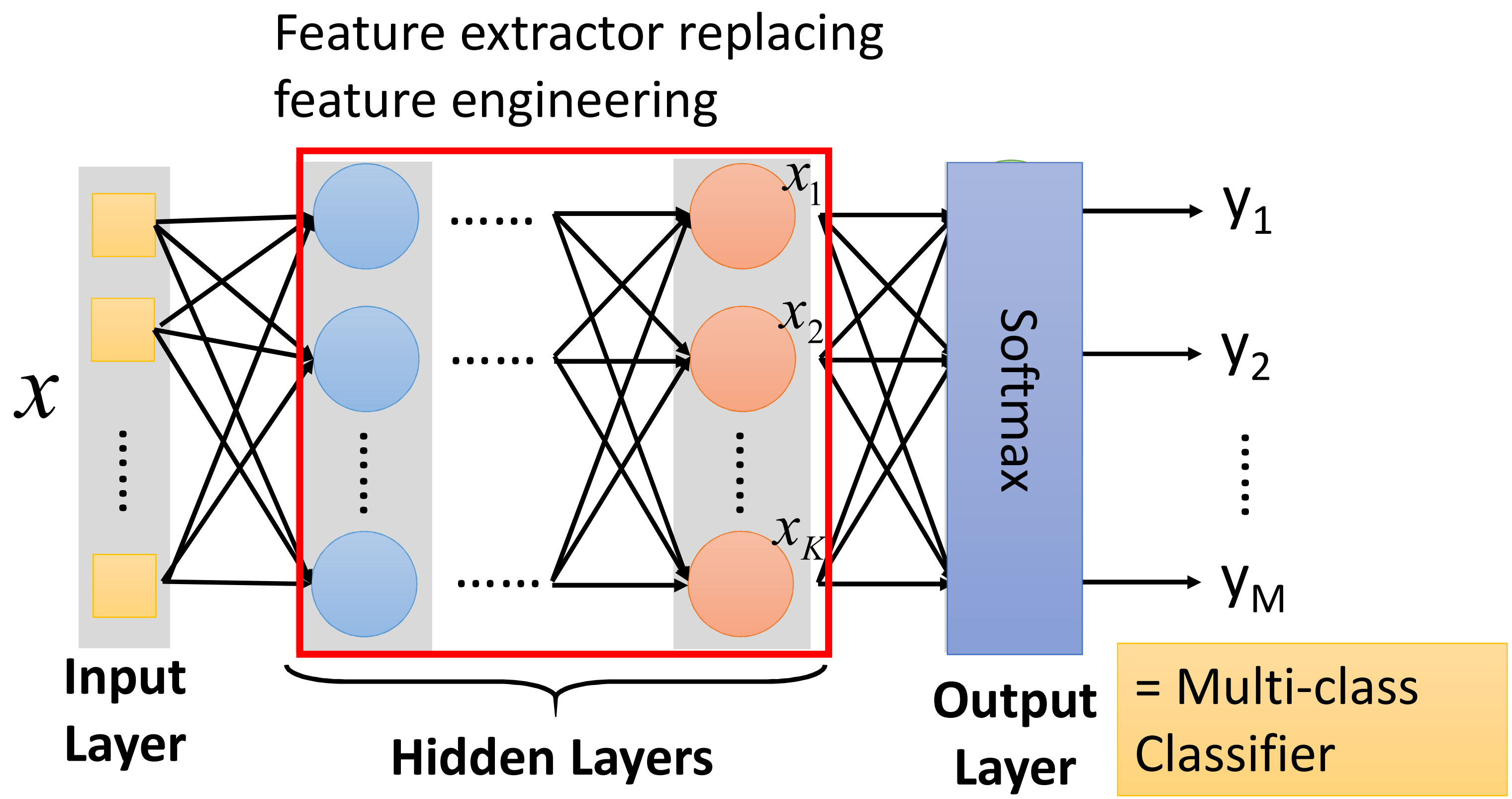


$$y = f(x)$$

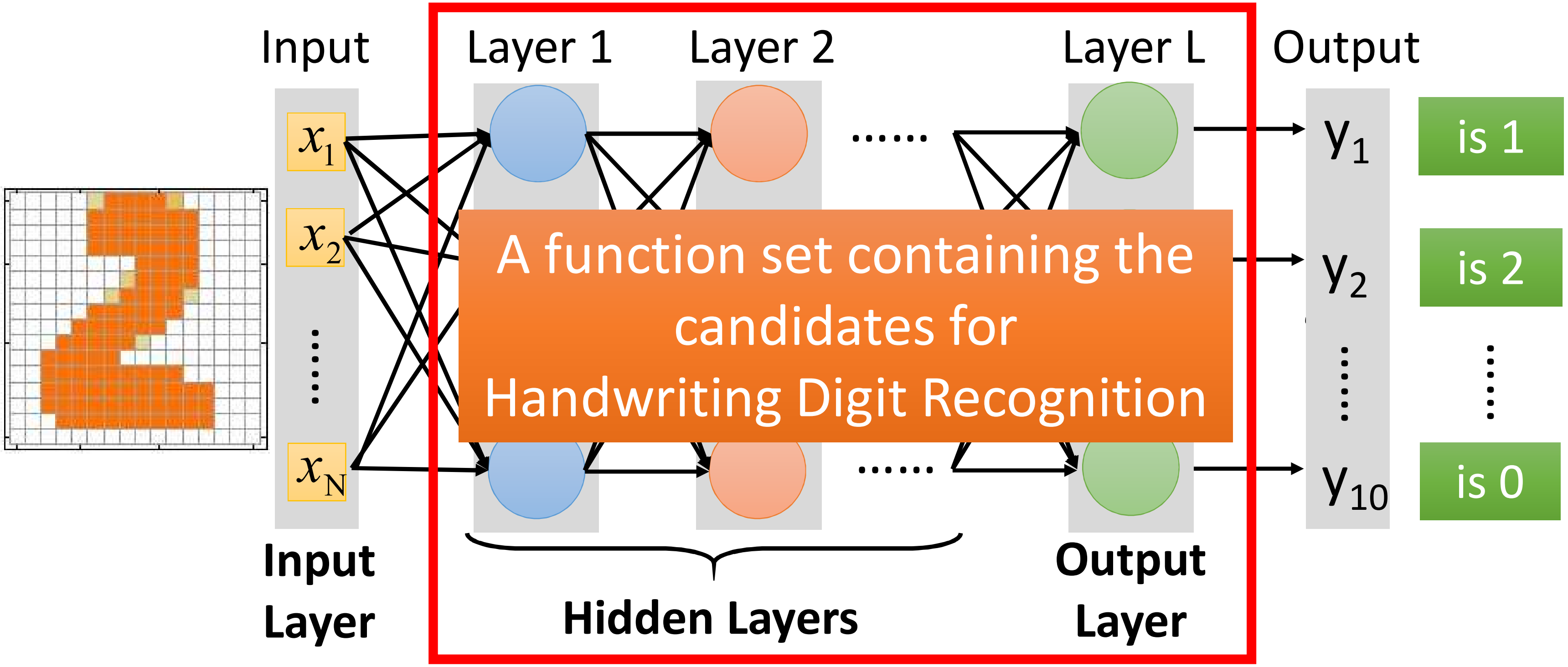
Using parallel computing techniques to speed up matrix operation

$$= \sigma(W^L \cdots \sigma(W^2\, \sigma(W^1\, x + b^1) + b^2) \cdots + b^L)$$

Output Layer as a Multi-Class Classifier

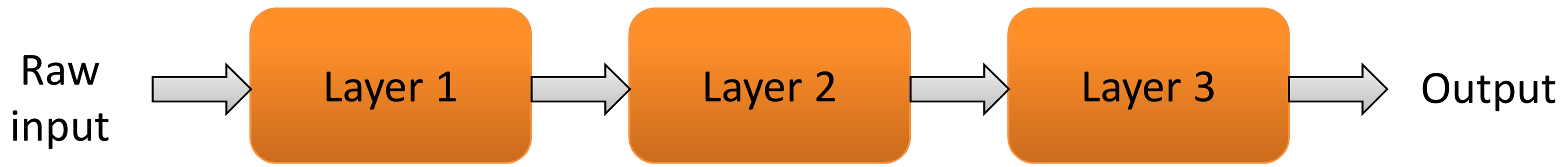


Example Application



Need to decide the network structure to work well on your dataset.

“Deep” pipeline



- Learn a *feature hierarchy*
- Each layer extracts features from the output of previous layer
- All layers are trained jointly

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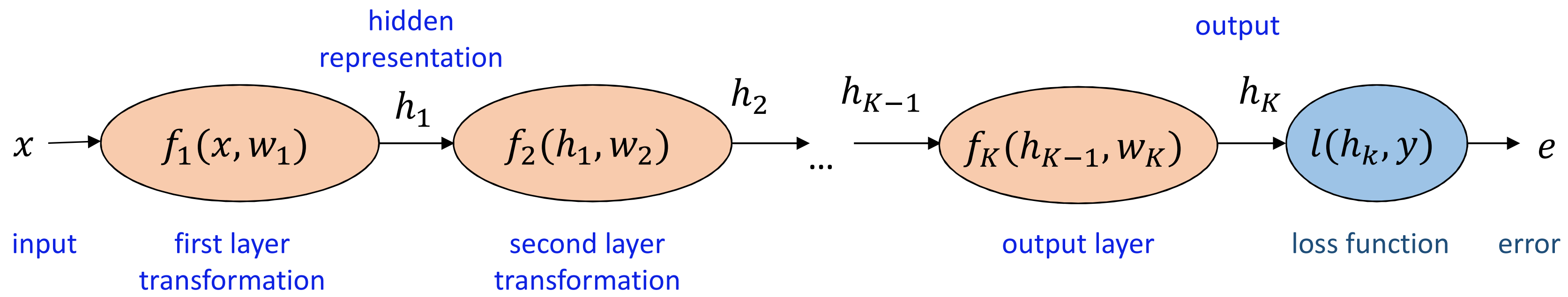
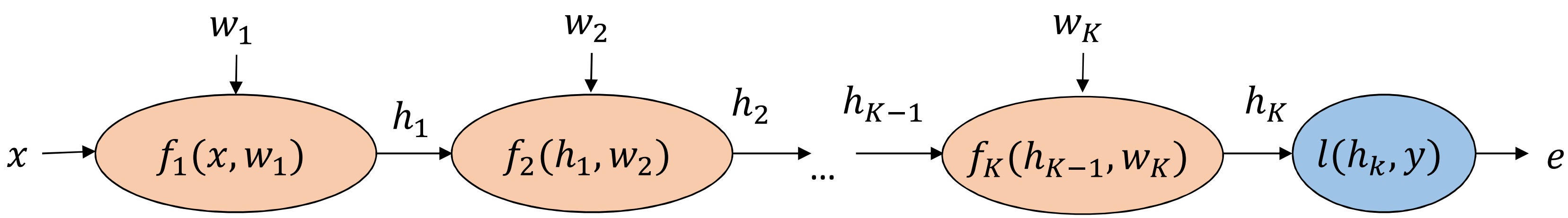
How to train a multi-layer network?



- We need to find the gradient of the error w. r.t. the parameters of each layer, $\frac{\partial e}{\partial w_k}$, to perform updates $\quad w_k \leftarrow w_k - \eta \frac{\partial e}{\partial w_k}$

Computation graph



Chain Rule

Case 1

$$y = g(x) \qquad z = h(y)$$

$$\Delta x \to \Delta y \to \Delta z \qquad \frac{dz}{dx} = \frac{dz}{dy}\frac{dy}{dx}$$

Case 2

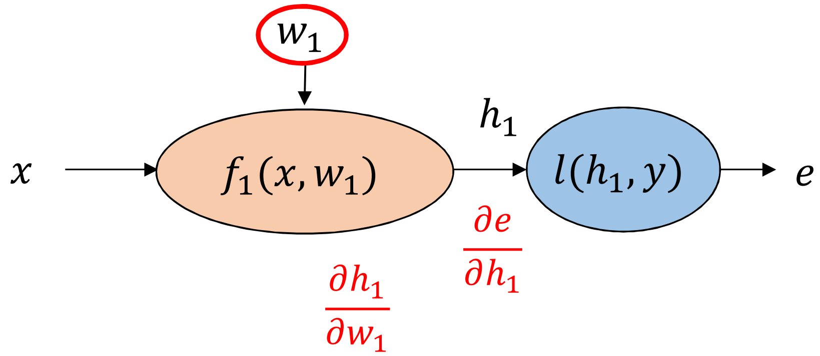
$$x = g(s) \qquad y = h(s) \qquad z = k(x, y)$$

$$\begin{tikzcd}
 & \Delta x \arrow[dr] & \\
\Delta s \arrow[ur] \arrow[dr] & & \Delta z \\
 & \Delta y \arrow[ur] &
\end{tikzcd}$$

$$\frac{dz}{ds} = \frac{\partial z}{\partial x}\frac{dx}{ds} + \frac{\partial z}{\partial y}\frac{dy}{ds}$$

Chain rule

Let's start with $k = 1$



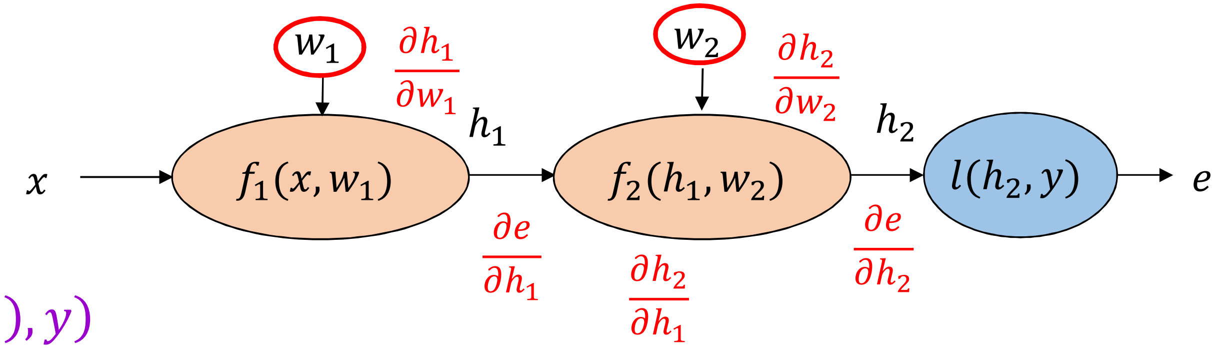
- $e = l(f_1(x, w_1), y)$
- $\frac{\partial}{\partial w_1} l(f_1(x, w_1), y) = \frac{\partial e}{\partial h_1} \frac{\partial h_1}{\partial w_1}$
- Example: $e = (y - w_1^T x)^2$
- $h_1 = f_1(x, w_1) = w_1^T x$
- $e = l(h_1, y) = (y - h_1)^2$
- $\frac{\partial e}{\partial w_1} = \frac{\partial e}{\partial h_1} \frac{\partial h_1}{\partial w_1} = -2x(y - w_1^T x)$

$$\frac{\partial h_1}{\partial w_1} = x$$

$$\frac{\partial e}{\partial h_1} = -2(y - h_1) = -2(y - w_1^T x)$$

Chain rule

$k = 2$



- $e = l(f_2(f_1(x, w_1), w_2), y)$

$$\frac{\partial e}{\partial w_2} = \frac{\partial e}{\partial h_2}\frac{\partial h_2}{\partial w_2} \qquad \frac{\partial e}{\partial w_1} = \boxed{\frac{\partial e}{\partial h_2}\frac{\partial h_2}{\partial h_1}}\frac{\partial h_1}{\partial w_1}$$

- Example: $e = -\log\left(\sigma\left(w_1^T x\right)\right)$ (assume $y = 1$) $\quad \sigma(x) = 1/(1 + e^{-x})$

$$h_1 = f_1(x, w_1) = w_1^T x \qquad \frac{\partial h_1}{\partial w_1} = x$$

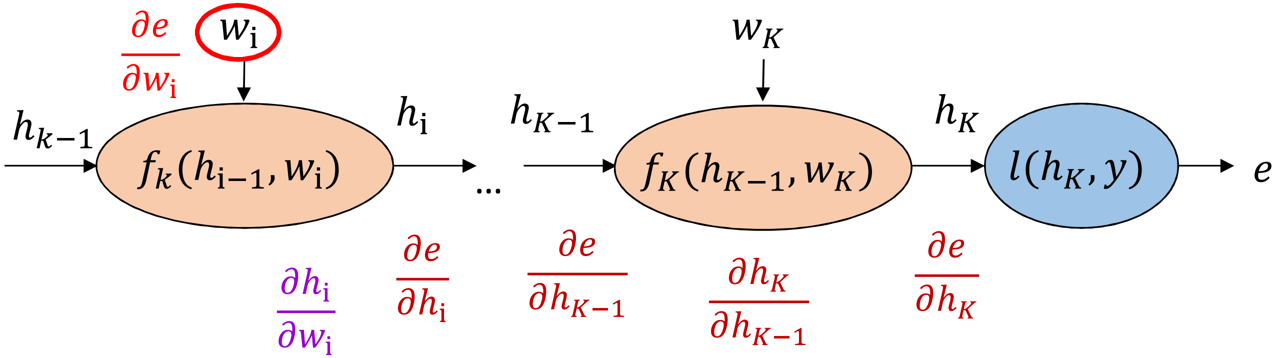
$$h_2 = f_2(h_1, w_2) = \sigma(h_1) \qquad \frac{\partial h_2}{\partial h_1} = \sigma'(h_1) = \sigma(h_1)(1 - \sigma(h_1))$$

$$e = l(h_2, 1) = -\log(h_2) \qquad \frac{\partial e}{\partial h_2} = -\frac{1}{h_2}$$

$$\frac{\partial e}{\partial w_1} = \frac{\partial e}{\partial h_2}\frac{\partial h_2}{\partial h_1}\frac{\partial h_1}{\partial w_1} = -\frac{1}{\sigma(w_1^T x)}\sigma\left(w_1^T x\right)\left(1 - \sigma\left(w_1^T x\right)\right)x = \sigma\left(w_1^T x\right)x - x$$

Chain rule

- General case:

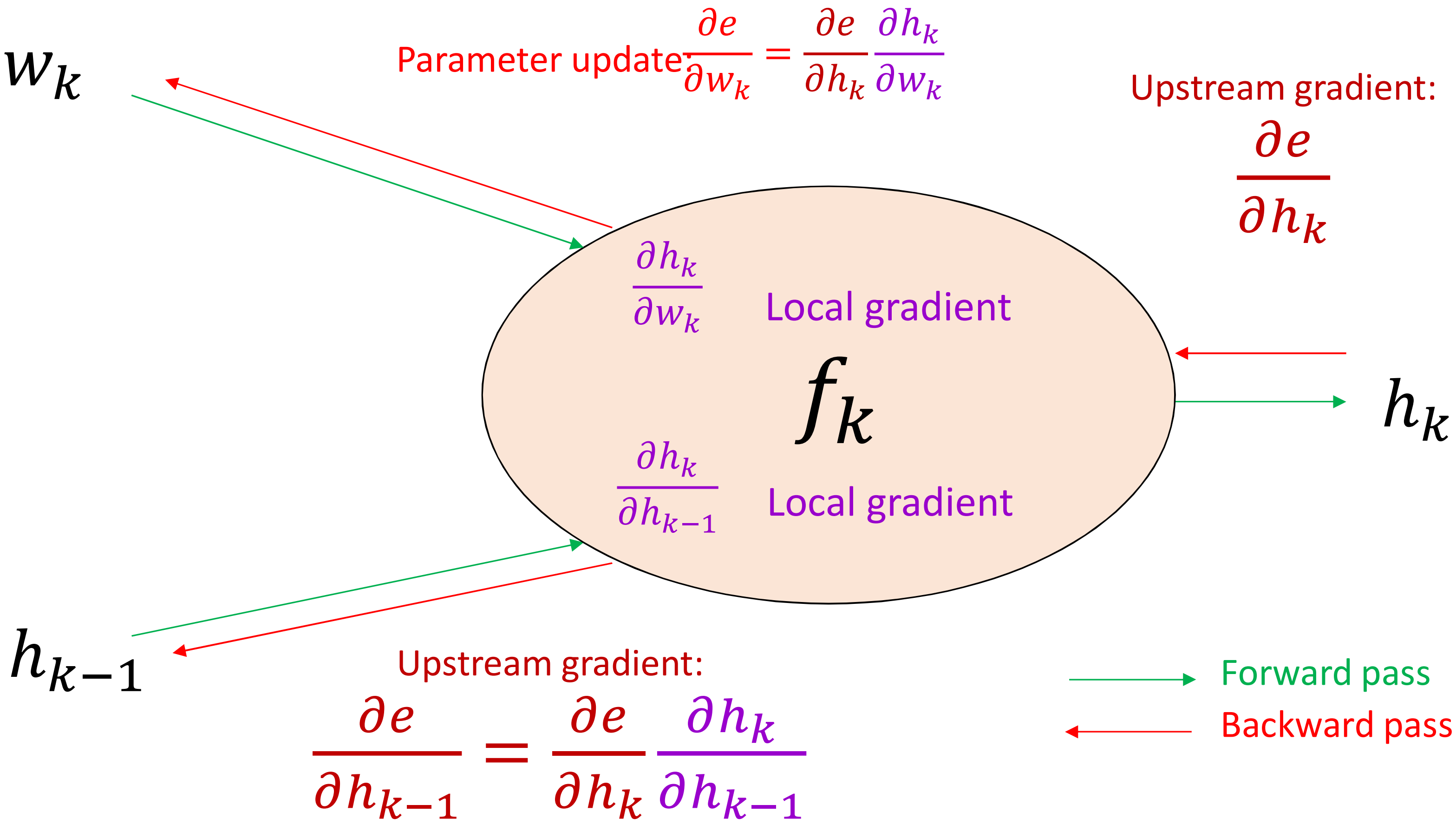


- $$\frac{\partial e}{\partial w_i} = \boxed{\frac{\partial e}{\partial h_K} \frac{\partial h_K}{\partial h_{K-1}} \cdots \frac{\partial h_{i+1}}{\partial h_i}} \frac{\partial h_i}{\partial w_i}$$

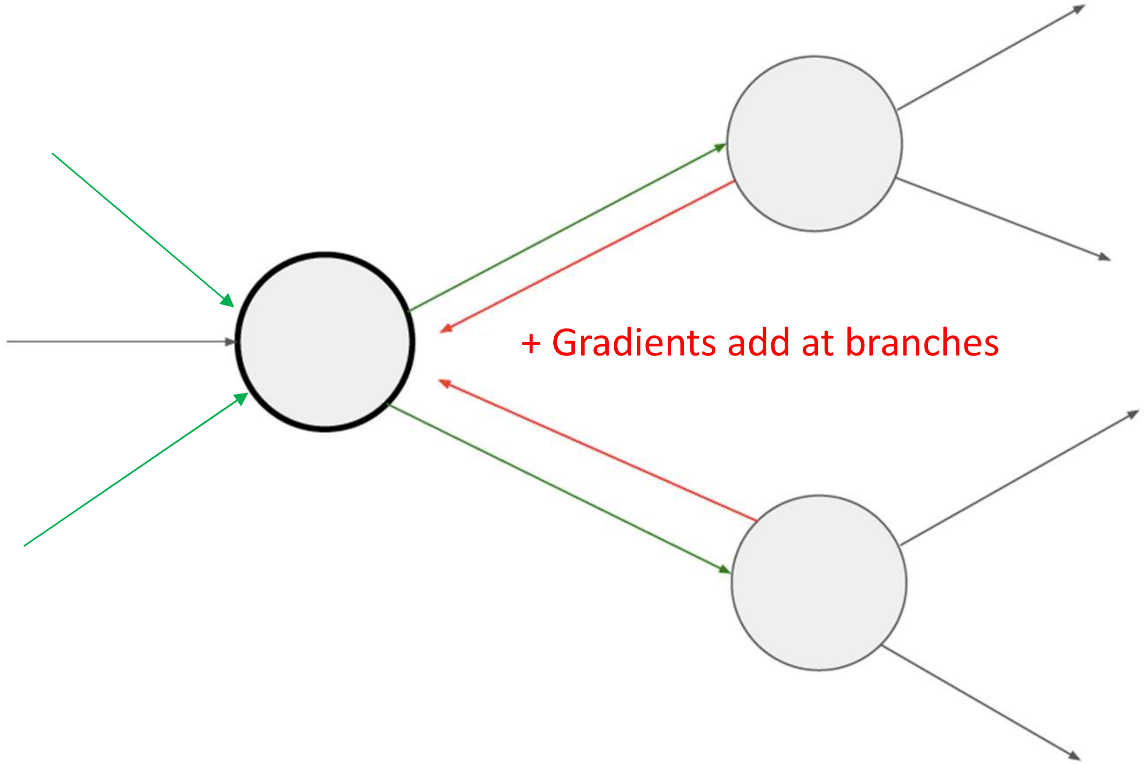
Upstream gradient $\frac{\partial e}{\partial h_i}$

Local gradient

Backpropagation summary

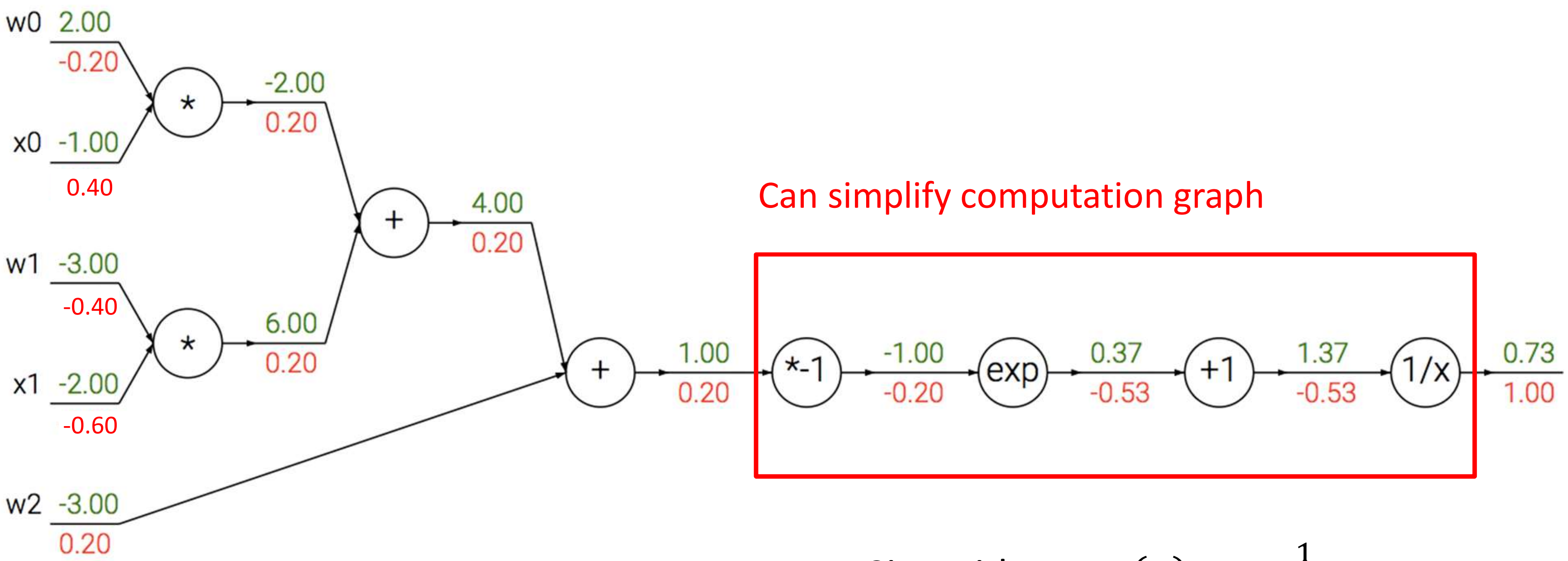


What about more general computation graphs?



A detailed example

$$f(x, w) = \frac{1}{1 + \exp[-(w_0 x_0 + w_1 x_1 + w_2)]}$$



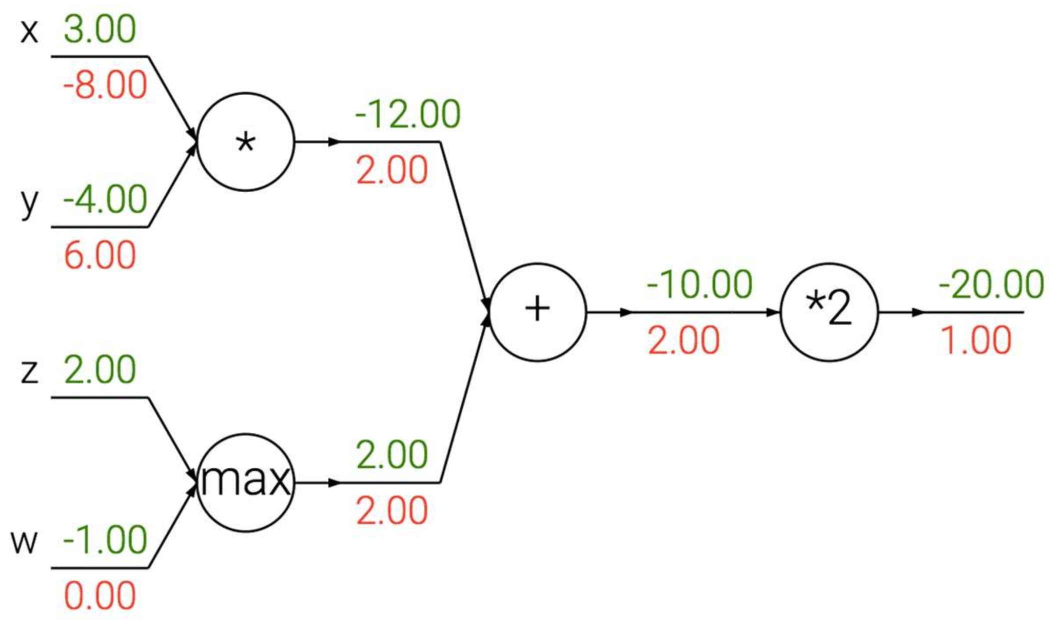
Sigmoid gate $\sigma(x) = \frac{1}{1+\exp(-x)}$

$$\sigma'(x) = \sigma(x)\big(1 - \sigma(x)\big)$$

$$\sigma(1)\big(1 - \sigma(1)\big) = 0.73 * (1 - 0.73) = 0.20$$

Source: Stanford 231n

Patterns in gradient flow



Add gate: “gradient distributor”

Multiply gate: “gradient switcher”

Max gate: “gradient router”

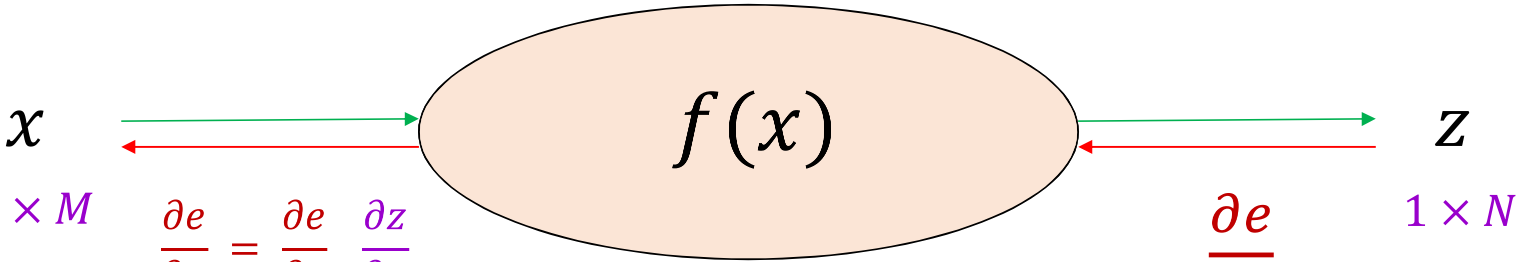
Source: [Stanford 231n]()

Dealing with vectors

$$\frac{\partial z}{\partial x} = \begin{pmatrix} \frac{\partial z_1}{\partial x_1} & \cdots & \frac{\partial z_1}{\partial x_M} \\ \vdots & \ddots & \vdots \\ \frac{\partial z_N}{\partial x_1} & \cdots & \frac{\partial z_N}{\partial x_M} \end{pmatrix}$$

$N \times M$

Jacobian



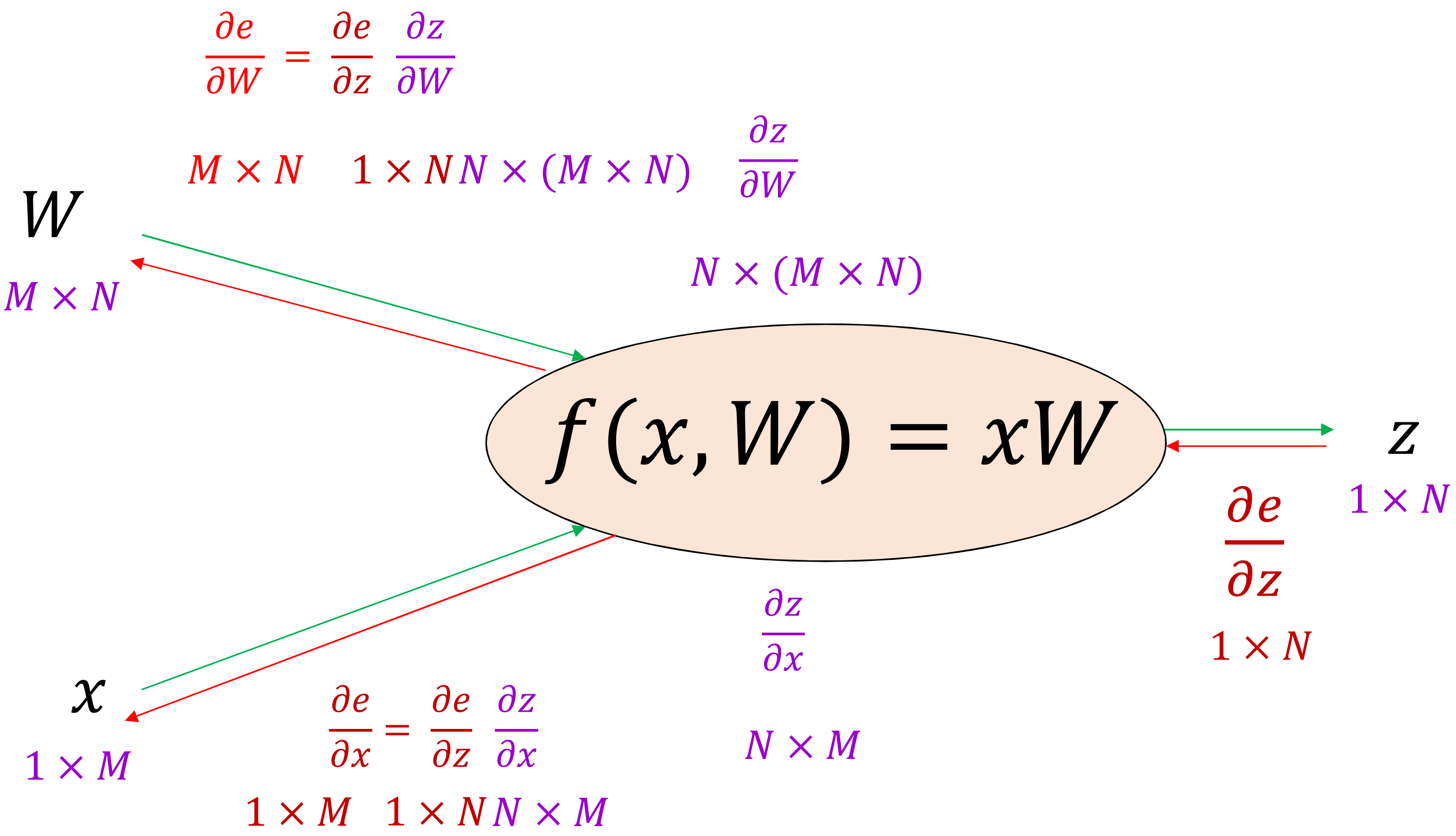
$1 \times M$ $\qquad$ $1 \times N$

$$\frac{\partial e}{\partial x} = \frac{\partial e}{\partial z} \frac{\partial z}{\partial x}$$

$$\frac{\partial e}{\partial z}$$

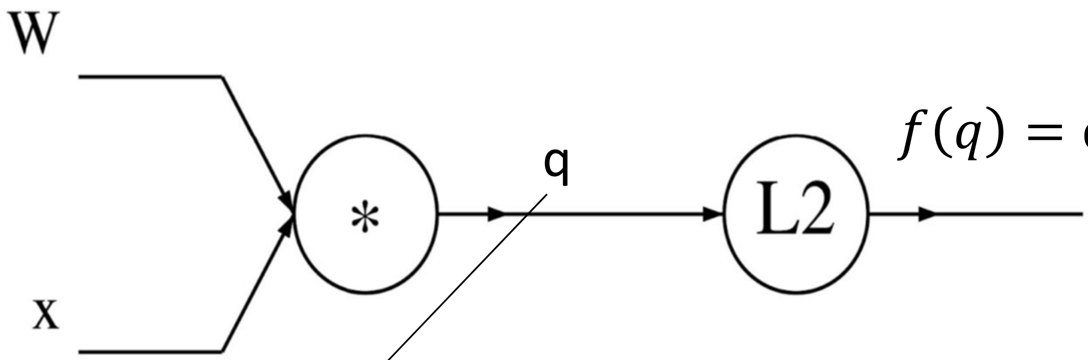
$1 \times M$ $\quad$ $1 \times N$ $N \times M$ $\qquad$ $1 \times N$

Matrix-vector multiplication



A vectorized example:

$$f(\mathrm{x}, W) = \sum_{i=1}^{n} (W \cdot \mathrm{x})_i^2$$



$$f(q) = \mathrm{q}_1^2 + \cdots + \mathrm{q}_n^2$$

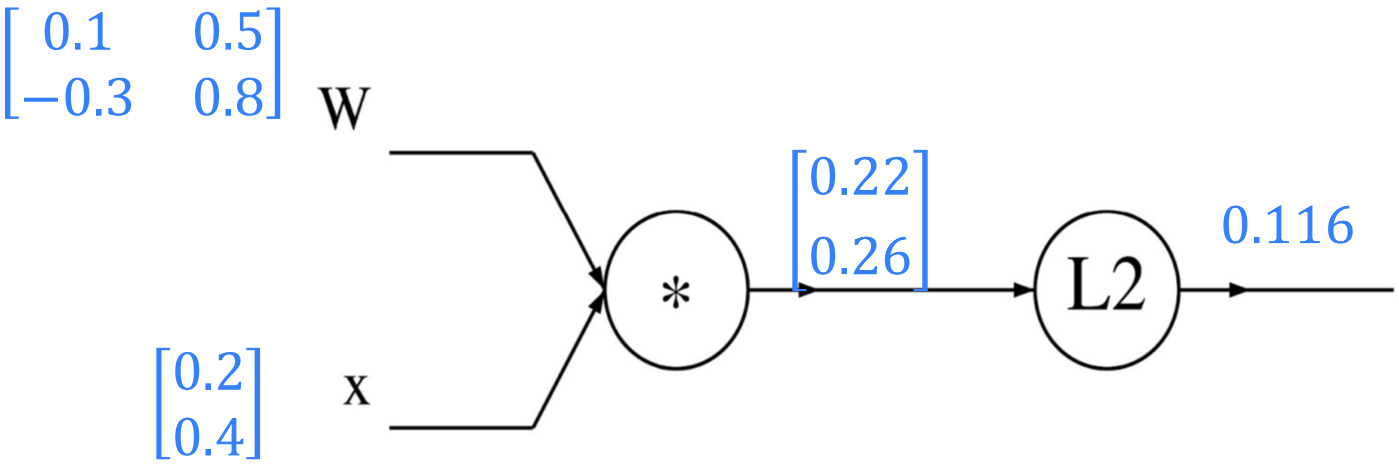
$$q = W\mathrm{x} = \begin{pmatrix} w_{11}x_1 + \cdots + w_{1n}x_n \\ \vdots \\ w_{n1}x_1 + \cdots + w_{nn}x_n \end{pmatrix}$$

A vectorized example: $f(\mathrm{x}, W) = \sum_{i=1}^{n} (W \cdot \mathrm{x})_i^2$

Feed-forward:

$$q = Wx = \begin{pmatrix} w_{11}x_1 + w_{12}x_2 \\ w_{21}x_1 + w_{22}x_2 \end{pmatrix} = \begin{bmatrix} 0.22 \\ 0.26 \end{bmatrix}$$

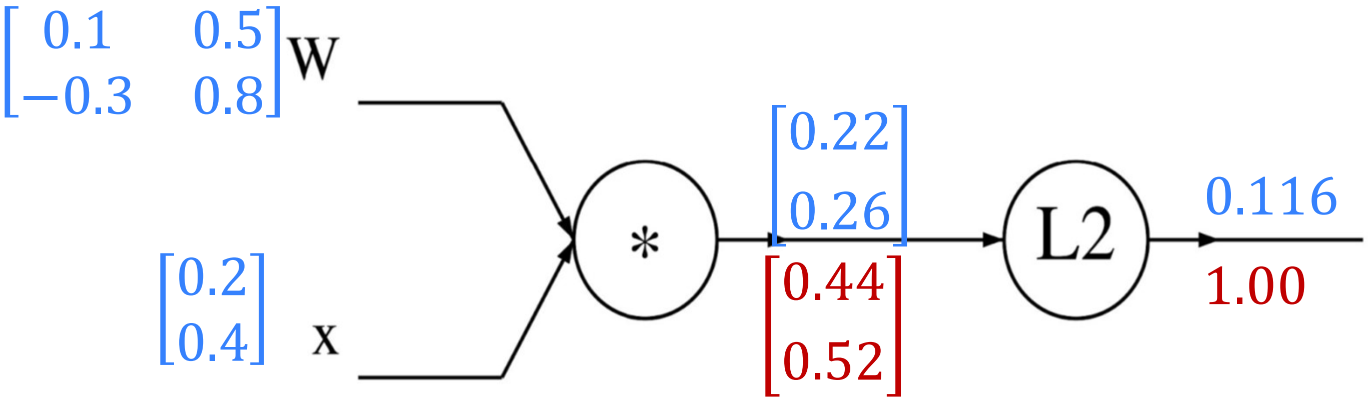
$$f(q) = \sum_{i=1}^{2} \mathrm{q}_\mathrm{i}^2 = 0.116$$



A vectorized example: $f(\mathrm{x}, W) = \sum_{i=1}^{n} (W \cdot \mathrm{x})_i^2$

Backward:

$$f(q) = \sum_{i=1}^{2} \mathrm{q}_\mathrm{i}^2 \quad \Longrightarrow \quad \frac{\partial f}{\partial q_i} = 2q_i \quad \Longrightarrow \quad \boxed{\nabla_\mathrm{q}\, \mathrm{f} = 2q}$$

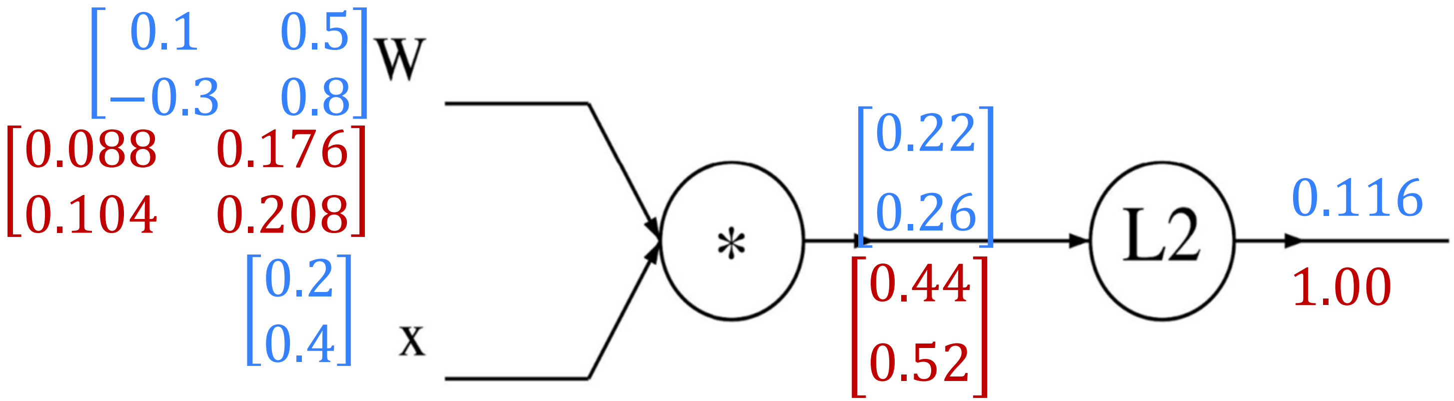


A vectorized example: $f(\mathrm{x}, W) = \sum_{i=1}^{n} (W \cdot \mathrm{x})_i^2$

Backward:

$$q = Wx = \begin{pmatrix} w_{11}x_1 + w_{12}x_2 \\ w_{21}x_1 + w_{22}x_2 \end{pmatrix} \Rightarrow \quad \frac{\partial q}{\partial w_{11}} = x_1 \quad \frac{\partial q}{\partial w_{12}} = x_2 \quad \frac{\partial q}{\partial w_{21}} = x_1 \quad \frac{\partial q}{\partial w_{22}} = x_2$$

$$\frac{\partial f}{\partial w_{ij}} = \sum_k \frac{\partial f}{\partial q_k}\frac{\partial q_k}{\partial w_{ij}} = 2q_i x_j \Longrightarrow \boxed{\nabla_W f = 2qx^T}$$

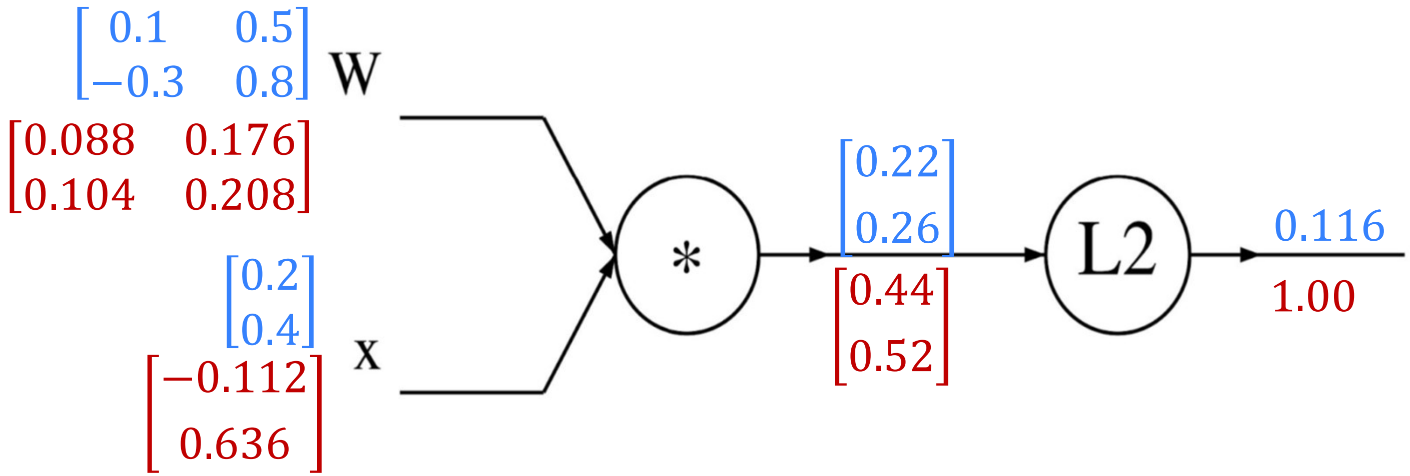


A vectorized example: $f(\mathrm{x}, W) = \sum_{i=1}^{n} (W \cdot \mathrm{x})_i^2$

Backward:

$$q = Wx = \begin{pmatrix} w_{11}x_1 + w_{12}x_2 \\ w_{21}x_1 + w_{22}x_2 \end{pmatrix} \Rightarrow \quad \frac{\partial q}{\partial x_1} = \begin{pmatrix} w_{11} \\ w_{21} \end{pmatrix} \quad \frac{\partial q}{\partial x_2} = \begin{pmatrix} w_{12} \\ w_{22} \end{pmatrix}$$

$$\frac{\partial f}{\partial x_i} = \sum_k \frac{\partial f}{\partial q_k} \frac{\partial q_k}{\partial x_i} = \sum_k 2\, q_k W_{ki} \Rightarrow \quad \boxed{\nabla_x \mathrm{f} = W^T 2q}$$



Outline

- Modeling one neuron
- Activation functions
- Fully connected feed-forward network
- How to train a multi-layer network
- Representational power of NN

Representational power

- Neural Networks with fully-connected layers define a family of functions that are parameterized by the weights of the network.
- A Neural Network with at least one hidden layer are *universal approximators, which* means that it can approximate any continuous function.

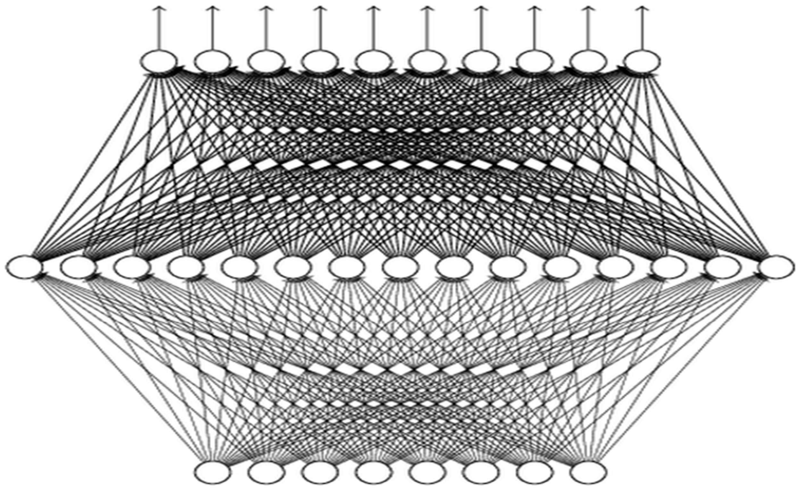
Universality Theorem

Any continuous function f

$$f : R^N \rightarrow R^{\mathrm{M}}$$

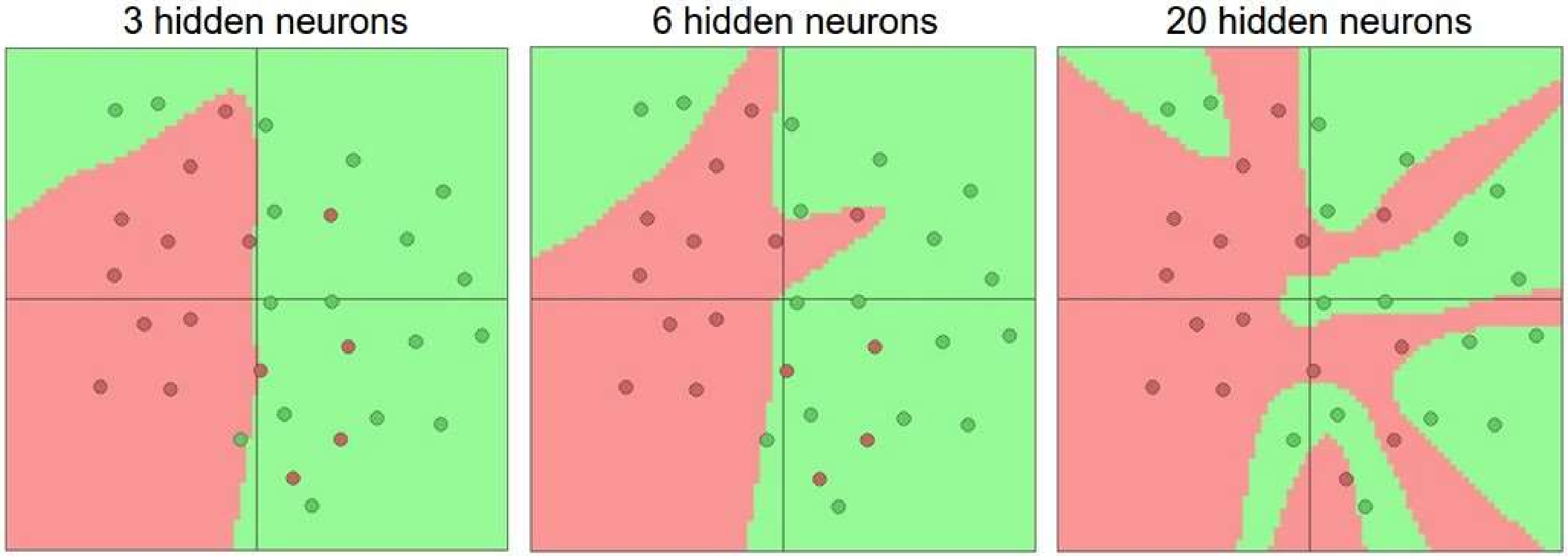
can be realized by a network with one hidden layer

(given **enough** hidden neurons)



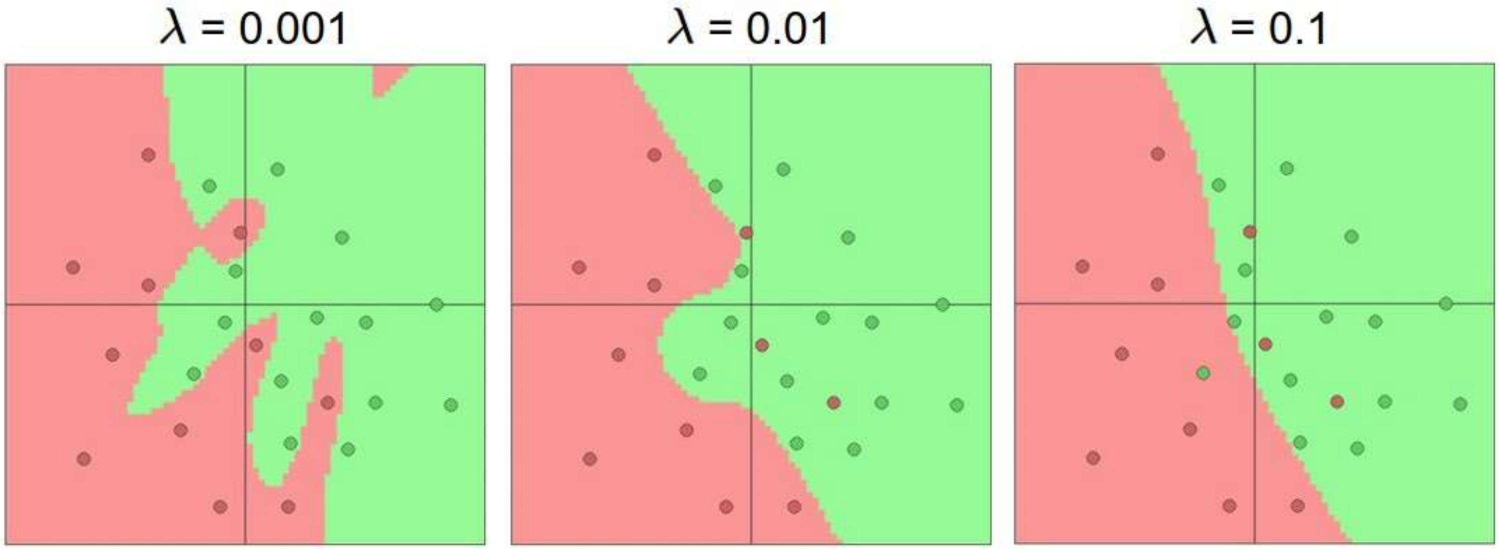
Reference for the reason: http://neuralnetworksanddeeplearning.com/chap4.html

Setting number of layers and their sizes

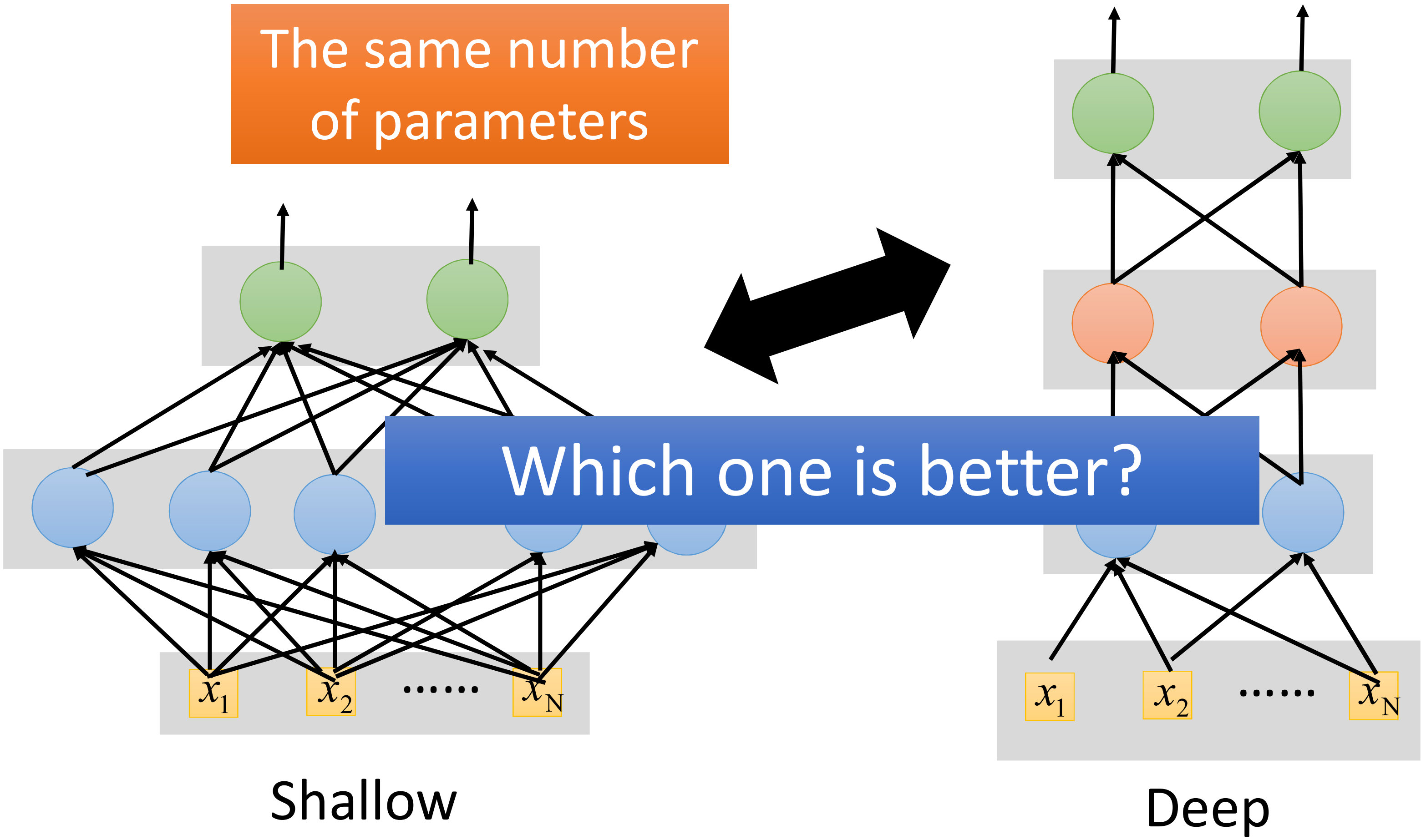


- Neural Networks with more neurons can express more complicated functions.
- But a model with high capacity fits the noise in the data instead of the (assumed) underlying relationship : **overfitting**.

- Use as bigger of a neural network, and use other regularization techniques to control overfitting.



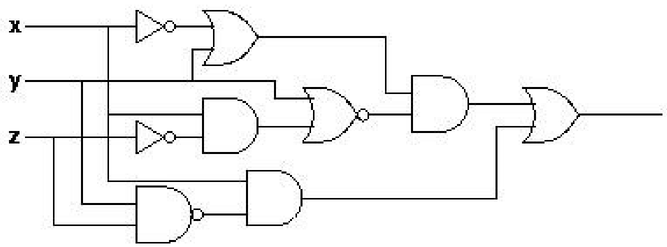
Fat + Short vs. Thin + Tall



Thin + Tall vs. Fat + Short

Layer X Size	Word Error Rate (%)	Layer X Size	Word Error Rate (%)
1 X 2k	24.2		
2 X 2k	20.4	Why?	
3 X 2k	18.4		
4 X 2k	17.8		
5 X 2k	17.2	1 X 3772	22.5
7 X 2k	17.1	1 X 4634	22.6
		1 X 16k	22.1

Analogy

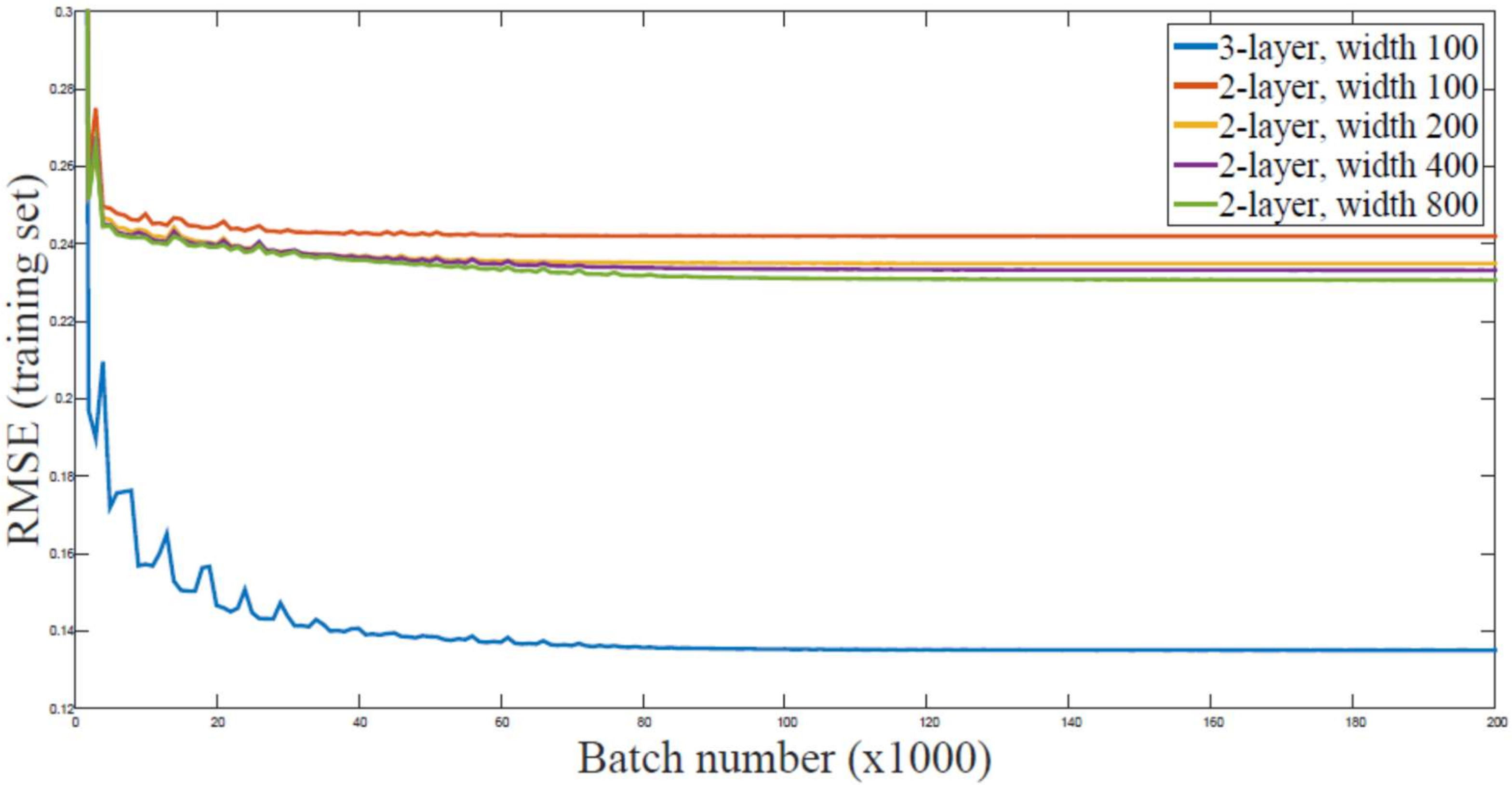


Logic circuits

Neural network

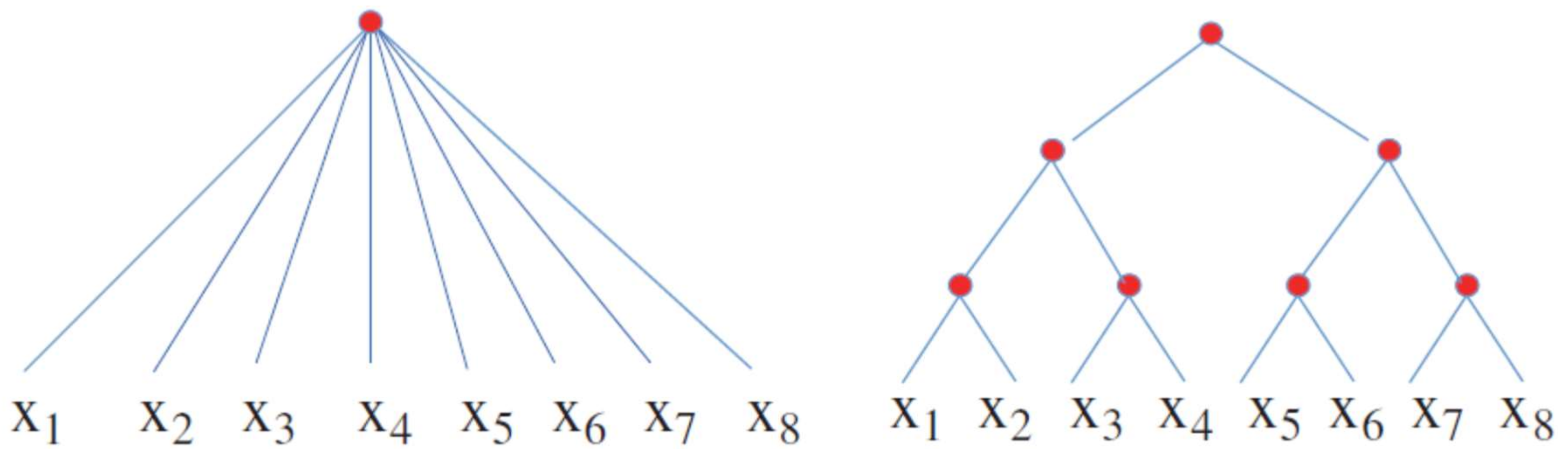
- Logic circuits consists of **gates**
- **A two layers of logic gates** can represent **any Boolean function.**
- Using multiple layers of logic gates to build some functions are much simpler → less gates needed

- Neural network consists of **neurons**
- **A hidden layer network** can represent **any continuous function.**
- Using multiple layers of neurons to represent some functions are much simpler → less parameters → less data?

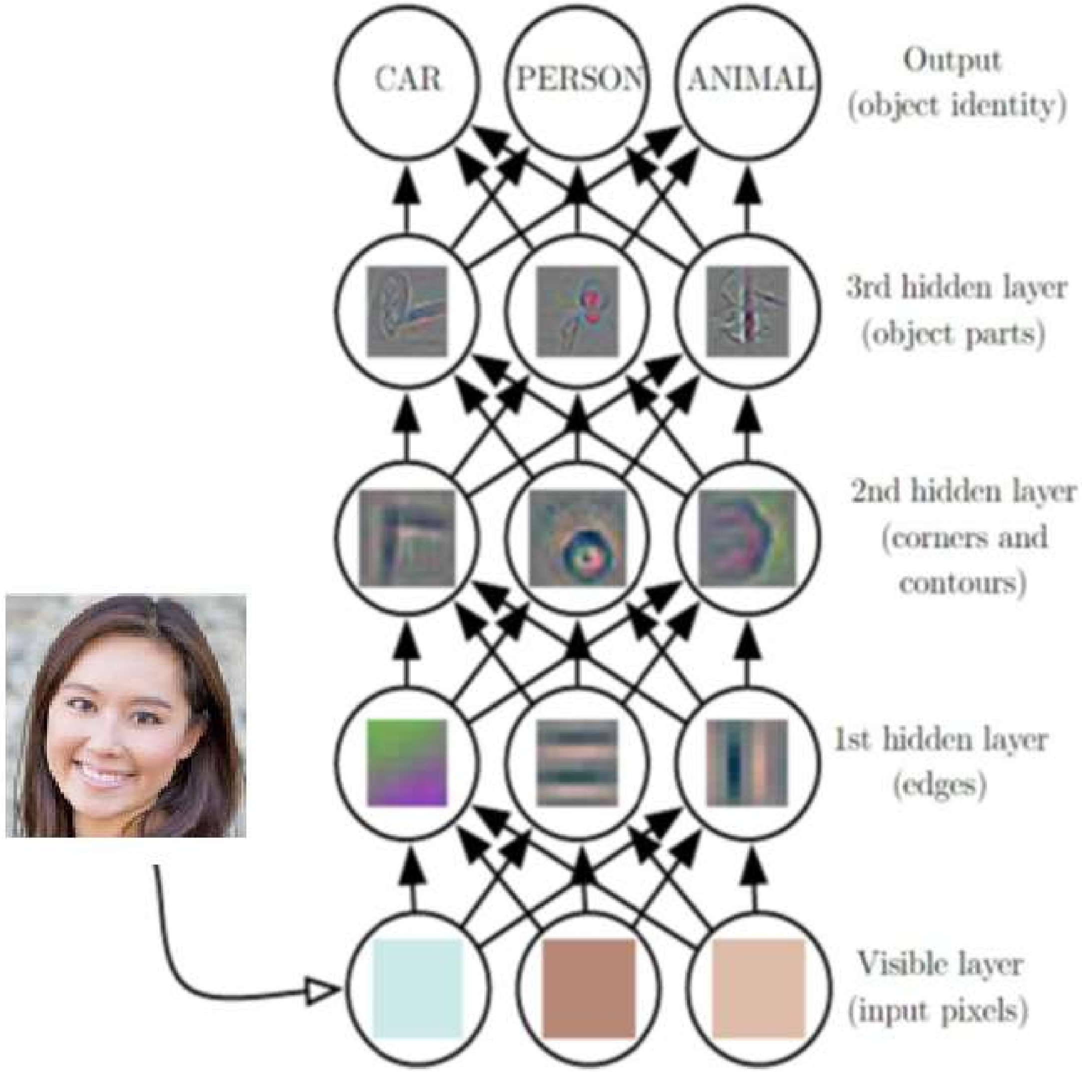


Itay Safran, Ohad Shamir, “Depth-Width Tradeoffs in Approximating Natural Functions with Neural Networks”, ICML, 2017

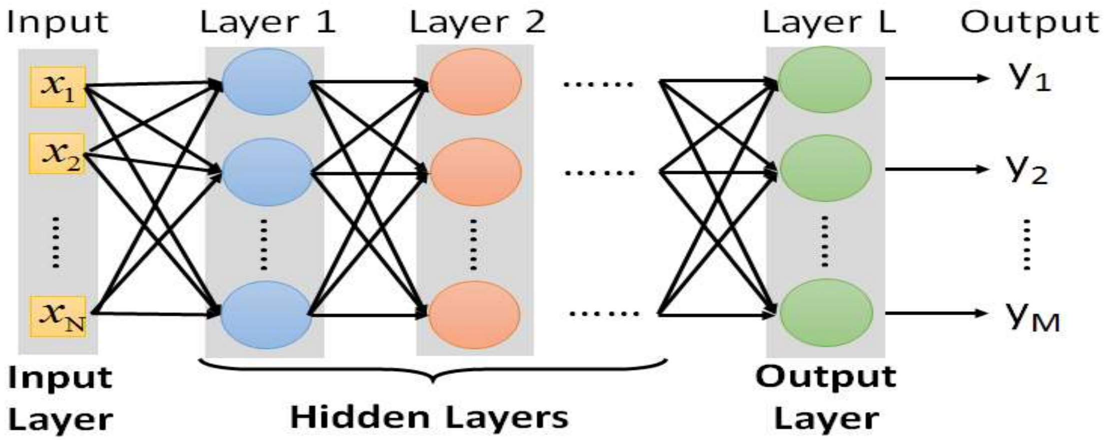
The Nature of Functions



Hrushikesh Mhaskar, Qianli Liao, Tomaso Poggio, When and Why Are Deep Networks Better Than Shallow Ones?, AAAI, 2017


CAR
PERSON
ANIMAL
Output
(object identity)
3rd hidden layer
(object parts)
2nd hidden layer
(corners and
contours)
1st hidden layer
(edges)
Visible layer
(input pixels)

Design the Network



- Q: How many layers? How many neurons for each layer?

Trial and Error + Intuition

- Q: Can the structure be automatically determined?
- Q: Can we design the network structure?

Q & A