## Lecture 6: Neural Networks

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## Outline

- Perceptron
- Activation functions
- Multilayer perceptron networks
- Training: backpropagation
- Examples
- Overfitting
- Applications

## Brief history of artificial neural nets

#### The First wave

- 1943 McCulloch and Pitts proposed the McCulloch-Pitts neuron model
- 1958 Rosenblatt introduced the simple single layer networks now called Perceptrons
- 1969 Minsky and Papert's book *Perceptrons* demonstrated the limitation of single layer perceptrons, and almost the whole field went into hibernation

#### The Second wave

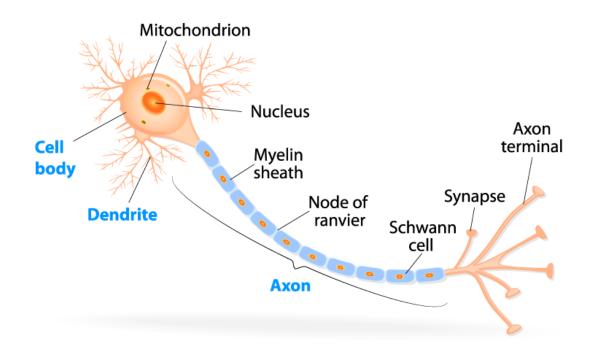
• 1986 The Back-Propagation learning algorithm for Multi-Layer Perceptrons was rediscovered and the whole field took off again

#### The Third wave

- 2006 Deep (neural networks) Learning gains popularity
- 2012 made significant break-through in many applications

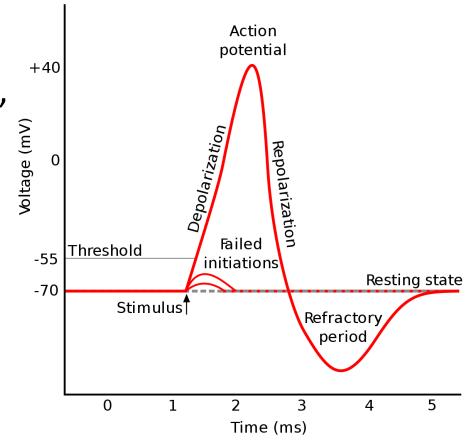
## Biological neuron structure

 The neuron receives signals from their dendrites, and send its own signal to the axon terminal



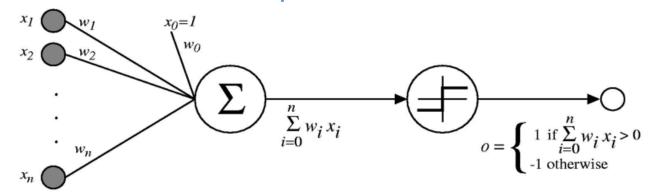
## Biological neural communication

- Electrical potential across cell membrane exhibits spikes called action potentials
- Spike originates in cell body, travels down axon, and causes synaptic terminals to release neurotransmitters
- Chemical diffuses across synapse to dendrites of other neurons
- Neurotransmitters can be excitatory or inhibitory
- If net input of neuro transmitters to a neuron from other neurons is excitatory and exceeds some threshold, it fires an action potential



## Perceptron

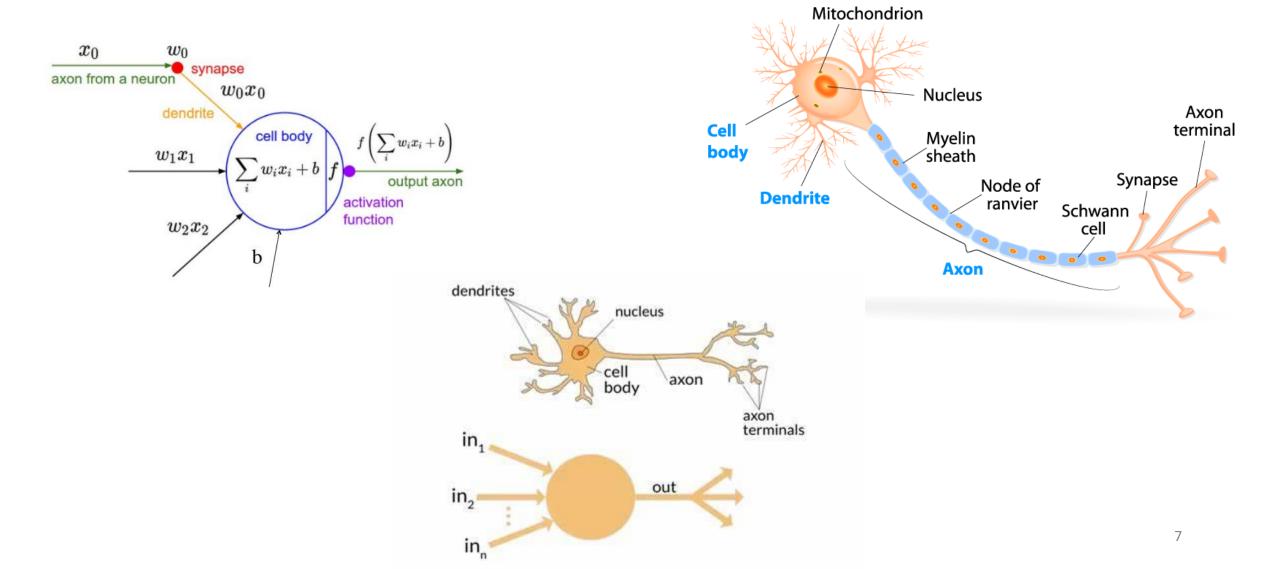
 Inspired by the biological neuron among humans and animals, researchers build a simple model called Perceptron



$$o(x_1, \dots, x_n) = \begin{cases} 1 & \text{if } w_0 + w_1 x_1 + \dots + w_n x_n > 0 \\ -1 & \text{otherwise.} \end{cases}$$

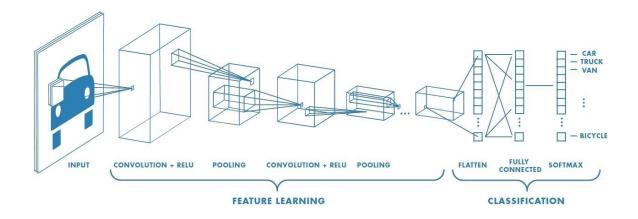
• It receives signals  $x_i$ 's, multiplies them with different weights  $w_i$ , and outputs the sum of the weighted signals after an activation function, step function

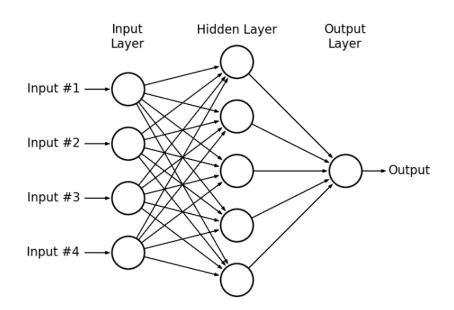
## Neuron vs. Perceptron

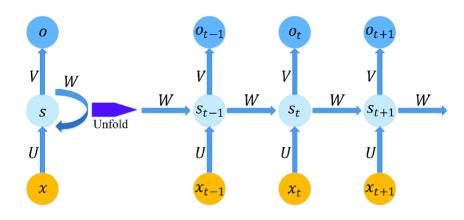


## Artificial neural networks

- Multilayer perceptron network
- Convolutional neural network
- Recurrent neural network



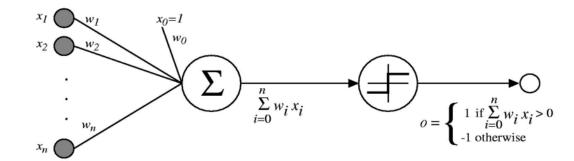




# Perceptron

## Training

- $w_i \leftarrow w_i \eta(o y)x_i$ 
  - *y*: the real label
  - *o*: the output for the perceptron
  - $\eta$ : the learning rate

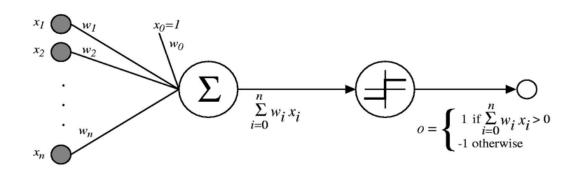


$$o(x_1, \dots, x_n) = \begin{cases} 1 & \text{if } w_0 + w_1 x_1 + \dots + w_n x_n > 0 \\ -1 & \text{otherwise.} \end{cases}$$

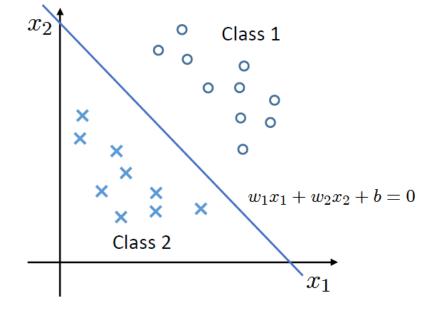
- Explanation
  - If the output is correct, do nothing
  - If the output is higher, lower the weight
  - If the output is lower, increase the weight

## Properties

• Rosenblatt [1958] proved the training can converge if two classes are linearly separable and  $\eta$  is reasonably small

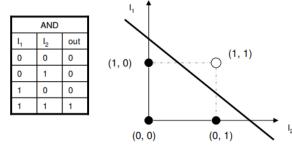


$$o(x_1, \dots, x_n) = \begin{cases} 1 & \text{if } w_0 + w_1 x_1 + \dots + w_n x_n > 0 \\ -1 & \text{otherwise.} \end{cases}$$

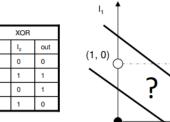


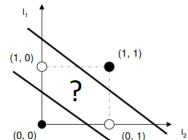
#### Limitation

- Minsky and Papert [1969] showed that some rather elementary computations, such as XOR problem, could not be done by Rosenblatt's one-layer perceptron
- However Rosenblatt believed the limitations could be overcome if more layers of units to be added, but no learning algorithm known to obtain the weights yet

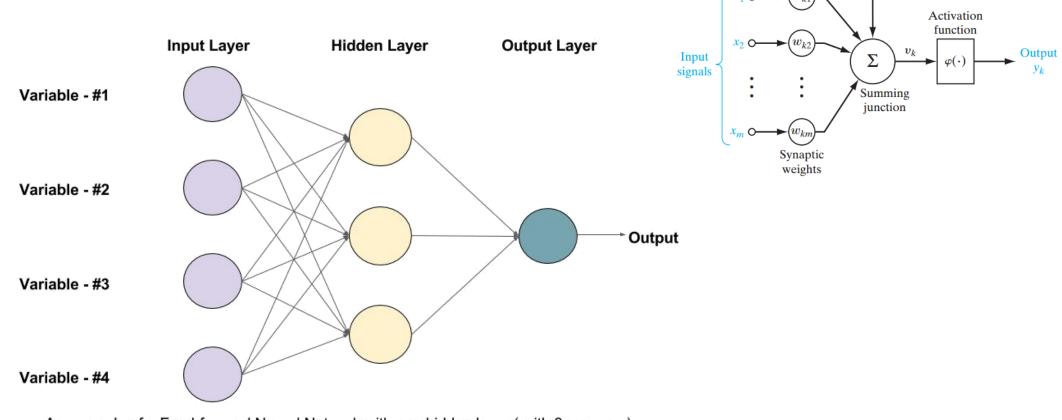


		_ i, ↑
OR		
l <sub>2</sub>	out	4.0
0	0	(1, 0) (1, 1)
1	1	
0	1	
1	1	
		(0, 0) (0, 1)





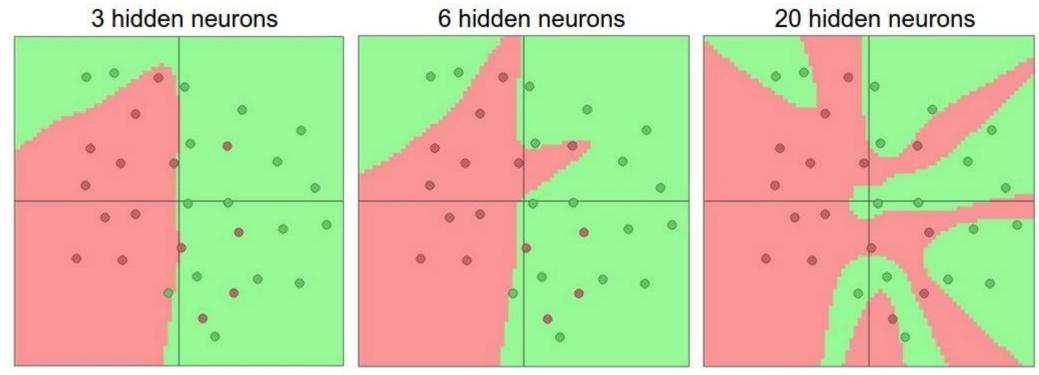
## Solution: Add hidden layers



An example of a Feed-forward Neural Network with one hidden layer ( with 3 neurons )

Two-layer feedforward neural network

#### Demo

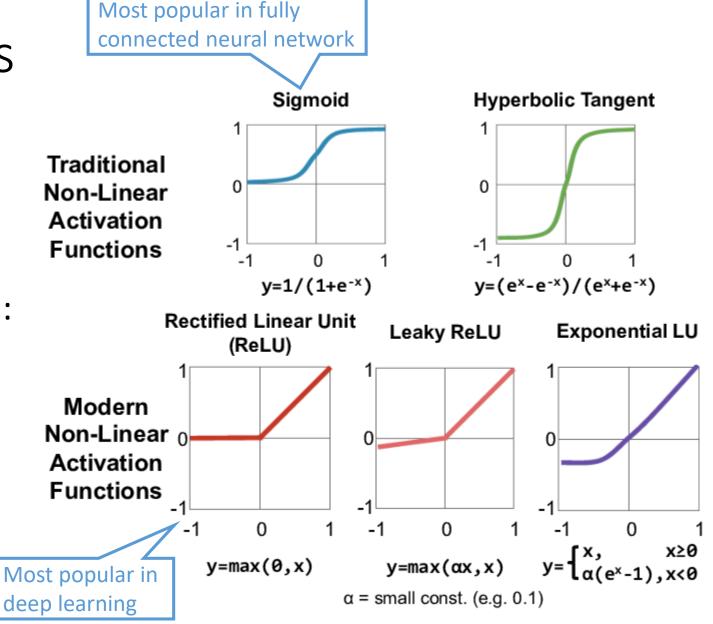


• Large Larger Neural Networks can represent more complicated functions. The data are shown as circles colored by their class, and the decision regions by a trained neural network are shown underneath. You can play with these examples in this <a href="ConvNetsJS demo">ConvNetsJS demo</a>.

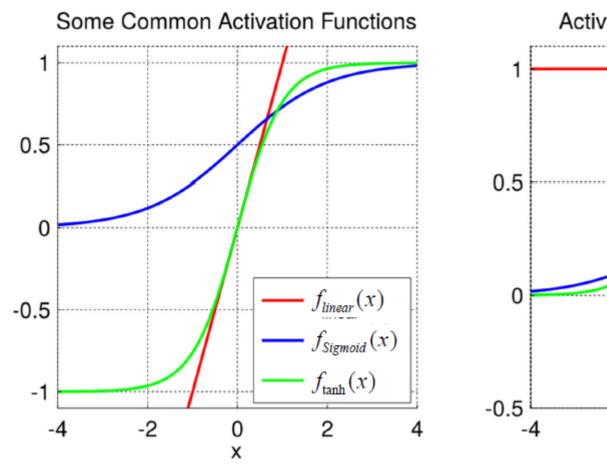
# Activation Functions

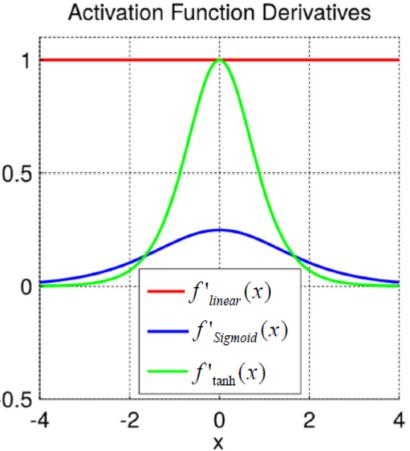
## Activation functions

- Sigmoid:  $\sigma(z) = \frac{1}{1+e^{-z}}$
- Tanh:  $tanh(z) = \frac{e^z e^{-z}}{e^z + e^{-z}}$
- ReLU (Rectified Linear Unity): ReLU(z) = max(0, z)



## Activation function values and derivatives

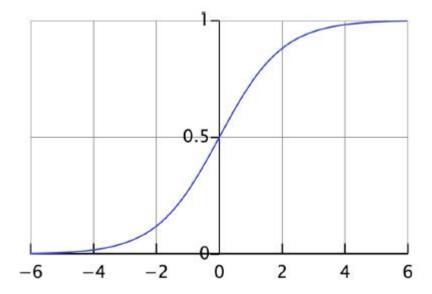




## Sigmoid activation function

Sigmoid

$$f_{Sigmoid}(x) = \frac{1}{1 + e^{-x}}$$



• Its derivative

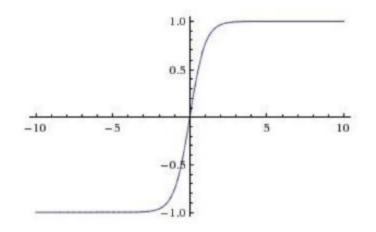
$$f'_{Sigmoid}(x) = f_{Sigmoid}(x)(1 - f_{Sigmoid}(x))$$

- Output range (0,1)
- Motivated by biological neurons and can be interpreted as the probability of an artificial neuron "firing" given its inputs
- However, saturated neurons make value vanished (why?)
  - $f(f(f(\cdots)))$
  - $f([0,1]) \subseteq [0.5, 0.732)$
  - $f([0.5, 0.732)) \subseteq (0.378, 0.676)$

#### Tanh activation function

Tanh function

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



Its derivative

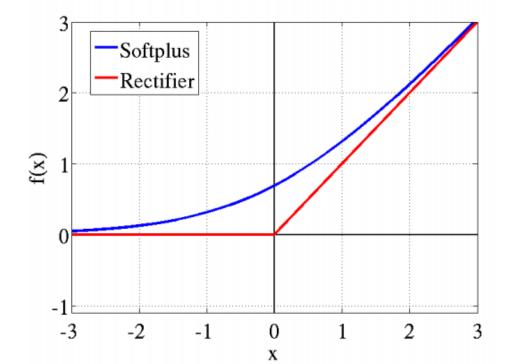
$$f_{\text{tanh}}(x) = 1 - f_{\text{tanh}}(x)^2$$

- Output range (-1,1)
- Thus strongly negative inputs to the tanh will map to negative outputs
- Only zero-valued inputs are mapped to near-zero outputs
- These properties make the network less likely to get "stuck" during training

#### ReLU activation function

 ReLU (Rectified linear unity) function

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



- Its derivative  $f_{ ext{ReLU}}(x) = egin{cases} 1 & ext{if } x > 0 \ 0 & ext{if } x \leq 0 \end{cases}$
- ReLU can be approximated by softplus function

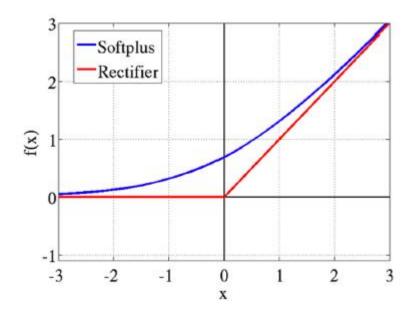
$$f_{\text{Softplus}}(x) = \log(1 + e^x)$$

- ReLU's gradient doesn't vanish as x increases
- Speed up training of neural networks
  - Since the gradient computation is very simple
  - The computational step is simple, no exponentials, no multiplication or division operations (compared to others)
- The gradient on positive portion is larger than sigmoid or tanh functions
  - Update more rapidly
  - The left "dead neuron" part can be ameliorated by Leaky ReLU

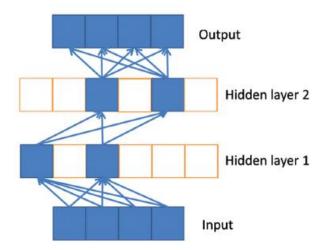
## ReLU activation function (cont.)

#### ReLU function

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



- The only non-linearity comes from the path selection with individual neurons being active or not
- It allows sparse representations:
  - for a given input only a subset of neurons are active

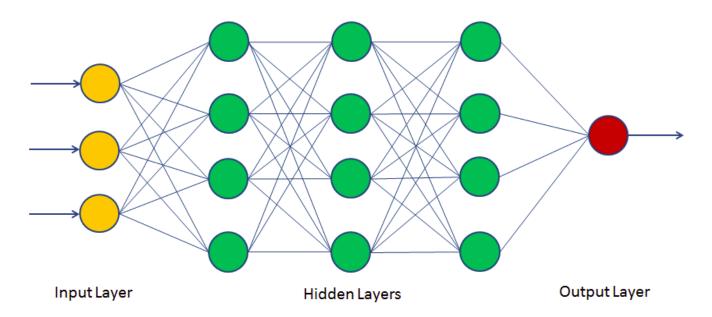


Sparse propagation of activations and gradients

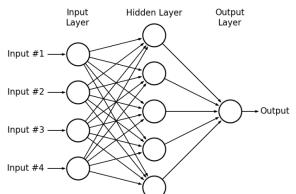
# Multilayer Perceptron Networks

#### Neural networks

 Neural networks are built by connecting many perceptrons together, layer by layer

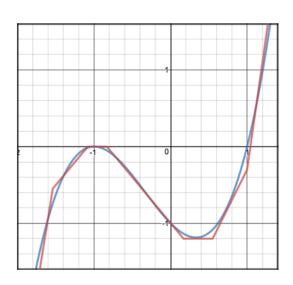


## Universal approximation theorem



• A feed-forward network with a single hidden layer containing a finite number of neurons can approximate continuous functions [1-20-1 NN approximate cont

1-20-1 NN approximates a noisy sine function



$$n_1(x) = Relu(-5x - 7.7)$$

$$n_2(x) = Relu(-1.2x - 1.3)$$

$$n_3(x) = Relu(1.2x + 1)$$

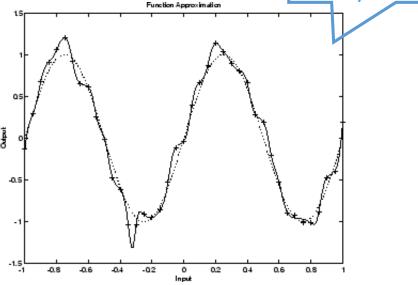
$$n_4(x) = Relu(1.2x - .2)$$

$$n_5(x) = Relu(2x - 1.1)$$

$$n_6(x) = Relu(5x - 5)$$

$$Z(x) = -n_1(x) - n_2(x) - n_3(x)$$

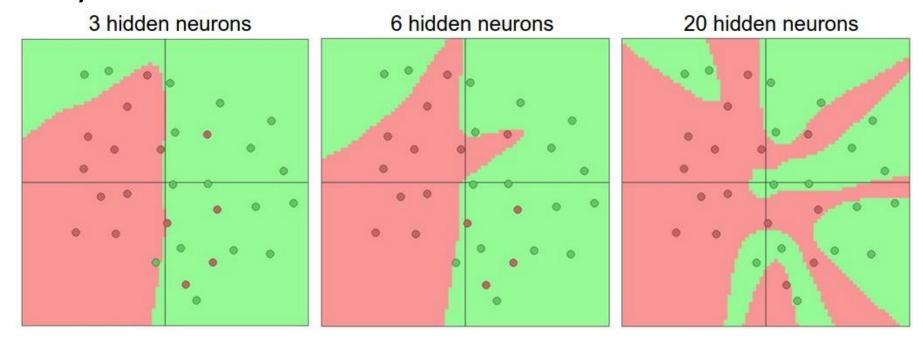
$$+ n_4(x) + n_5(x) + n_6(x)$$



Hornik, Kurt, Maxwell Stinchcombe, and Halbert White. "Multilayer feedforward networks are universal approximators." *Neural networks* 2.5 (1989): 359-366

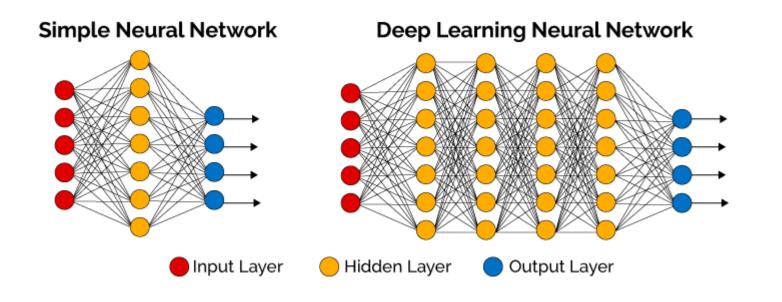
## Increasing power of approximation

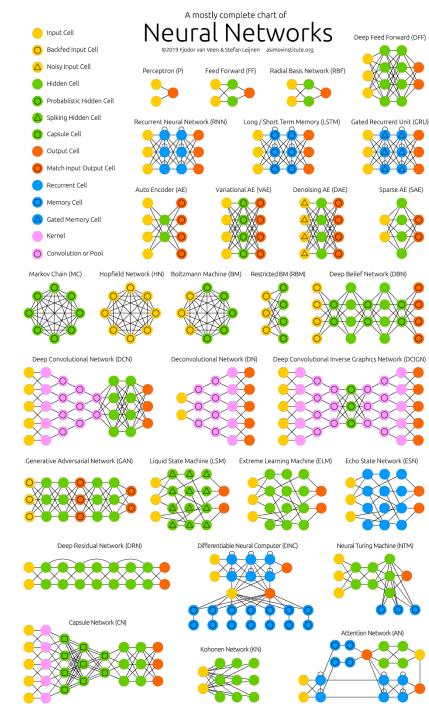
 With more neurons, its approximation power increases. The decision boundary covers more details



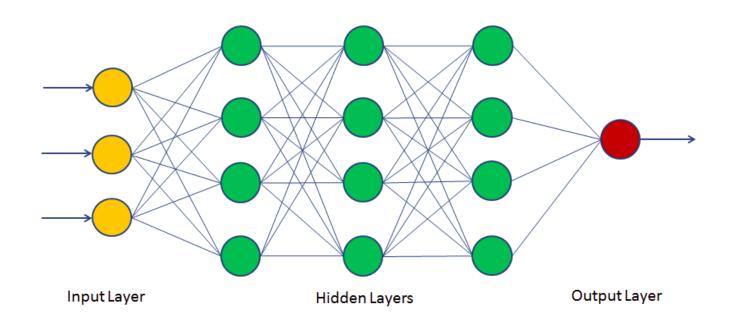
 Usually in applications, we use more layers with structures to approximate complex functions instead of one hidden layer with many neurons

# Common neuron network structures at a glance





## Multilayer perceptron network



## Single / Multiple layers of calculation

Single layer function

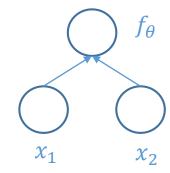
$$f_{\theta}(x) = \sigma(\theta_0 + \theta_1 x_1 + \theta_2 x_2)$$

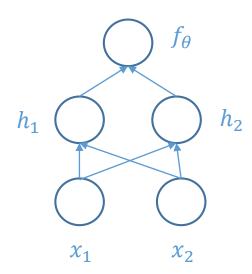


• 
$$h_1(x) = \sigma(\theta_0^1 + \theta_1^1 x_1 + \theta_2^1 x_2)$$

• 
$$h_2(x) = \sigma(\theta_0^2 + \theta_1^2 x_1 + \theta_2^2 x_2)$$

• 
$$f_{\theta}(h) = \sigma(\theta_0 + \theta_1 h_1 + \theta_2 h_2)$$





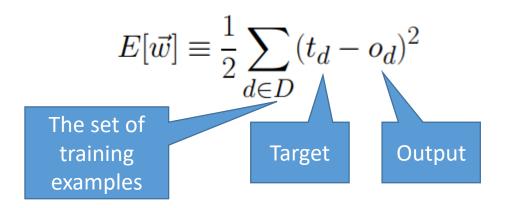
# Training

Backpropagation

#### How to train?

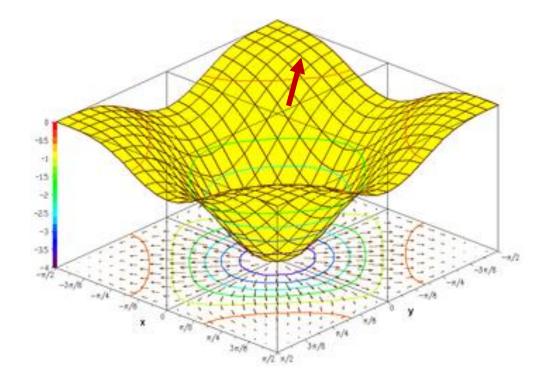
 As previous models, we use gradient descent method to train the neural network

 Given the topology of the network (number of layers, number of neurons, their connections), find a set of weights to minimize the error function



## Gradient interpretation

 Gradient is the vector (the red one) along which the value of the function increases most rapidly. Thus its opposite direction is where the value decreases most rapidly.



#### Gradient descent

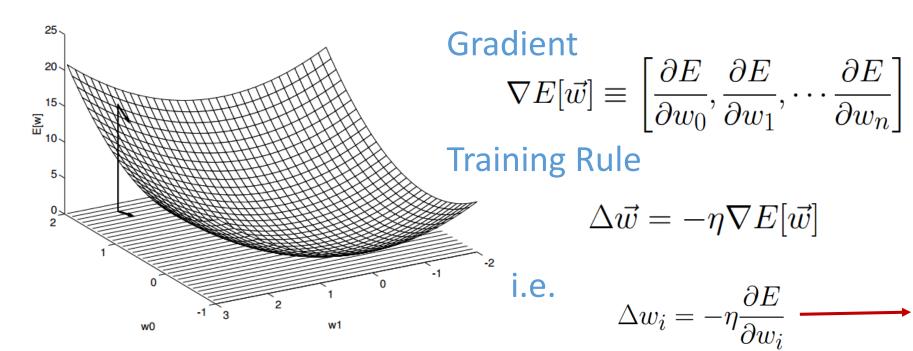
• To find a (local) minimum of a function using gradient descent, one takes steps proportional to the negative of the gradient (or an approximation) of the function at the current point

• For a smooth function f(x),  $\frac{\partial f}{\partial x}$  is the direction that f increases most rapidly. So we apply

$$x_{t+1} = x_t - \lambda \frac{\partial f}{\partial x}(x_t)$$

until x converges

## Gradient descent



Update

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

Partial derivatives

are the key

#### The chain rule

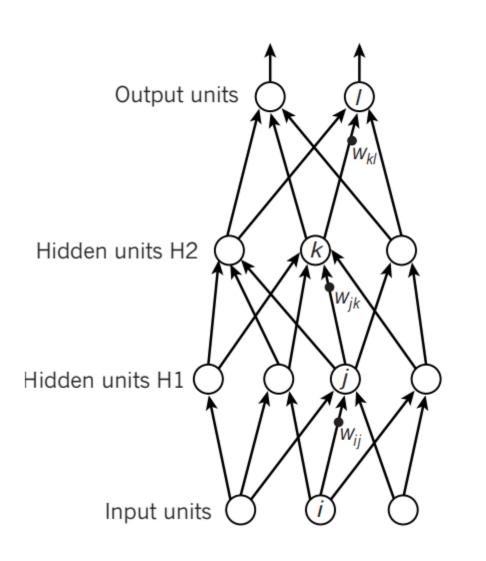
 The challenge in neural network model is that we only know the target of the output layer, but don't know the target for hidden and input layers, how can we update their connection weights using the gradient descent?

The answer is the chain rule that you have learned in calculus

$$y = f(g(x))$$

$$\Rightarrow \frac{dy}{dx} = f'(g(x))g'(x)$$

## Feed forward vs. Backpropagation



$$y_{l} = f(z_{l})$$

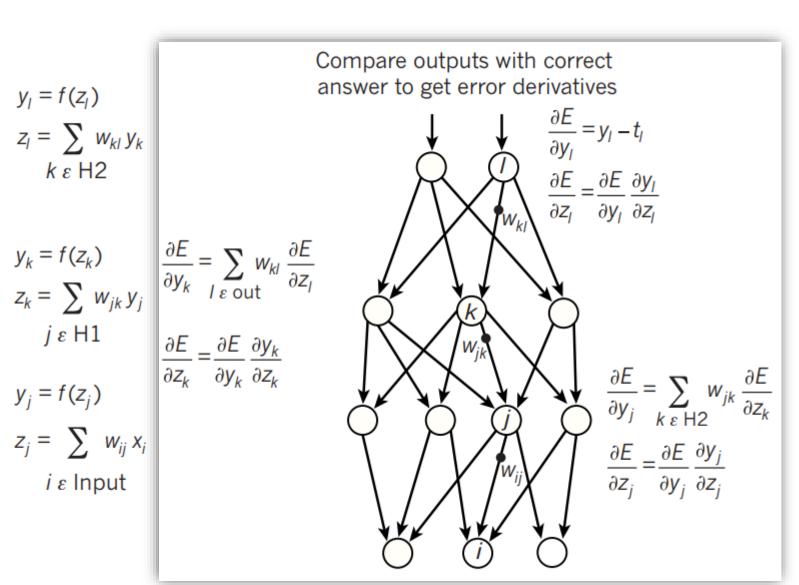
$$z_{l} = \sum_{k \in H2} w_{kl} y_{k}$$

$$y_k = f(z_k)$$

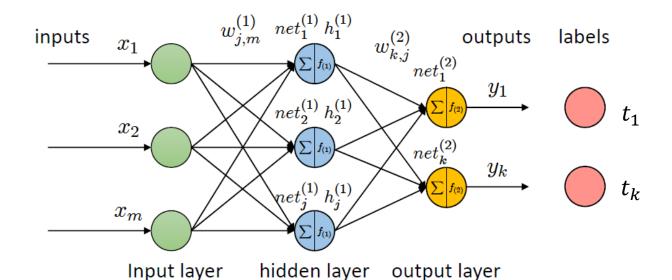
$$z_k = \sum_j w_{jk} y_j$$

$$j \varepsilon H1$$

$$y_j = f(z_j)$$
  
 $z_j = \sum_{i \in \text{Input}} w_{ij} x_i$ 



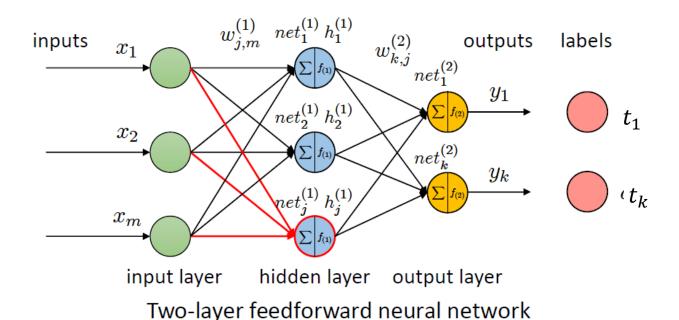
## Make a prediction



Two-layer feedforward neural network

#### Feed-forward prediction:

# Make a prediction (cont.)

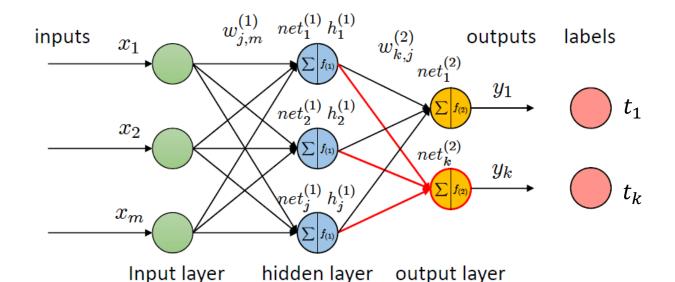


$$h_{j}^{(1)} = f_{(1)}(net_{j}^{(1)}) = f_{(1)}(\sum_{m} w_{j,m}^{(1)} x_{m}) \quad y_{k} = f_{(2)}(net_{k}^{(2)}) = f_{(2)}(\sum_{j} w_{k,j}^{(1)} h_{j}^{(1)})$$

$$x = (x_{1}, \dots, x_{m}) \xrightarrow{\qquad \qquad } h_{j}^{(1)} \xrightarrow{\qquad \qquad } y_{k}$$

$$where \qquad net_{j}^{(1)} = \sum_{m} w_{j,m}^{(1)} x_{m} \qquad \qquad net_{k}^{(2)} = \sum_{j} w_{k,j}^{(2)} h_{j}^{(1)}$$

# Make a prediction (cont.)



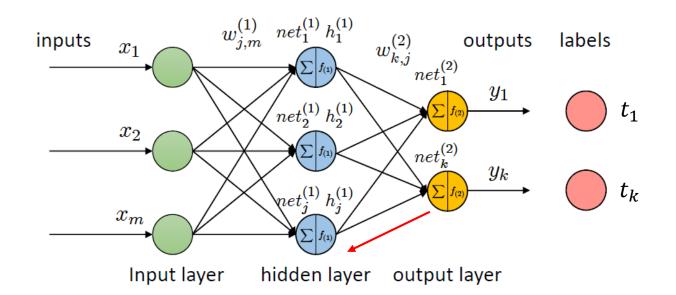
Two-layer feedforward neural network

$$h_{j}^{(1)} = f_{(1)}(net_{j}^{(1)}) = f_{(1)}(\sum_{m} w_{j,m}^{(1)} x_{m}) \quad y_{k} = f_{(2)}(net_{k}^{(2)}) = f_{(2)}(\sum_{j} w_{k,j}^{(1)} h_{j}^{(1)})$$

$$x = (x_{1}, \dots, x_{m}) \xrightarrow{\qquad \qquad } h_{j}^{(1)} \xrightarrow{\qquad \qquad } y_{k}$$

$$where \qquad net_{j}^{(1)} = \sum_{m} w_{j,m}^{(1)} x_{m} \qquad \qquad net_{k}^{(2)} = \sum_{j} w_{k,j}^{(2)} h_{j}^{(1)}$$

## Backpropagation

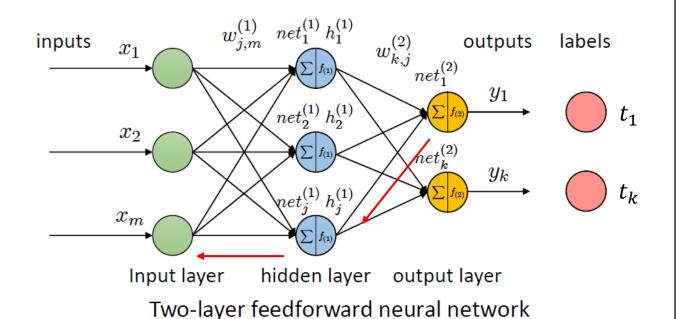


Two-layer feedforward neural network

- Assume all the activation functions are sigmoid
- Error function  $E = \frac{1}{2} \sum_{k} (y_k t_k)^2$
- $\frac{\partial E}{\partial y_k} = y_k t_k$
- $\bullet \Rightarrow \frac{\partial E}{\partial w_{k,j}^{(2)}} = -(t_k y_k)y_k(1 y_k)h_j^{(1)}$
- $\bullet \Rightarrow w_{k,j}^{(2)} \leftarrow w_{k,j}^{(2)} + \eta \delta_k^{(2)} h_j^{(1)} \qquad \delta$

Output of unit *j* 

# Backpropagation (cont.)



$$x = (x_1, \dots, x_m) \xrightarrow{h_j^{(1)} = f_{(1)}(net_j^{(1)}) = f_{(1)}(\sum_m w_{j,m}^{(1)} x_m)} y_k = f_{(2)}(net_k^{(2)}) = f_{(2)}(\sum_j w_{k,j}^{(1)} h_j^{(1)})$$

$$x = (x_1, \dots, x_m) \xrightarrow{h_j^{(1)}} h_j^{(1)} \xrightarrow{h_j^{(1)}} m_j^{(1)} \xrightarrow{h_j^{($$

- Error function  $E = \frac{1}{2} \sum_{k} (y_k t_k)^2$
- $\bullet \frac{\partial E}{\partial y_k} = y_k t_k$
- $\delta_k^{(2)} = (t_k y_k)y_k(1 y_k)$
- $\Rightarrow w_{k,i}^{(2)} \leftarrow w_{k,i}^{(2)} + \eta \delta_{k}^{(2)} h_{i}^{(1)}$
- $\frac{\partial h_j^{(1)}}{\partial w_j^{(1)}} = f'_{(1)} \left( net_j^{(1)} \right) x_m = h_j^{(1)} \left( 1 h_j^{(1)} \right) x_m$
- $\frac{\partial E}{\partial w_{i,m}^{(1)}} = -h_j^{(1)} \left( 1 h_j^{(1)} \right) \sum_k w_{k,j}^{(2)} (t_k y_k) y_k (1 y_k) x_m$  $=-h_j^{(1)}\left(1-h_j^{(1)}\right)\sum_{i}w_{k,j}^{(2)}\delta_k^{(2)}x_m$
- $\Rightarrow w_{im}^{(1)} \leftarrow w_{im}^{(1)} + \eta \delta_i^{(1)} x_m$

# Backpropagation algorithms

Activation function: sigmoid

Initialize all weights to small random numbers Do until convergence

- For each training example:
  - 1. Input it to the network and compute the network output
  - 2. For each output unit k,  $o_k$  is the output of unit k

$$\delta_k \leftarrow o_k (1 - o_k) (t_k - o_k)$$

3. For each hidden unit j,  $o_i$  is the output of unit j

$$\delta_j \leftarrow o_j (1 - o_j) \sum_{k,j} w_{k,j} \delta_k$$

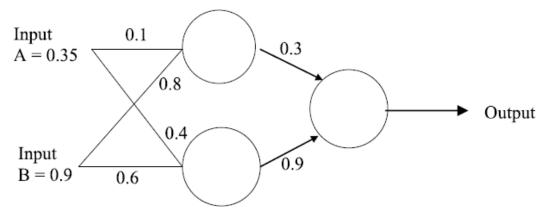
4. Update each network weight, where  $x_i$  is the output for unit i

$$w_{j,i} \leftarrow w_{j,i} + \eta \delta_j x_i$$

- Error function  $E = \frac{1}{2} \sum_{k} (y_k t_k)^2$
- $\delta_k^{(2)} = (t_k y_k)y_k(1 y_k)$
- $\Rightarrow w_{k,j}^{(2)} \leftarrow w_{k,j}^{(2)} + \eta \delta_k^{(2)} h_j^{(1)}$
- $\delta_j^{(1)} = h_j^{(1)} \left( 1 h_j^{(1)} \right) \sum_k w_{k,j}^{(2)} \delta_k^{(2)}$
- $\bullet \Rightarrow w_{j,m}^{(1)} \leftarrow w_{j,m}^{(1)} + \eta \delta_j^{(1)} x_m$

# Calculation example

Consider the simple network below:



- Assume that the neurons have sigmoid activation function and
  - Perform a forward pass on the network and find the predicted output
  - Perform a reverse pass (training) once (target = 0.5)
  - Perform a further forward pass and comment on the result

# Calculation example (cont.)

#### Answer:

(i)

Input to top neuron = (0.35x0.1)+(0.9x0.8)=0.755. Out = 0.68. Input to bottom neuron = (0.9x0.6)+(0.35x0.4)=0.68. Out = 0.6637. Input to final neuron = (0.3x0.68)+(0.9x0.6637)=0.80133. Out = 0.69.

(ii) Output error  $\delta$ =(t-o)(1-o)o = (0.5-0.69)(1-0.69)0.69 = -0.0406.

New weights for output layer

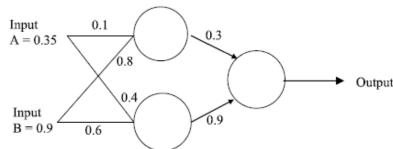
$$w1^+ = w1 + (\delta x \text{ input}) = 0.3 + (-0.0406x0.68) = 0.272392.$$
  
 $w2^+ = w2 + (\delta x \text{ input}) = 0.9 + (-0.0406x0.6637) = 0.87305.$ 

#### Errors for hidden layers:

$$\delta 1 = \delta \times w1 = -0.0406 \times 0.272392 \times (1-o)o = -2.406 \times 10^{-3}$$
  
 $\delta 2 = \delta \times w2 = -0.0406 \times 0.87305 \times (1-o)o = -7.916 \times 10^{-3}$ 

New hidden layer weights:

$$w3^{+}=0.1 + (-2.406 \times 10^{-3} \times 0.35) = 0.09916.$$
  
 $w4^{+}=0.8 + (-2.406 \times 10^{-3} \times 0.9) = 0.7978.$   
 $w5^{+}=0.4 + (-7.916 \times 10^{-3} \times 0.35) = 0.3972.$   
 $w6^{+}=0.6 + (-7.916 \times 10^{-3} \times 0.9) = 0.5928.$ 



• For each output unit k,  $o_k$  is the output of unit k

$$\delta_k \leftarrow o_k (1 - o_k) (t_k - o_k)$$

• For each hidden unit j,  $o_j$  is the output of unit j

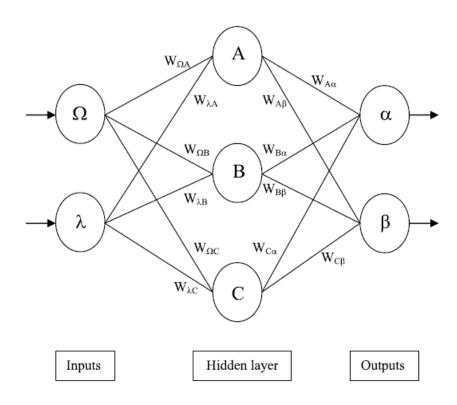
$$\delta_j \leftarrow o_j (1 - o_j) \sum_{k \in next \ layer} w_{k,j} \delta_k$$

• Update each network weight, where  $x_{i,j}$  is the input for unit j

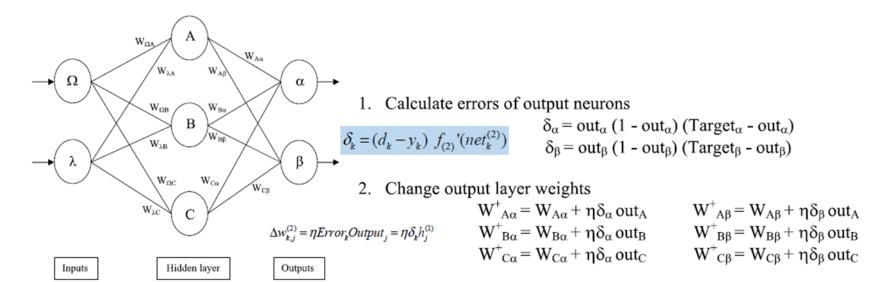
$$w_{j,i} \leftarrow w_{j,i} + \eta \delta_j x_{i,j}$$

(iii)

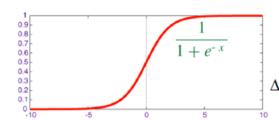
# Formula example for backpropagation



# Formula example for backpropagation (cont.)



Consider sigmoid activation function  $f_{Sigmoid}(x) = \frac{1}{1 + e^{-x}}$ 



3. Calculate (back-propagate) hidden layer errors

$$\delta_{A} = \operatorname{out}_{A} (1 - \operatorname{out}_{A}) (\delta_{\alpha} W_{A\alpha} + \delta_{\beta} W_{A\beta})$$

$$\delta_{B} = \operatorname{out}_{B} (1 - \operatorname{out}_{B}) (\delta_{\alpha} W_{B\alpha} + \delta_{\beta} W_{B\beta})$$

$$\delta_{C} = \operatorname{out}_{C} (1 - \operatorname{out}_{C}) (\delta_{\alpha} W_{C\alpha} + \delta_{\beta} W_{C\beta})$$

4. Change hidden layer weights

$$\Delta w_{j,m}^{(1)} = \eta Error_{j}Output_{m} = \eta \delta_{j}x_{m}$$

$$W_{\lambda B}^{+} = W_{\lambda A} + \eta \delta_{A} \operatorname{in}_{\lambda}$$

$$W_{\lambda B}^{+} = W_{\lambda B} + \eta \delta_{B} \operatorname{in}_{\lambda}$$

$$W_{\Delta C}^{+} = W_{\lambda C}^{+} + \eta \delta_{C} \operatorname{in}_{\lambda}$$

$$W_{\Omega C}^{+} = W_{\Omega C}^{+} + \eta \delta_{C} \operatorname{in}_{\lambda}$$

$$W_{\Omega C}^{+} = W_{\Omega C}^{+} + \eta \delta_{C} \operatorname{in}_{\Omega}$$

$$f'_{Sigmoid}(x) = f_{Sigmoid}(x)(1 - f_{Sigmoid}(x))$$

## More on backpropagations

- It is gradient descent over entire network weight vectors
- Easily generalized to arbitrary directed graphs
- Will find a local, not necessarily global error minimum
  - In practice, often work well (can run multiple times)
- Often include weight momentum lpha

$$\Delta w_{j,i}(n) \leftarrow \eta \delta_j x_i + \alpha \Delta w_{j,i}(n-1)$$

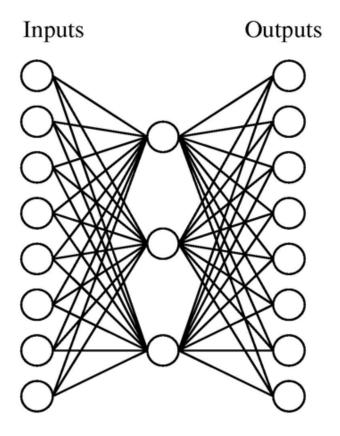
- Minimizes error over *training* examples
  - Will it generalize well to unseen examples?
- Training can take thousands of iterations, slow!
- Using network after training is very fast

# Training Example

### Network structure

• What happens when we train a network?

• Example:



# Input and output

• A target function:

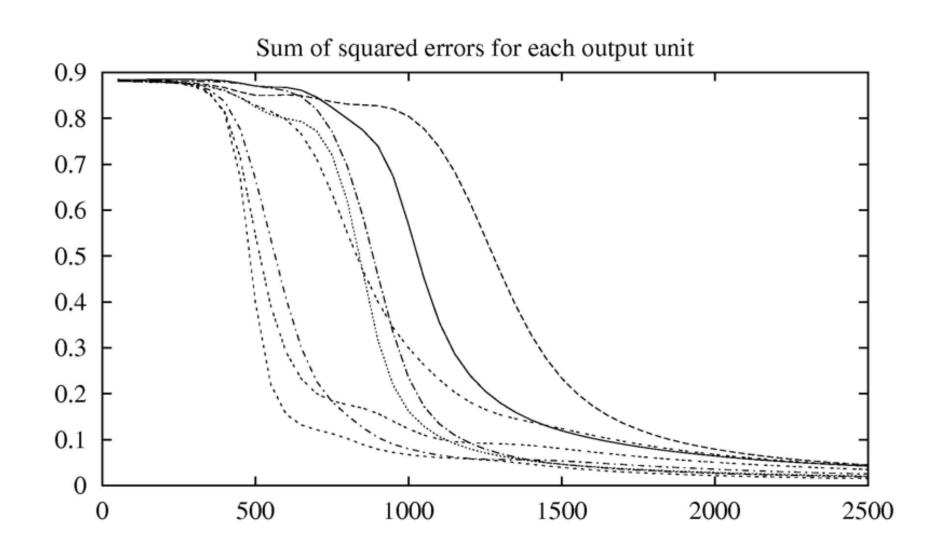
Input		Output
10000000	$\rightarrow$	10000000
01000000	$\rightarrow$	01000000
00100000	$\rightarrow$	00100000
00010000	$\rightarrow$	00010000
00001000	$\rightarrow$	00001000
00000100	$\rightarrow$	00000100
00000010	$\rightarrow$	00000010
00000001	$\rightarrow$	00000001

• Can this be learned?

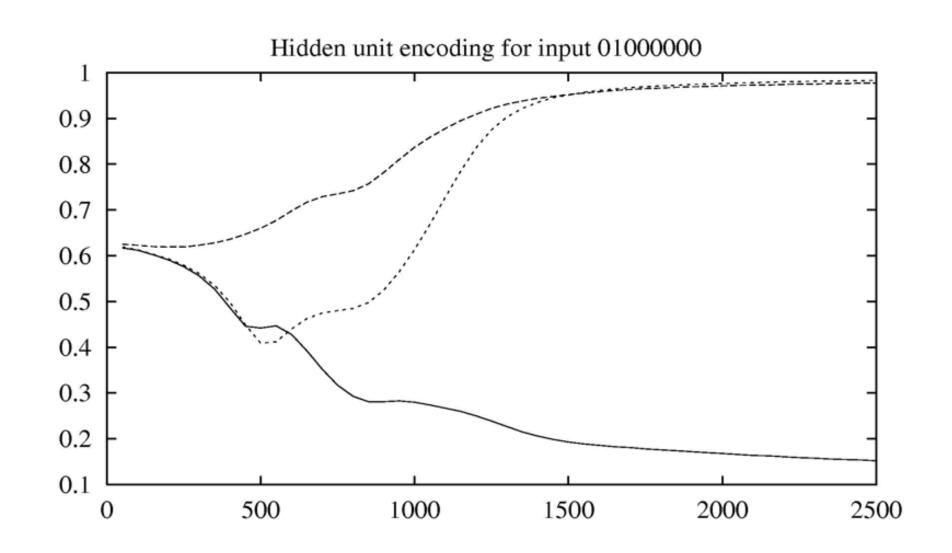
# Learned hidden layer

Input		I	Output					
Values								
10000000	$\rightarrow$	.89	.04	.08	$\rightarrow$	10000000		
01000000	$\rightarrow$	.01	.11	.88	$\rightarrow$	01000000		
00100000	$\rightarrow$	.01	.97	.27	$\rightarrow$	00100000		
00010000	$\rightarrow$	.99	.97	.71	$\rightarrow$	00010000		
00001000	$\rightarrow$	.03	.05	.02	$\rightarrow$	00001000		
00000100	$\rightarrow$	.22	.99	.99	$\rightarrow$	00000100		
00000010	$\rightarrow$	.80	.01	.98	$\rightarrow$	00000010		
00000001	$\rightarrow$	.60	.94	.01	$\rightarrow$	00000001		

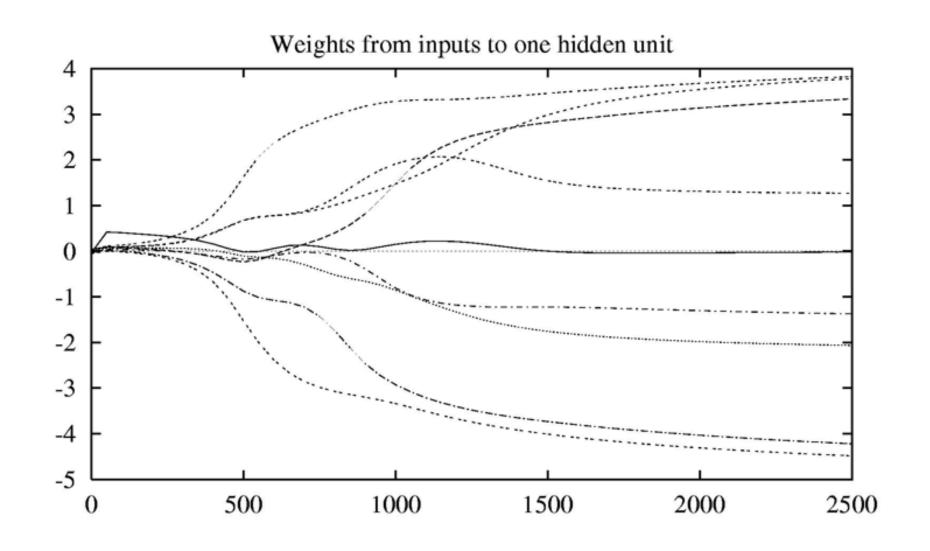
# Convergence of sum of squared errors



# Hidden unit encoding for 01000000



# Convergence of first layer weights



# Convergence of backpropagation

- Gradient descent to some local minimum
  - Perhaps not global minimum
  - Add momentum
  - Stochastic gradient descent
  - Train multiple nets with different initial weights
- Nature of convergence
  - Initialize weights near zero
  - Therefore, initial networks near-linear
  - Increasingly approximate non-linear functions as training progresses

### Expressiveness of neural nets

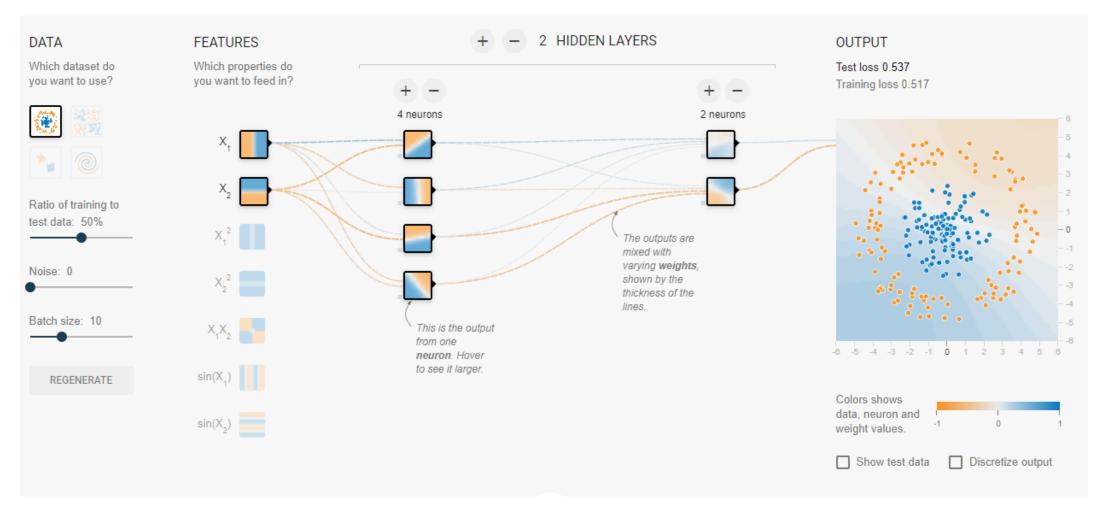
### Boolean functions:

- Every Boolean function can be represented by network with single hidden layer
- But might require exponential (in number of inputs) hidden units

### Continuous functions:

- Every bounded continuous function can be approximated with arbitrarily small error, by network with one hidden layer
- Any function can be approximated to arbitrary accuracy by network with two hidden layers

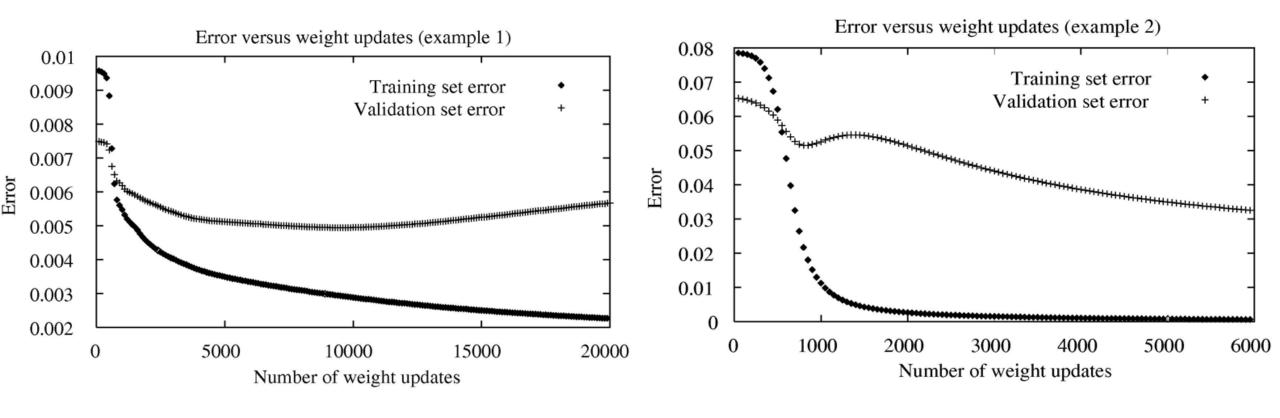
# Tensorflow playground



http://playground.tensorflow.org/

# Overfitting

# Two examples



# Avoid overfitting

• Penalize large weights:

$$E(\vec{w}) \equiv \frac{1}{2} \sum_{d \in D} \sum_{k \in outputs} (t_{kd} - o_{kd})^2 + \gamma \sum_{i,j} w_{ji}^2$$

Train on target slopes as well as values:

$$E(\vec{w}) \equiv \frac{1}{2} \sum_{d \in D} \sum_{k \in outputs} \left[ (t_{kd} - o_{kd})^2 + \mu \sum_{j \in inputs} \left( \frac{\partial t_{kd}}{\partial x_d^j} - \frac{\partial o_{kd}}{\partial x_d^j} \right)^2 \right]$$

- Weight sharing
  - Reduce total number of weights
  - Using structures, like convolutional neural networks
- Early stopping
- Dropout

# Applications

# Autonomous self-driving cars

• Use neural network to summarize observation information and learn

path planning



# Autonomous self-driving cars (cont.)

