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# Introduction to Neural Networks

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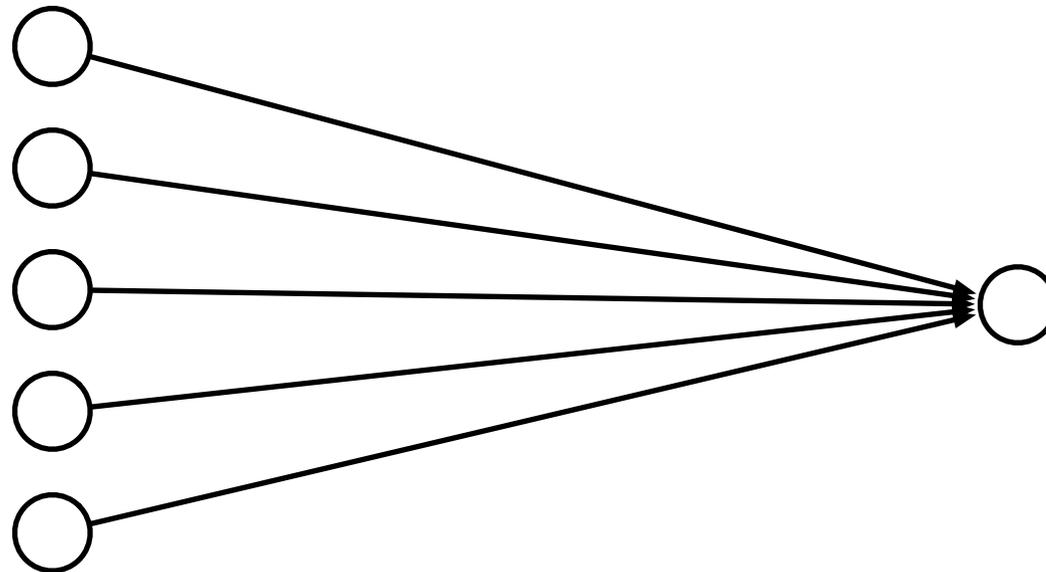
# Linear Models



- We used before weighted linear combination of feature values  $h_j$  and weights  $\lambda_j$

$$\text{score}(\lambda, \mathbf{d}_i) = \sum_j \lambda_j h_j(\mathbf{d}_i)$$

- Such models can be illustrated as a "network"



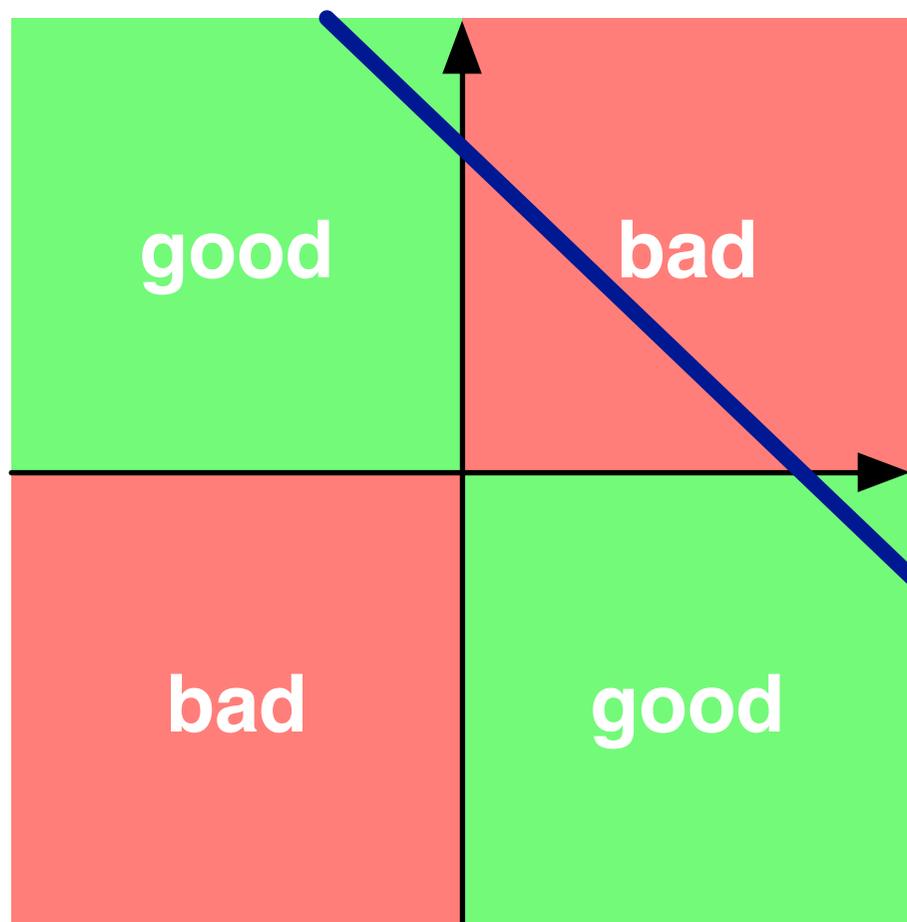
# Limits of Linearity



- We can give each feature a weight
- But not more complex value relationships, e.g.,
  - any value in the range  $[0;5]$  is equally good
  - values over 8 are bad
  - higher than 10 is not worse

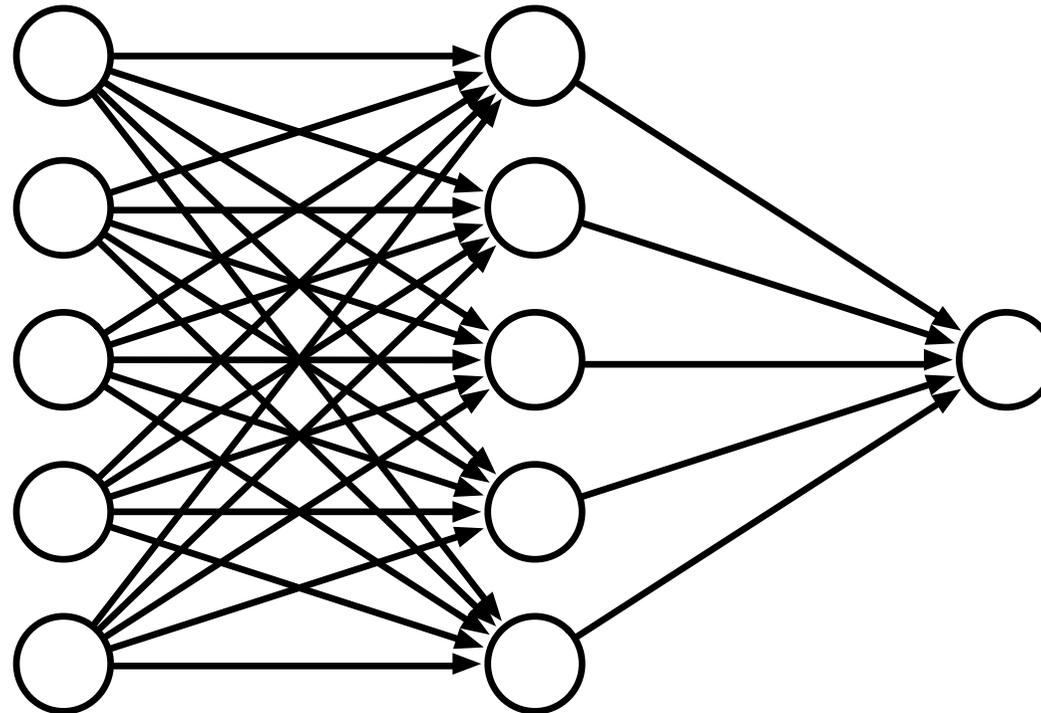
# XOR

- Linear models cannot model XOR



# Multiple Layers

- Add an intermediate ("hidden") layer of processing (each arrow is a weight)



- Have we gained anything so far?

# Non-Linearity

- Instead of computing a linear combination

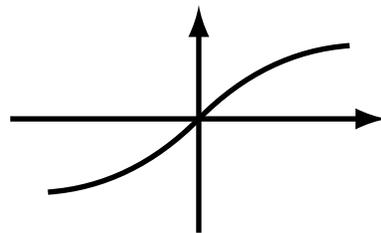
$$\text{score}(\lambda, \mathbf{d}_i) = \sum_j \lambda_j h_j(\mathbf{d}_i)$$

- Add a non-linear function

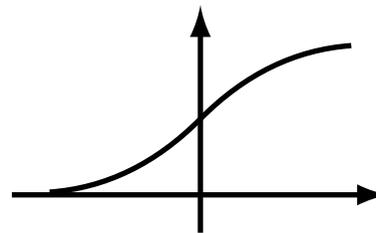
$$\text{score}(\lambda, \mathbf{d}_i) = f\left(\sum_j \lambda_j h_j(\mathbf{d}_i)\right)$$

- Popular choices

$\tanh(x)$



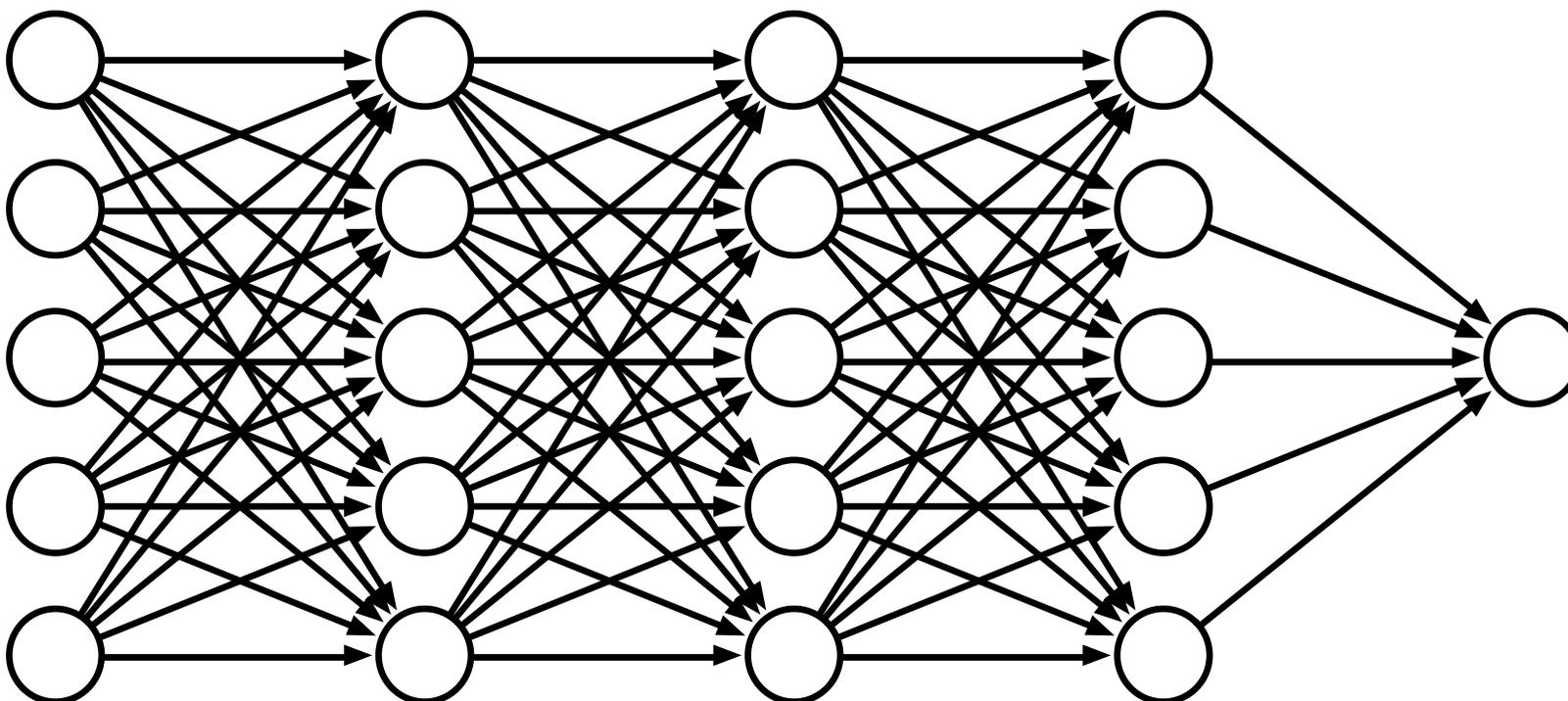
$\text{sigmoid}(x) = \frac{1}{1+e^{-x}}$



(sigmoid is also called the "logistic function")

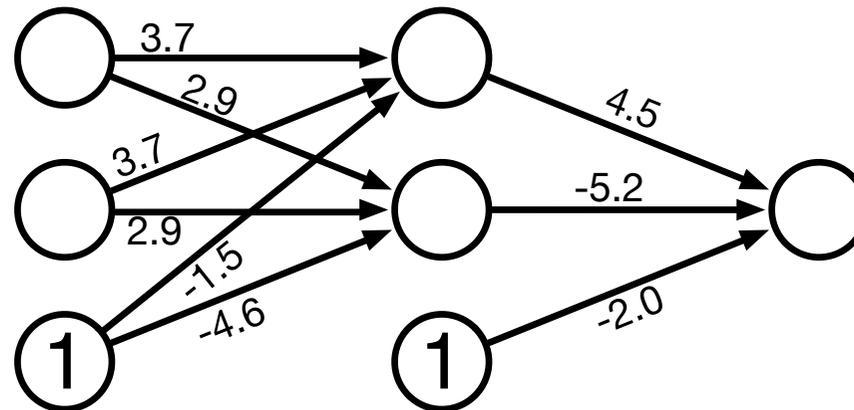
# Deep Learning

- More layers = deep learning



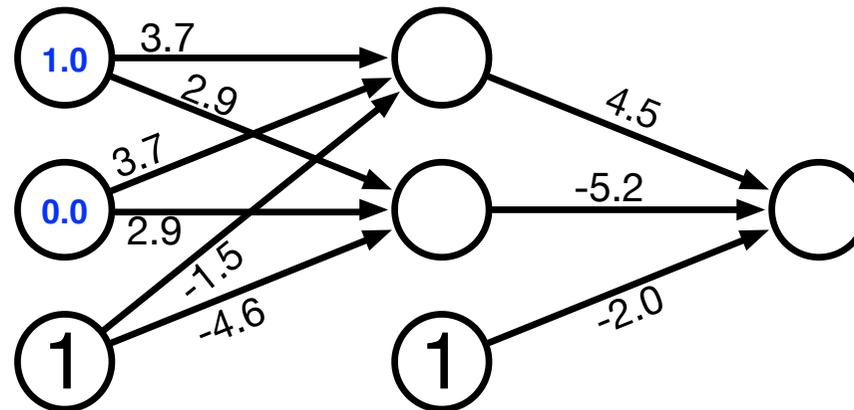
example

# Simple Neural Network



- One innovation: bias units (no inputs, always value 1)

# Sample Input

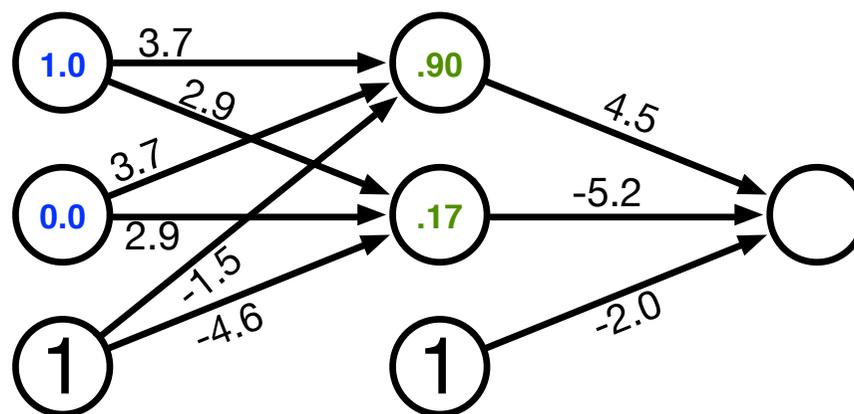


- Try out two input values
- Hidden unit computation

$$\text{sigmoid}(1.0 \times 3.7 + 0.0 \times 3.7 + 1 \times -1.5) = \text{sigmoid}(2.2) = \frac{1}{1 + e^{-2.2}} = 0.90$$

$$\text{sigmoid}(1.0 \times 2.9 + 0.0 \times 2.9 + 1 \times -4.5) = \text{sigmoid}(-1.6) = \frac{1}{1 + e^{1.6}} = 0.17$$

# Computed Hidden

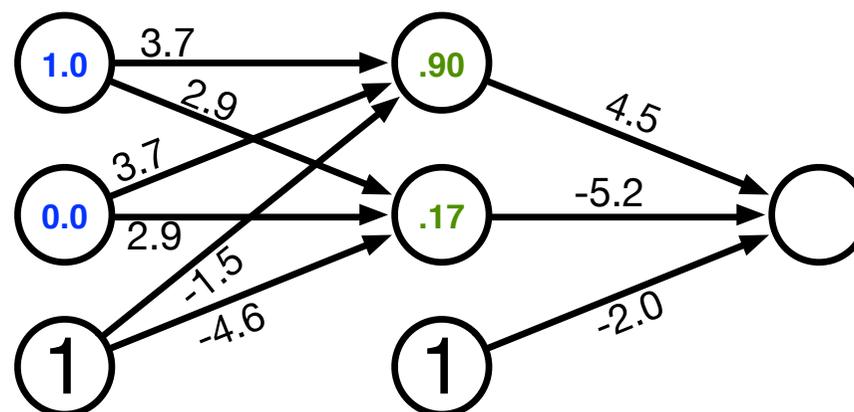


- Try out two input values
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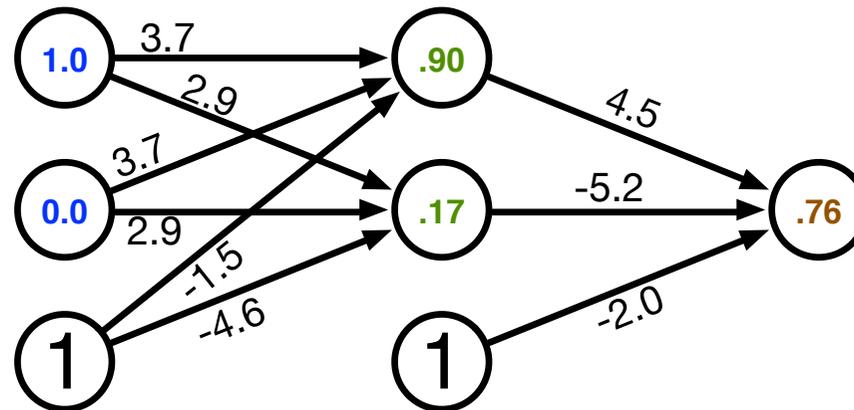
# Compute Output



- Output unit computation

$$\text{sigmoid}(.90 \times 4.5 + .17 \times -5.2 + 1 \times -2.0) = \text{sigmoid}(1.17) = \frac{1}{1 + e^{-1.17}} = 0.76$$

# Computed Output



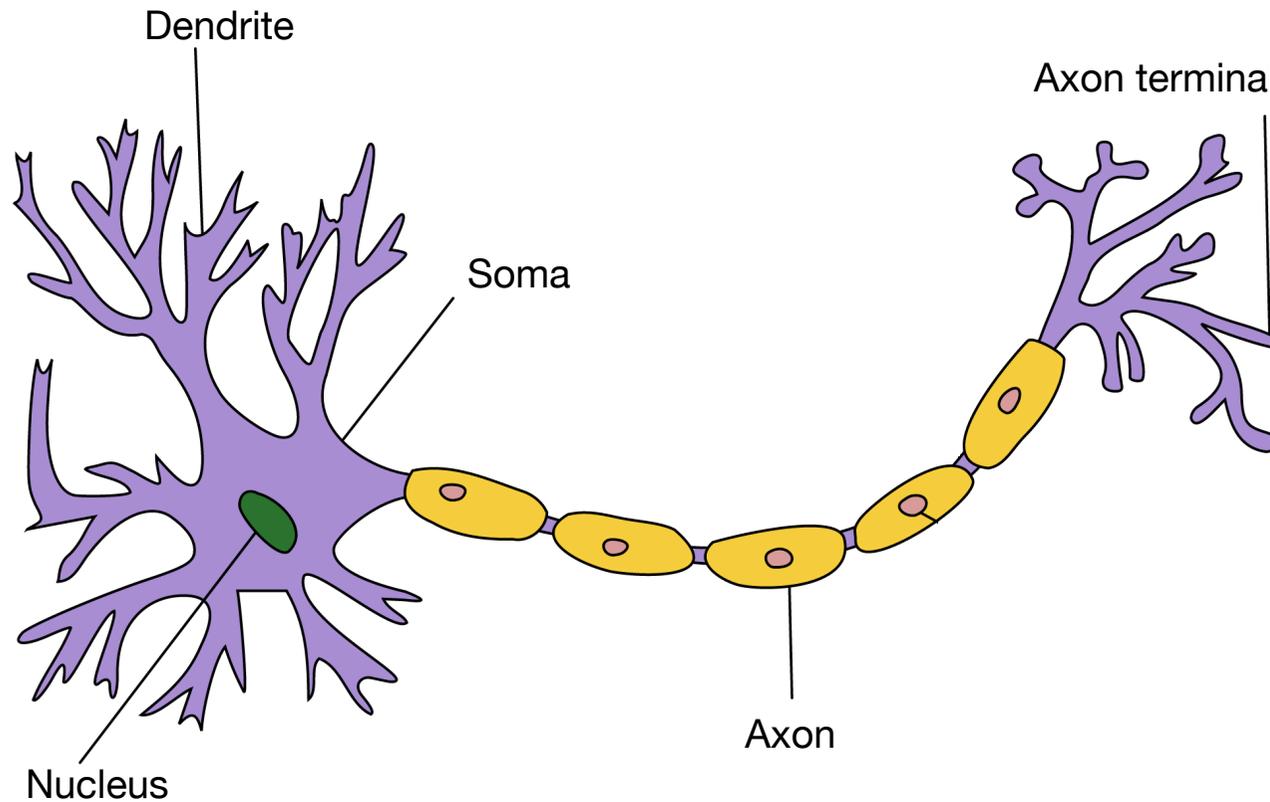
- Output unit computation

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why “neural” networks?

# Neuron in the Brain

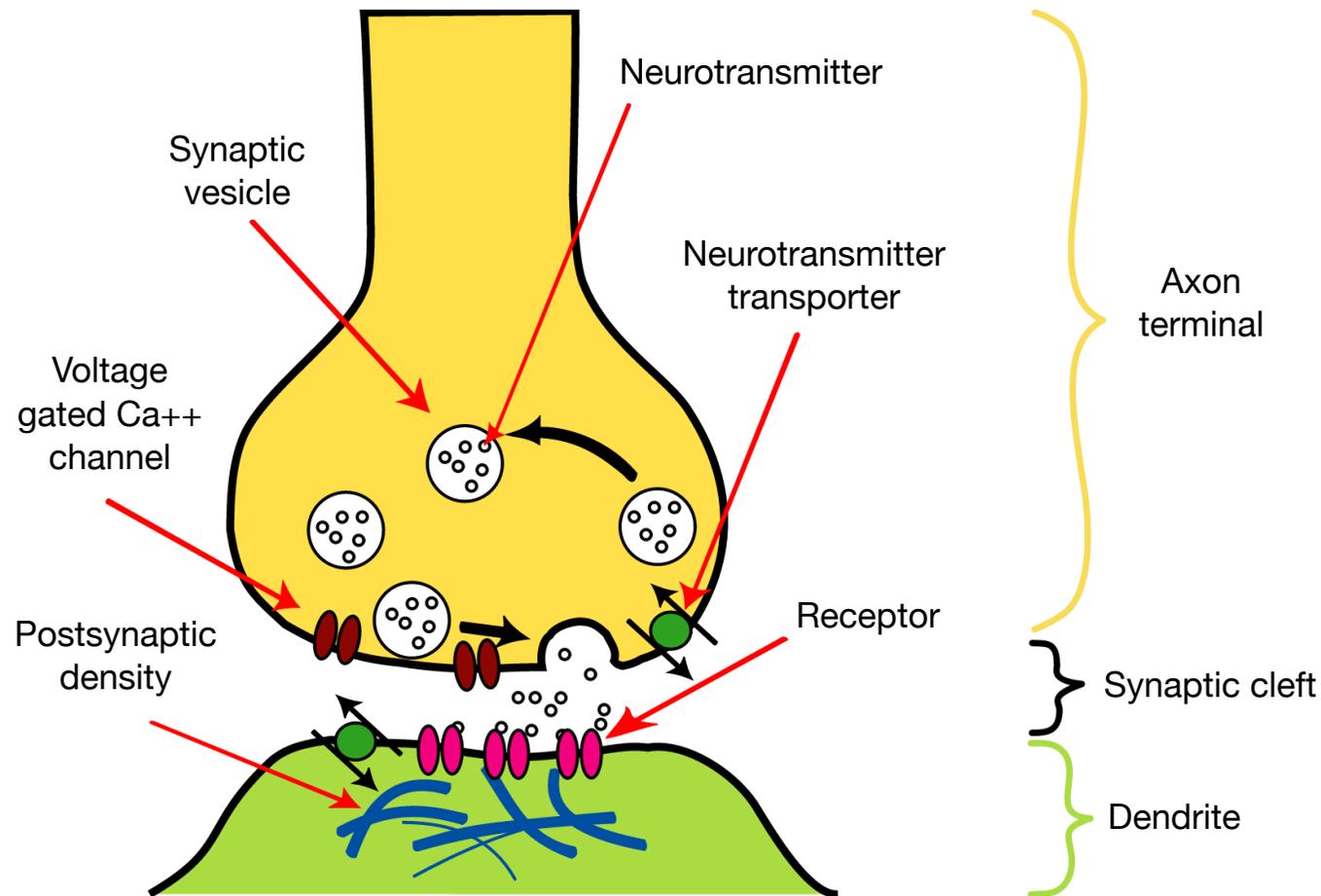
- The human brain is made up of about 100 billion neurons



- Neurons receive electric signals at the dendrites and send them to the axon

# Neural Communication

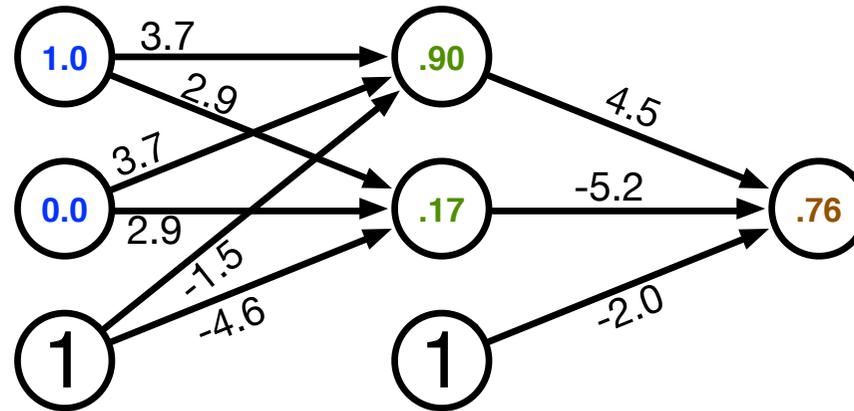
- The axon of the neuron is connected to the dendrites of many other neurons



- Similarities
  - Neurons, connections between neurons
  - Learning = change of connections, not change of neurons
  - Massive parallel processing
  
- But artificial neural networks are much simpler
  - computation within neuron vastly simplified
  - discrete time steps
  - typically some form of supervised learning with massive number of stimuli

# back-propagation training

# Error



- Computed output:  $y = .76$
- Correct output:  $t = 1.0$

⇒ How do we adjust the weights?

# Key Concepts

- Gradient descent
  - error is a function of the weights
  - we want to reduce the error
  - gradient descent: move towards the error minimum
  - compute gradient → get direction to the error minimum
  - adjust weights towards direction of lower error
  
- Back-propagation
  - first adjust last set of weights
  - propagate error back to each previous layer
  - adjust their weights

# Derivative of Sigmoid

- Sigmoid

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

- Reminder: quotient rule

$$\left(\frac{f(x)}{g(x)}\right)' = \frac{g(x)f'(x) - f(x)g'(x)}{g(x)^2}$$

- Derivative

$$\begin{aligned}\frac{d \text{sigmoid}(x)}{dx} &= \frac{d}{dx} \frac{1}{1 + e^{-x}} \\ &= \frac{0 \times (1 - e^{-x}) - (-e^{-x})}{(1 + e^{-x})^2} \\ &= \frac{1}{1 + e^{-x}} \left( \frac{e^{-x}}{1 + e^{-x}} \right) \\ &= \frac{1}{1 + e^{-x}} \left( 1 - \frac{1}{1 + e^{-x}} \right) \\ &= \text{sigmoid}(x)(1 - \text{sigmoid}(x))\end{aligned}$$

# Final Layer Update

- Linear combination of weights  $s = \sum_k w_k h_k$
- Activation function  $y = \text{sigmoid}(s)$
- Error (L2 norm)  $E = \frac{1}{2}(t - y)^2$
- Derivative of error with regard to one weight  $w_k$

$$\frac{dE}{dw_k} = \frac{dE}{dy} \frac{dy}{ds} \frac{ds}{dw_k}$$

# Final Layer Update (1)

- Linear combination of weights  $s = \sum_k w_k h_k$
- Activation function  $y = \text{sigmoid}(s)$
- Error (L2 norm)  $E = \frac{1}{2}(t - y)^2$
- Derivative of error with regard to one weight  $w_k$

$$\frac{dE}{dw_k} = \frac{dE}{dy} \frac{dy}{ds} \frac{ds}{dw_k}$$

- Error  $E$  is defined with respect to  $y$

$$\frac{dE}{dy} = \frac{d}{dy} \frac{1}{2}(t - y)^2 = -(t - y)$$

## Final Layer Update (2)

- Linear combination of weights  $s = \sum_k w_k h_k$
- Activation function  $y = \text{sigmoid}(s)$
- Error (L2 norm)  $E = \frac{1}{2}(t - y)^2$
- Derivative of error with regard to one weight  $w_k$

$$\frac{dE}{dw_k} = \frac{dE}{dy} \frac{dy}{ds} \frac{ds}{dw_k}$$

- $y$  with respect to  $x$  is  $\text{sigmoid}(s)$

$$\frac{dy}{ds} = \frac{d \text{sigmoid}(s)}{ds} = \text{sigmoid}(s)(1 - \text{sigmoid}(s)) = y(1 - y)$$

## Final Layer Update (3)

- Linear combination of weights  $s = \sum_k w_k h_k$
- Activation function  $y = \text{sigmoid}(s)$
- Error (L2 norm)  $E = \frac{1}{2}(t - y)^2$
- Derivative of error with regard to one weight  $w_k$

$$\frac{dE}{dw_k} = \frac{dE}{dy} \frac{dy}{ds} \frac{ds}{dw_k}$$

- $x$  is weighted linear combination of hidden node values  $h_k$

$$\frac{ds}{dw_k} = \frac{d}{dw_k} \sum_k w_k h_k = h_k$$

# Putting it All Together

- Derivative of error with regard to one weight  $w_k$

$$\begin{aligned}\frac{dE}{dw_k} &= \frac{dE}{dy} \frac{dy}{ds} \frac{ds}{dw_k} \\ &= -(t - y) \quad y(1 - y) \quad h_k\end{aligned}$$

- error
  - derivative of sigmoid:  $y'$
- Weight adjustment will be scaled by a fixed learning rate  $\mu$

$$\Delta w_k = \mu (t - y) y' h_k$$

# Multiple Output Nodes

- Our example only had one output node
- Typically neural networks have multiple output nodes
- Error is computed over all  $j$  output nodes

$$E = \sum_j \frac{1}{2} (t_j - y_j)^2$$

- Weights  $k \rightarrow j$  are adjusted according to the node they point to

$$\Delta w_{j \leftarrow k} = \mu (t_j - y_j) y'_j h_k$$

# Hidden Layer Update

- In a hidden layer, we do not have a target output value
- But we can compute how much each node contributed to downstream error
- Definition of error term of each node

$$\delta_j = (t_j - y_j) y'_j$$

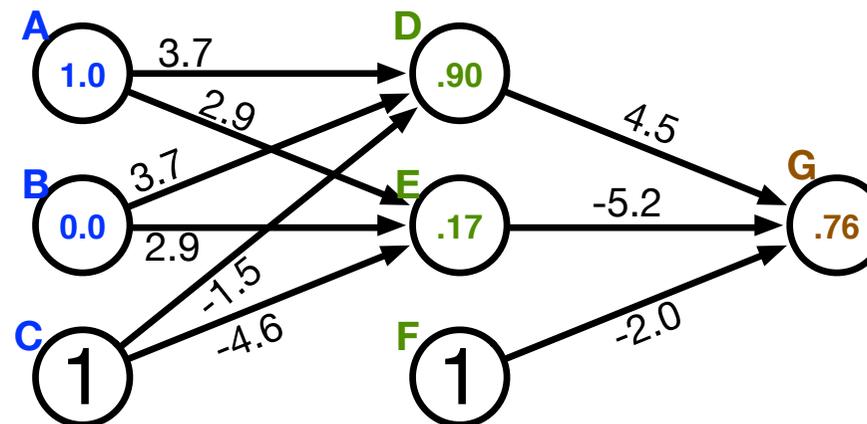
- Back-propagate the error term  
(why this way? there is math to back it up...)

$$\delta_i = \left( \sum_j w_{j \leftarrow i} \delta_j \right) y'_i$$

- Universal update formula

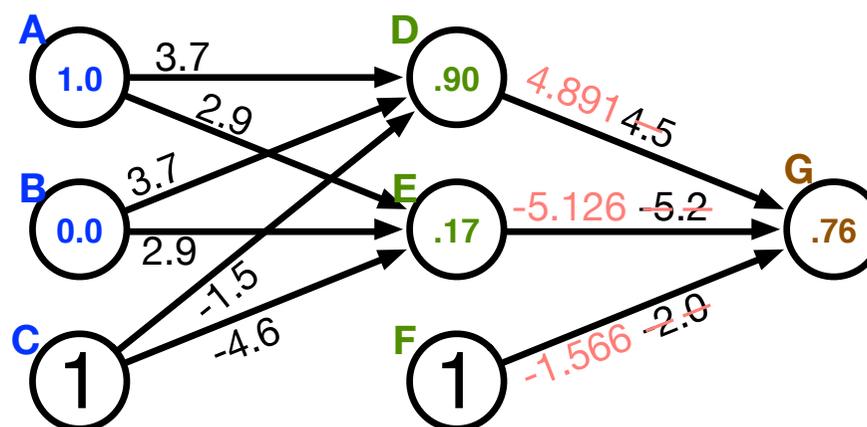
$$\Delta w_{j \leftarrow k} = \mu \delta_j h_k$$

# Our Example



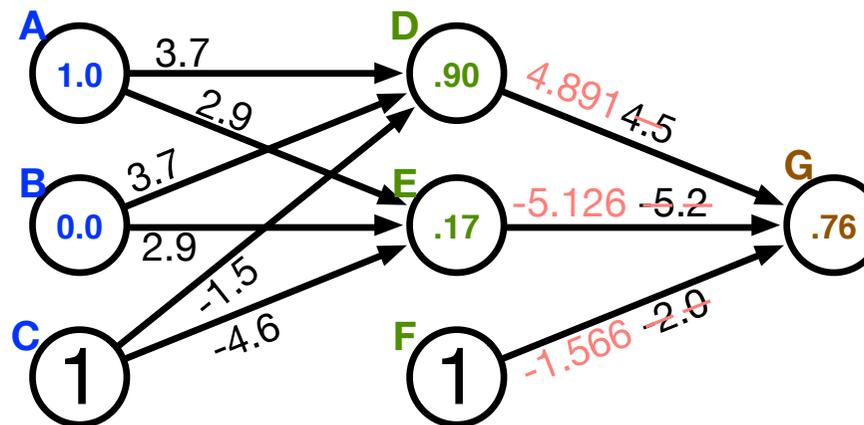
- Computed output:  $y = .76$
- Correct output:  $t = 1.0$
- Final layer weight updates (learning rate  $\mu = 10$ )
  - $\delta_G = (t - y) y' = (1 - .76) 0.181 = .0434$
  - $\Delta w_{GD} = \mu \delta_G h_D = 10 \times .0434 \times .90 = .391$
  - $\Delta w_{GE} = \mu \delta_G h_E = 10 \times .0434 \times .17 = .074$
  - $\Delta w_{GF} = \mu \delta_G h_F = 10 \times .0434 \times 1 = .434$

# Our Example



- Computed output:  $y = .76$
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  - $\delta_G = (t - y) y' = (1 - .76) 0.181 = .0434$
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# Hidden Layer Updates



- Hidden node **D**

- $\delta_D = \left( \sum_j w_{j \leftarrow i} \delta_j \right) y'_D = w_{GD} \delta_G y'_D = 4.5 \times .0434 \times .0898 = .0175$
- $\Delta w_{DA} = \mu \delta_D h_A = 10 \times .0175 \times 1.0 = .175$
- $\Delta w_{DB} = \mu \delta_D h_B = 10 \times .0175 \times 0.0 = 0$
- $\Delta w_{DC} = \mu \delta_D h_C = 10 \times .0175 \times 1 = .175$

- Hidden node **E**

- $\delta_E = \left( \sum_j w_{j \leftarrow i} \delta_j \right) y'_E = w_{GE} \delta_G y'_E = -5.2 \times .0434 \times 0.2055 = -.0464$
- $\Delta w_{EA} = \mu \delta_E h_A = 10 \times -.0464 \times 1.0 = -.464$
- etc.



# some additional aspects

# Initialization of Weights

- Weights are initialized randomly  
e.g., uniformly from interval  $[-0.01, 0.01]$
- Glorot and Bengio (2010) suggest
  - for shallow neural networks

$$\left[ -\frac{1}{\sqrt{n}}, \frac{1}{\sqrt{n}} \right]$$

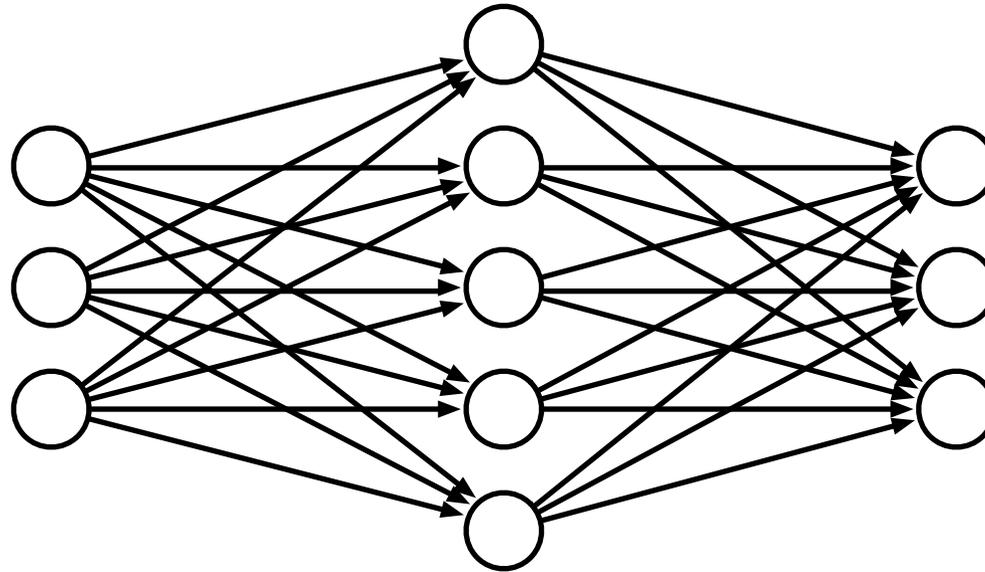
$n$  is the size of the previous layer

- for deep neural networks

$$\left[ -\frac{\sqrt{6}}{\sqrt{n_j + n_{j+1}}}, \frac{\text{sqrt6}}{\sqrt{n_j + n_{j+1}}} \right]$$

$n_j$  is the size of the previous layer,  $n_{j+1}$  size of next layer

# Neural Networks for Classification



- Predict class: one output node per class
- Training data output: "One-hot vector", e.g.,  $\vec{y} = (0, 0, 1)^T$
- Prediction
  - predicted class is output node  $y_i$  with highest value
  - obtain posterior probability distribution by soft-max

$$\text{softmax}(y_i) = \frac{e^{y_i}}{\sum_j e^{y_j}}$$

# Speedup: Momentum Term

- Updates may move a weight slowly in one direction
- To speed this up, we can keep a memory of prior updates

$$\Delta w_{j \leftarrow k}(n-1)$$

- ... and add these to any new updates (with decay factor  $\rho$ )

$$\Delta w_{j \leftarrow k}(n) = \mu \delta_j h_k + \rho \Delta w_{j \leftarrow k}(n-1)$$

# computational aspects

# Vector and Matrix Multiplications

- Forward computation:  $\vec{s} = W\vec{h}$
- Activation function:  $\vec{y} = \text{sigmoid}(\vec{h})$
- Error term:  $\vec{\delta} = (\vec{t} - \vec{y}) \text{sigmoid}'(\vec{s})$
- Propagation of error term:  $\vec{\delta}_i = W\vec{\delta}_{i+1} \cdot \text{sigmoid}'(\vec{s})$
- Weight updates:  $\Delta W = \mu\vec{\delta}\vec{h}^T$

- Neural network layers may have, say, 200 nodes
- Computations such as  $W\vec{h}$  require  $200 \times 200 = 40,000$  multiplications
- Graphics Processing Units (GPU) are designed for such computations
  - image rendering requires such vector and matrix operations
  - massively multi-core but lean processing units
  - example: NVIDIA Tesla K20c GPU provides 2496 thread processors
- Extensions to C to support programming of GPUs, such as CUDA

- GPU library for Python
- Homepage: <http://deeplearning.net/software/theano/>
- See web site for sample implementation of back-propagation training
- Used to implement
  - neural network language models
  - neural machine translation (Bahdanau et al., 2015)