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# Introduction to Neural Networks

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19 September 2024



# Basic Machine Learning



- Given an input  $\mathbf{x}$
- Represented by a number of features  $x_i$
- Predict an output  $y$

# Linear Models

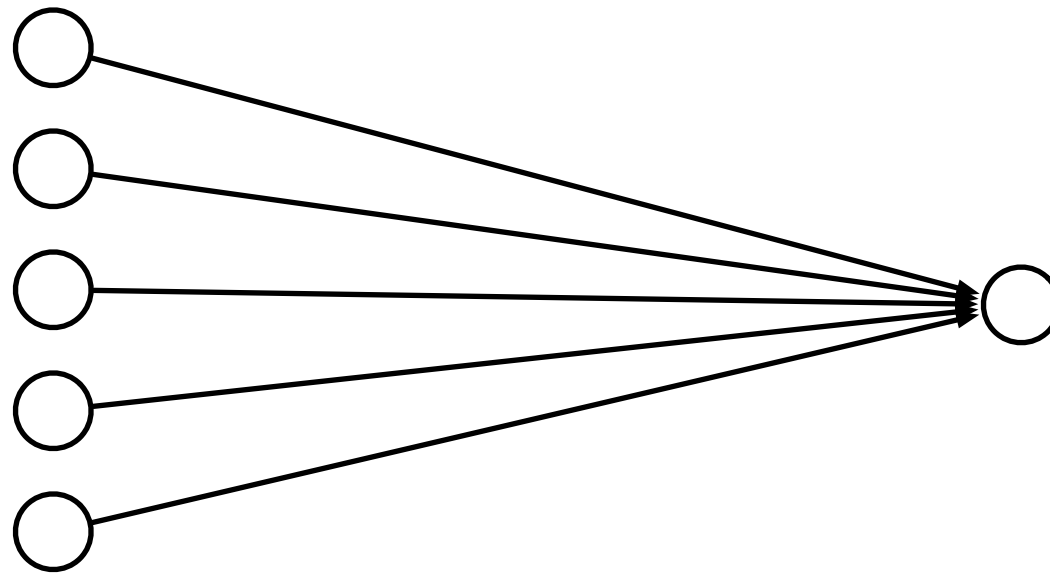


2

- Weighted linear combination of feature values  $x_i$  and weights  $\lambda_j$

$$\text{score}(\lambda, \mathbf{x}) = \sum_i \lambda_i x_i$$

- Such models can be illustrated as a "network"



# Limits of Linearity

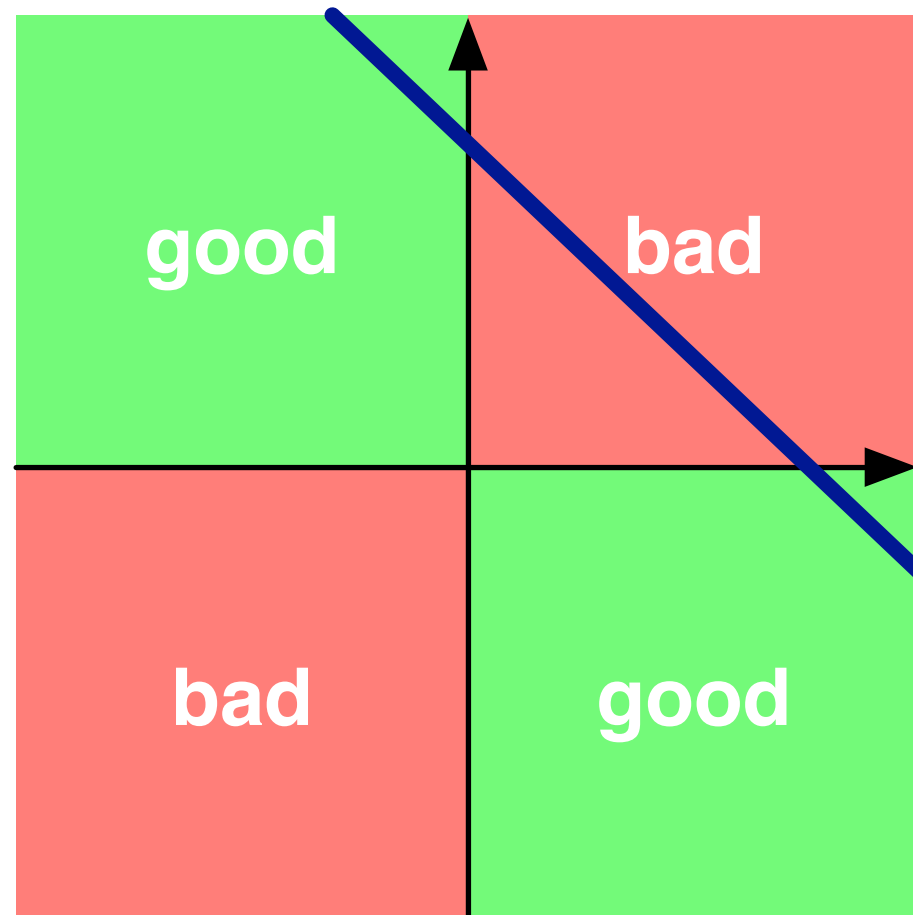


- We can give each feature a weight
- But not more complex value relationships, e.g.,
  - any value in the range  $[0;5]$  is equally good
  - values over 8 are bad
  - higher than 10 is not worse

# XOR

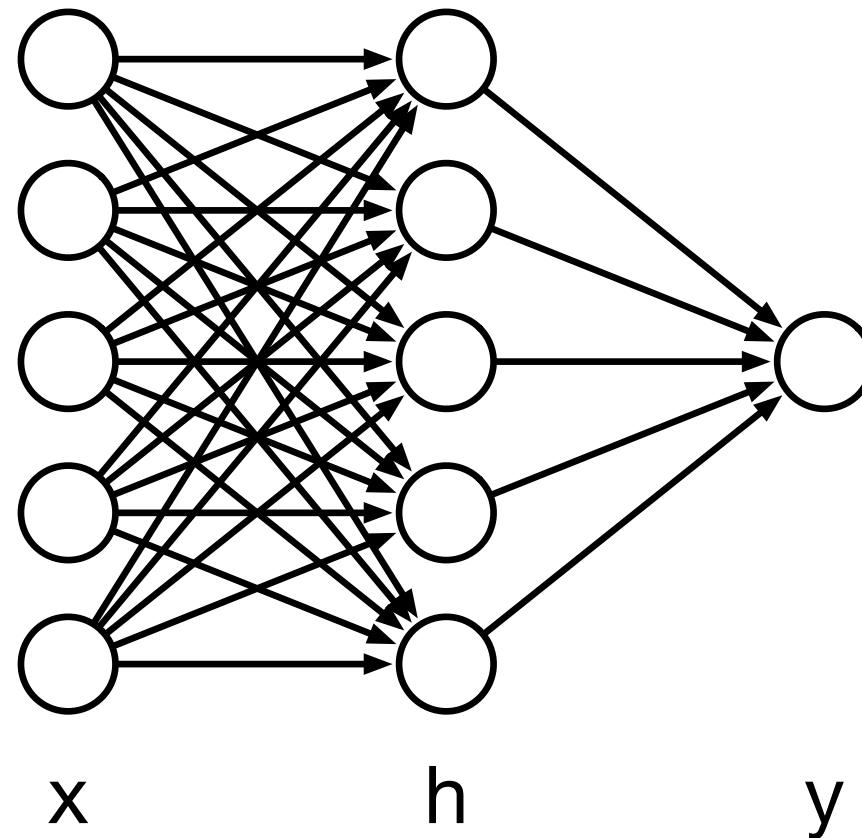


- Linear models cannot model XOR



# 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

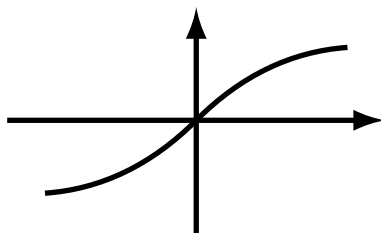
$$\text{score}(\lambda, \mathbf{x}) = \sum_i \lambda_i x_i$$

- Add a non-linear function

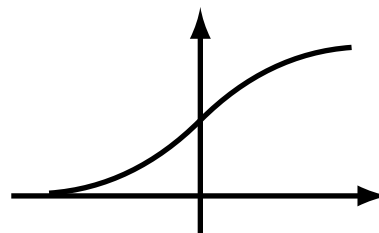
$$\text{score}(\lambda, \mathbf{x}) = f\left(\sum_i \lambda_i x_i\right)$$

- Popular choices

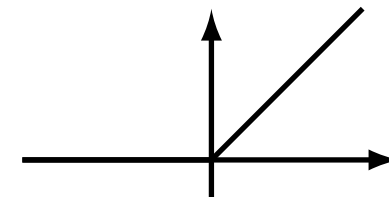
$$\tanh(x)$$



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



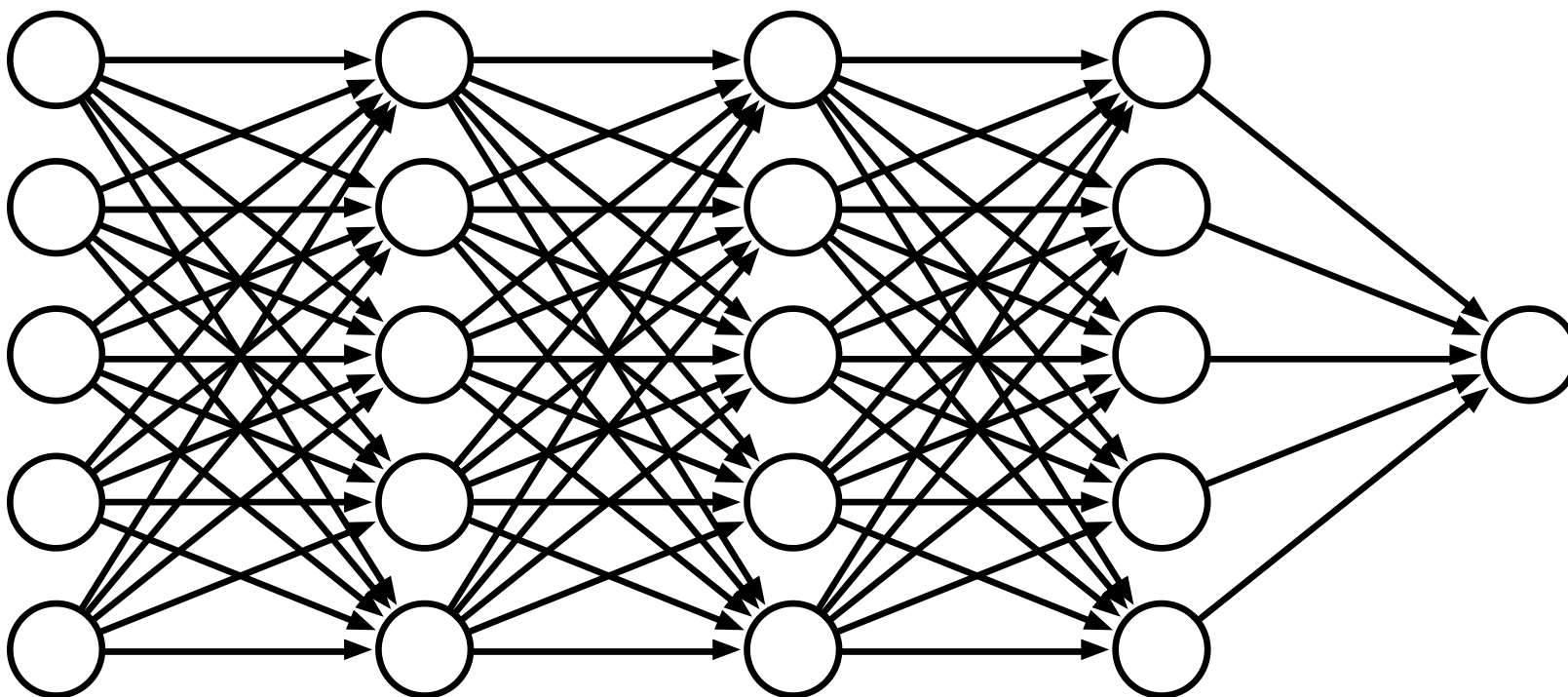
$$\text{relu}(x) = \max(0, x)$$



(sigmoid is also called the "logistic function")

# Deep Learning

- More layers = deep learning





# What Depth Enables

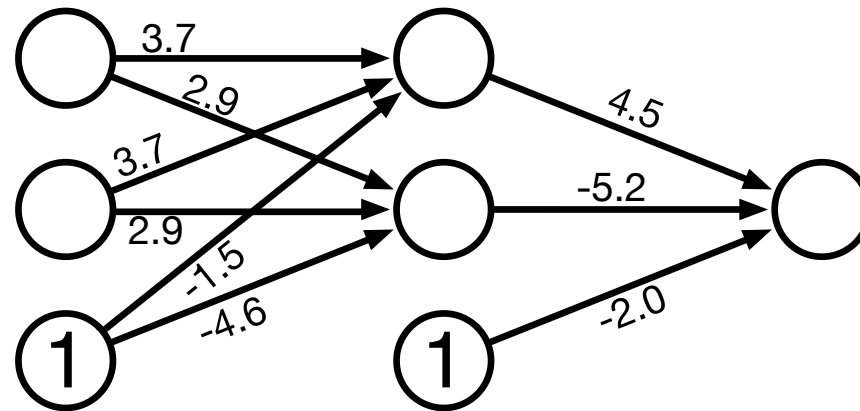


8

- Each layer is a processing step
- Having multiple processing steps allows complex functions
- Metaphor: NN and computing circuits
  - computer = sequence of Boolean gates
  - neural computer = sequence of layers
- Deep neural networks can implement complex functions  
e.g., sorting on input values

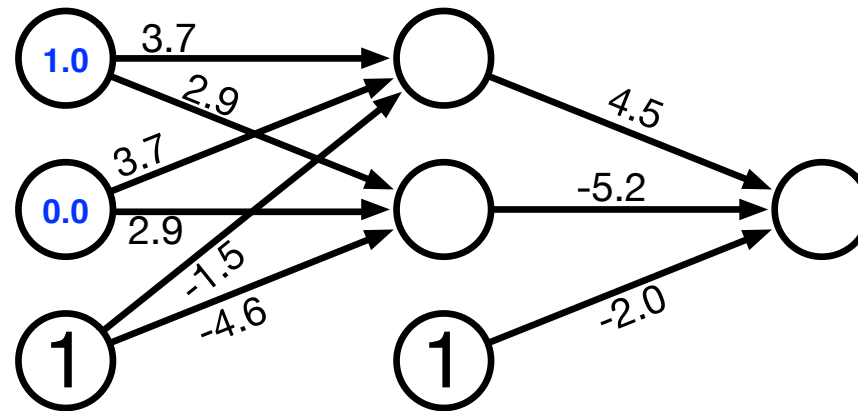
# example

# Simple Neural Network



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

# Sample Input

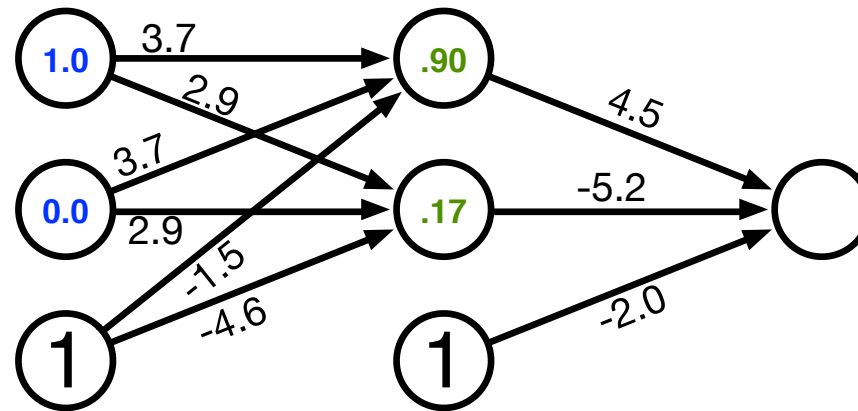


- Try out two input values
- Hidden unit computation

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

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

# Computed Hidden

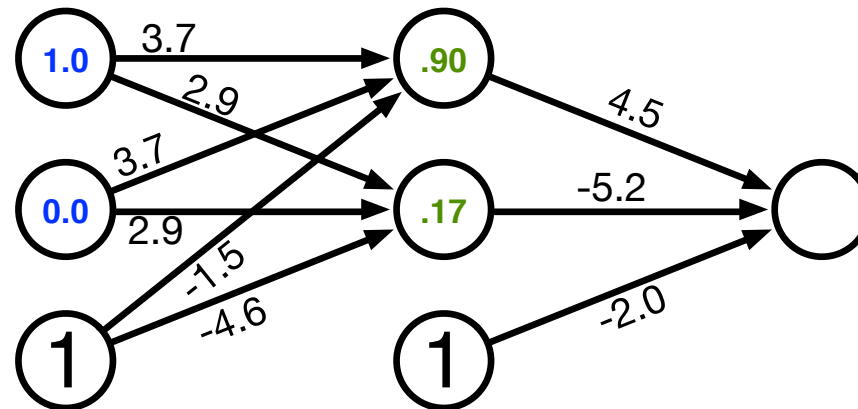


- Try out two input values
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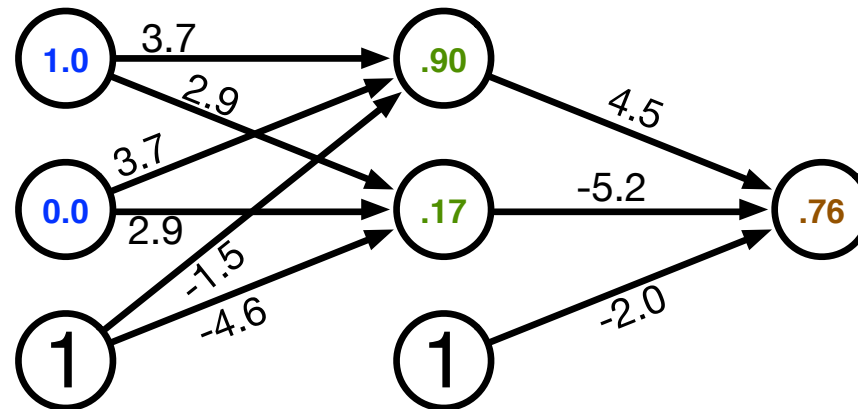
# Compute Output



- 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

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

# Output for all Binary Inputs

Input $x_0$	Input $x_1$	Hidden $h_0$	Hidden $h_1$	Output $y_0$
0	0	0.12	0.02	$0.18 \rightarrow 0$
0	1	0.88	0.27	$0.74 \rightarrow 1$
1	0	0.73	0.12	$0.74 \rightarrow 1$
1	1	0.99	0.73	$0.33 \rightarrow 0$

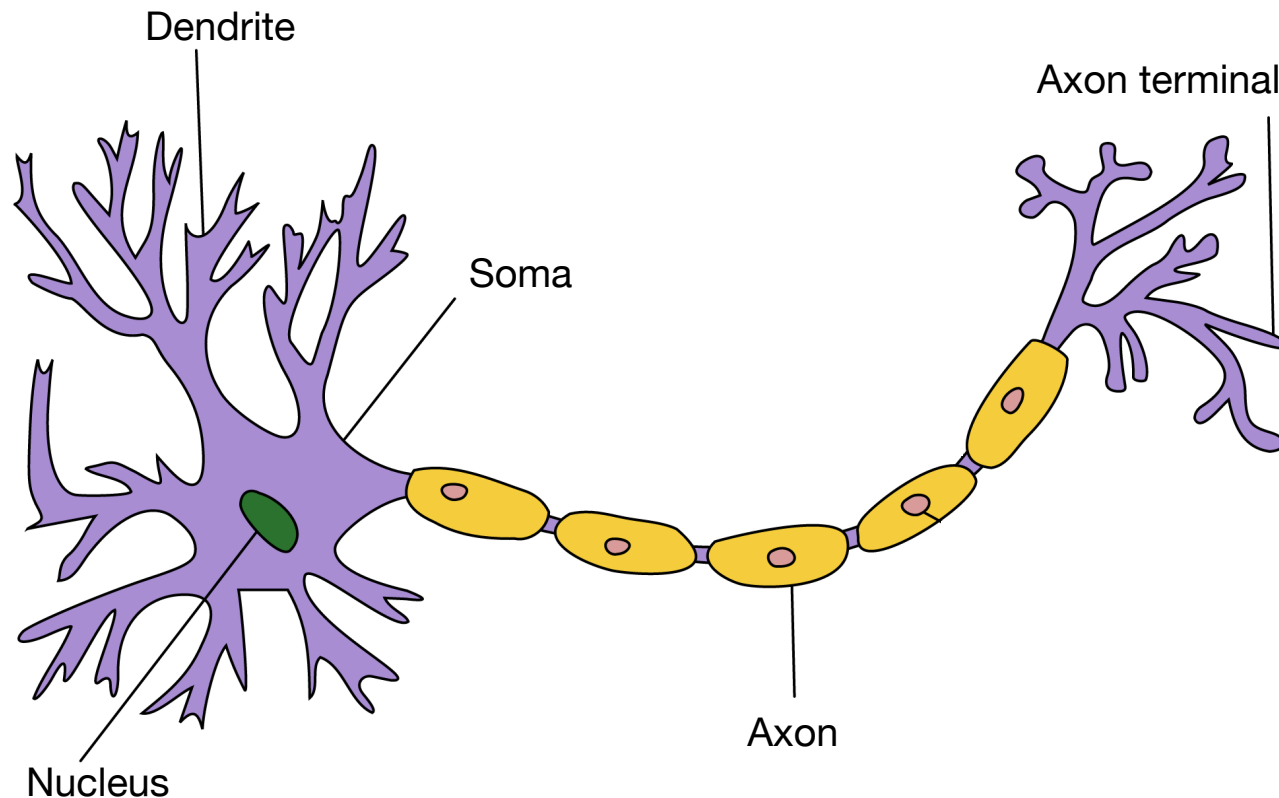
- Network implements XOR
  - hidden node  $h_0$  is OR
  - hidden node  $h_1$  is AND
  - final layer operation is  $h_0 - -h_1$
- Power of deep neural networks: chaining of processing steps  
just as: more Boolean circuits  $\rightarrow$  more complex computations possible



# why “neural” networks?

# Neuron in the Brain

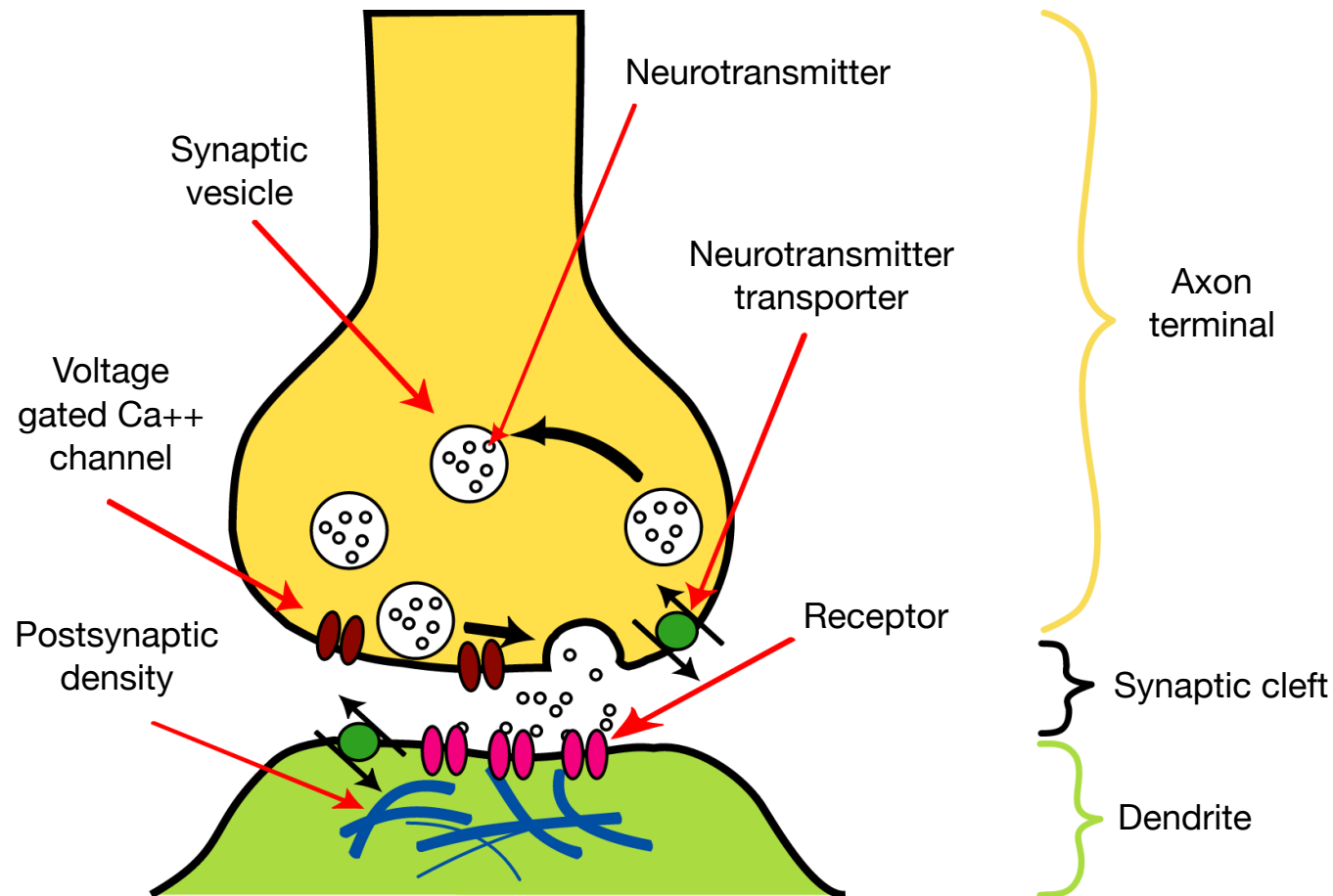
- The human brain is made up of about 100 billion neurons



- 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

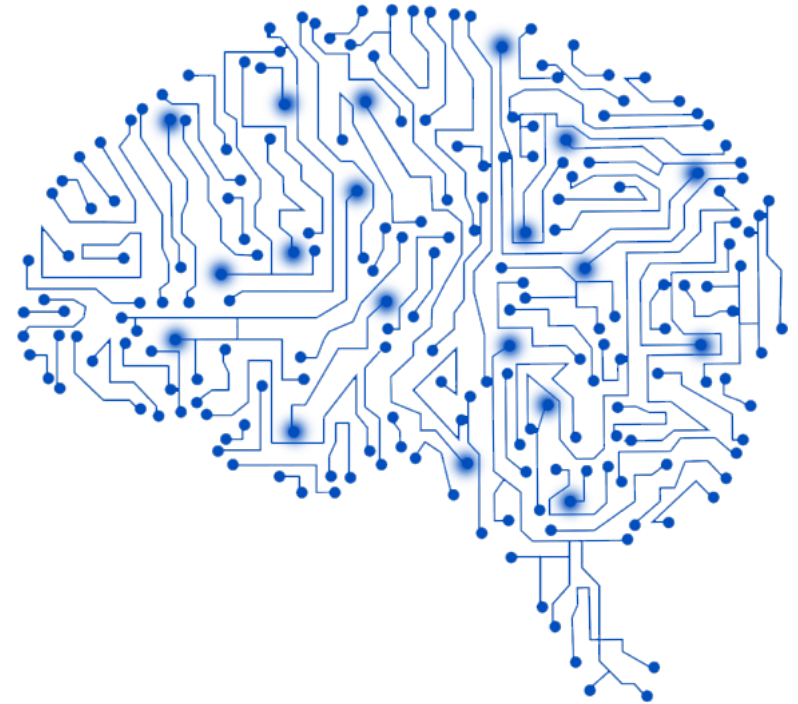


# The Brain vs. Artificial Neural Networks

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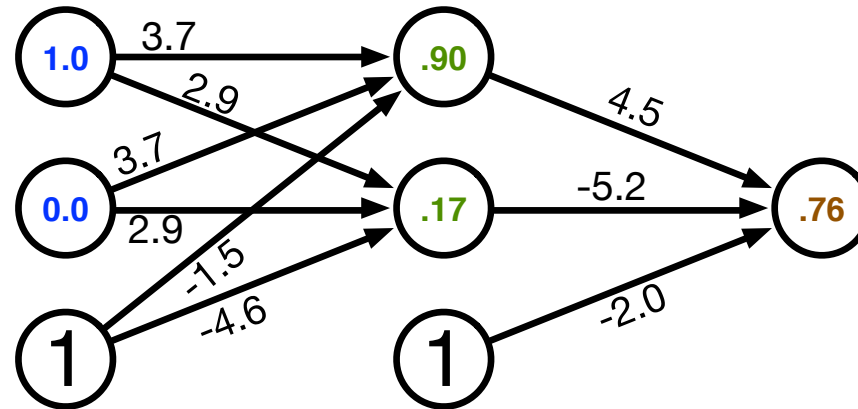


- Similarities
  - Neurons, connections between neurons
  - Learning = change of connections, not change of neurons
  - Massive parallel processing
- But artificial neural networks are much simpler
  - computation within neuron vastly simplified
  - discrete time steps
  - typically some form of supervised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



# back-propagation training

# Error



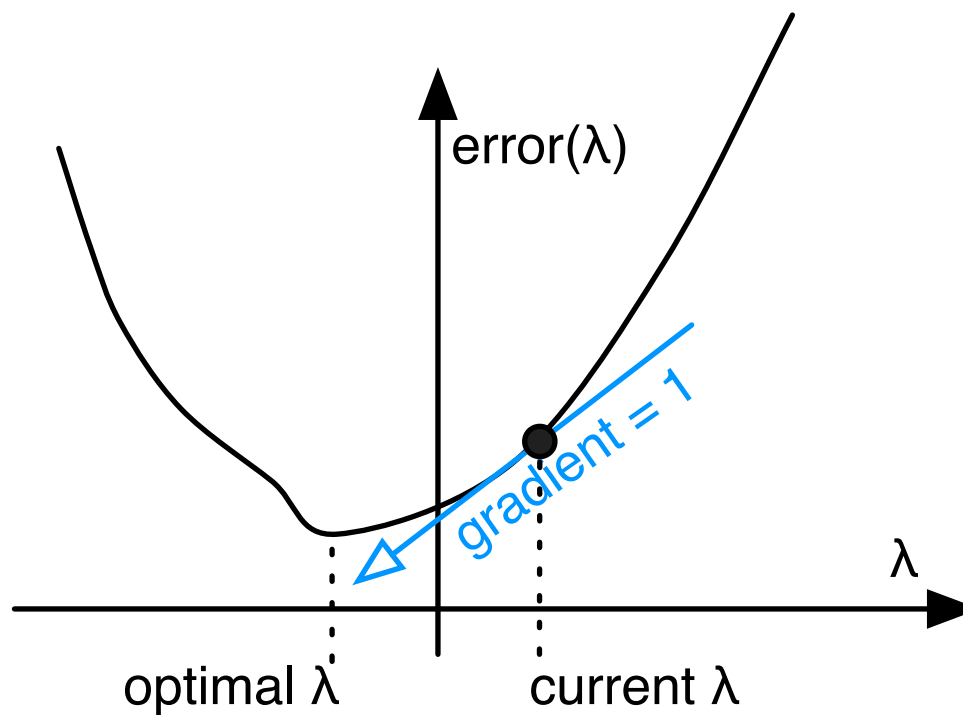
- Computed output:  $y = .76$
- Correct output:  $t = 1.0$

⇒ How do we adjust the weights?

# Key Concepts

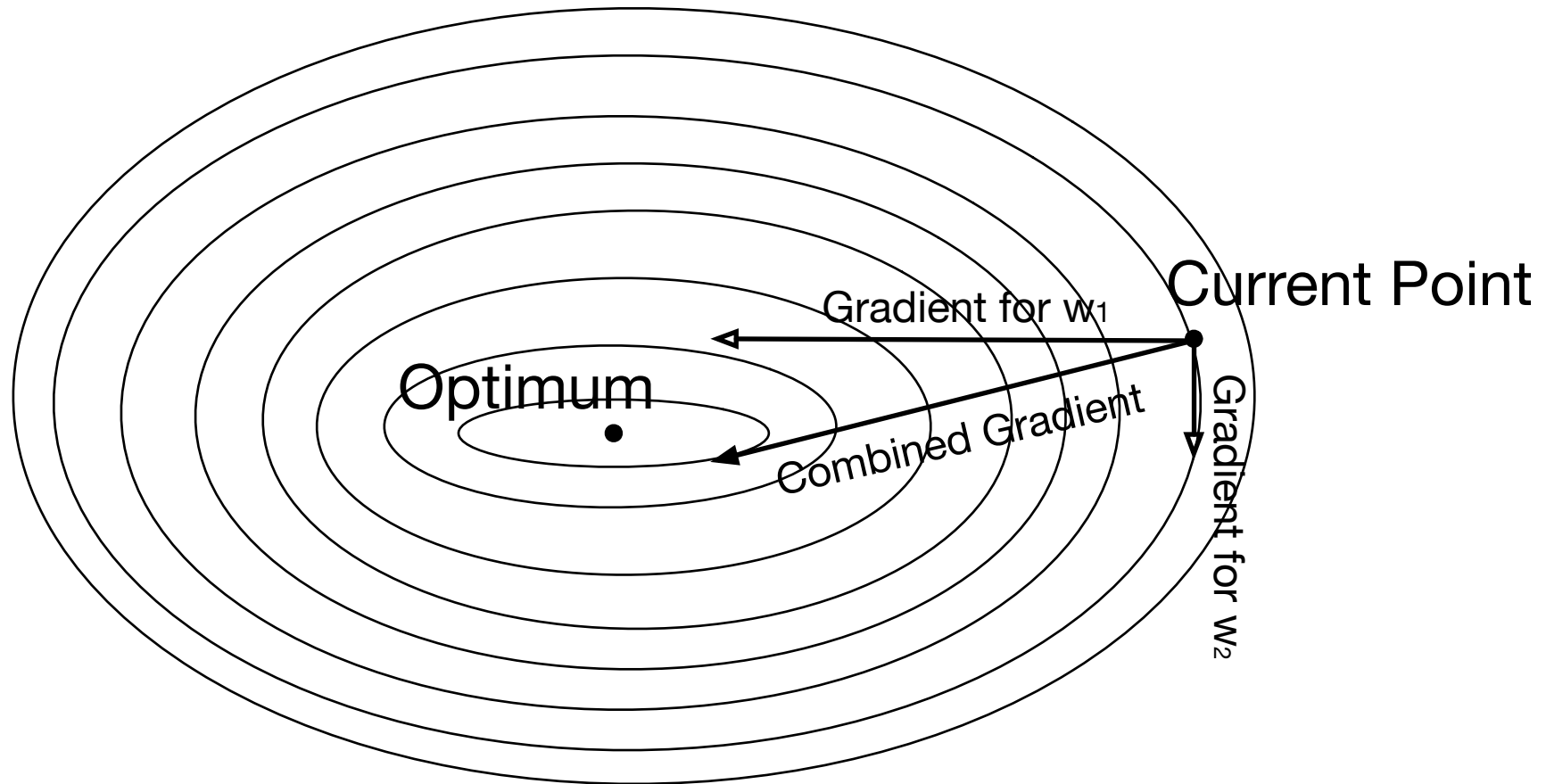
- Gradient descent
  - error is a function of the weights
  - we want to reduce the error
  - gradient descent: move towards the error minimum
  - compute gradient  $\rightarrow$  get direction to the error minimum
  - adjust weights towards direction of lower error
- Back-propagation
  - first adjust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

# Gradient Descent





# Gradient Descent



# 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

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

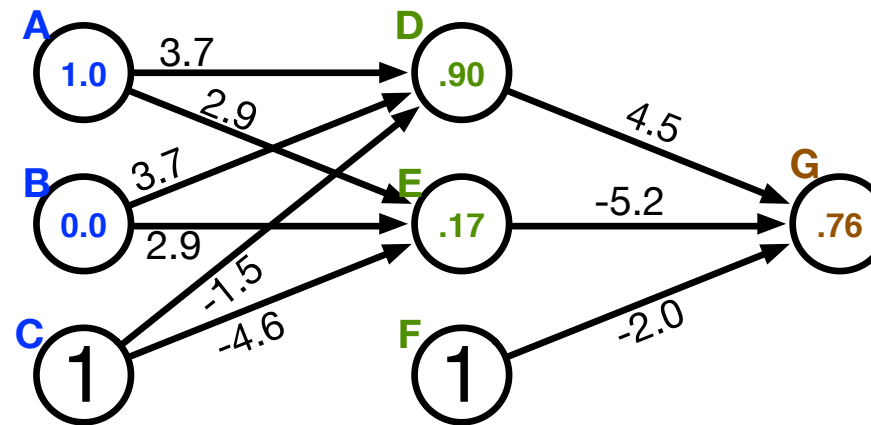
- Back-propagate the error term  
(why this way? there is math to back it up...)

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

- Universal update formula

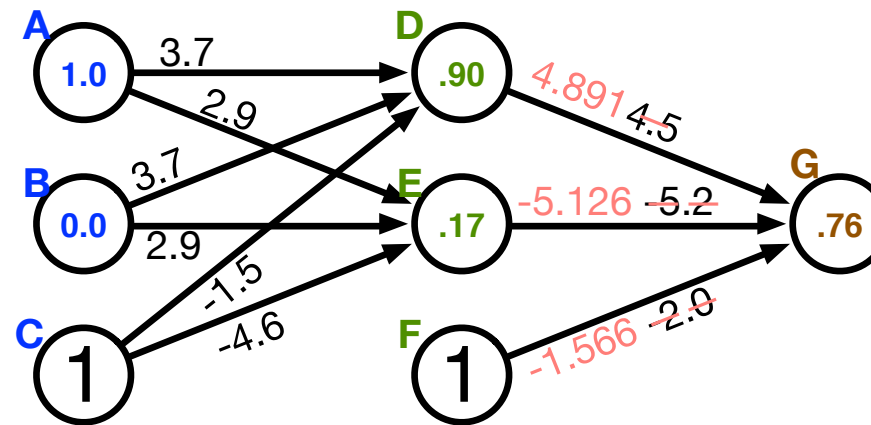
$$\Delta w_{j \leftarrow k} = \mu \delta_j h_k$$

# Our Example



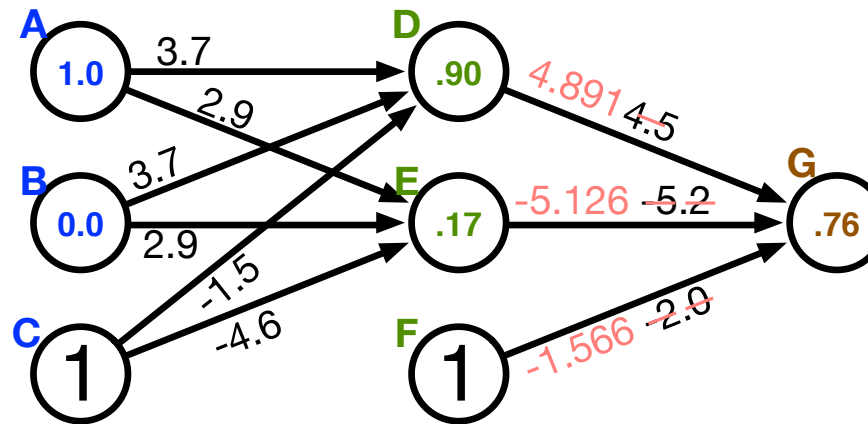
- Computed output:  $y = .76$
- Correct output:  $t = 1.0$
- Final layer weight updates (learning rate  $\mu = 10$ )
  - $\delta_G = (t - y) y' = (1 - .76) 0.181 = .0434$
  - $\Delta w_{GD} = \mu \delta_G h_D = 10 \times .0434 \times .90 = .391$
  - $\Delta w_{GE} = \mu \delta_G h_E = 10 \times .0434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

# Our Example



- Computed output:  $y = .76$
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  - $\Delta w_{GF} = \mu \delta_G h_F = 10 \times .0434 \times 1 = .434$

# 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.

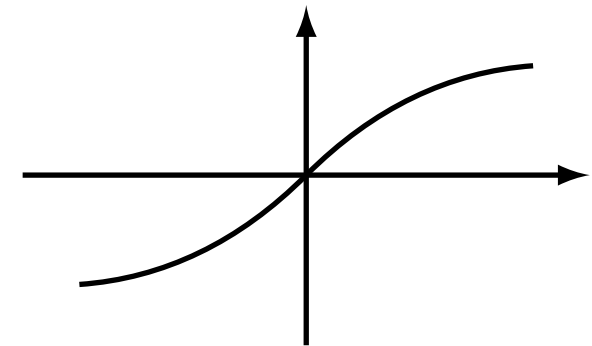
some additional aspects

# 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

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

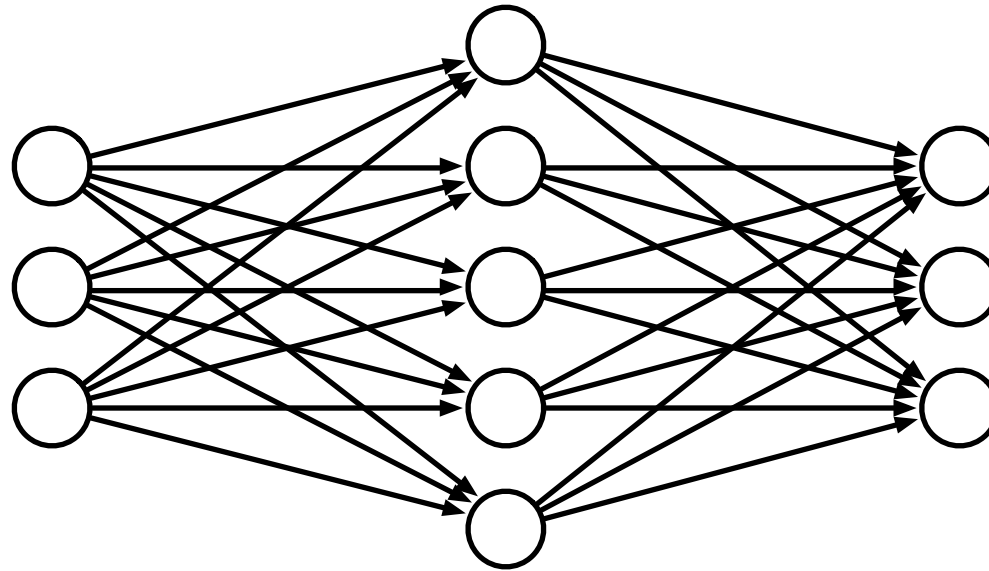
$n$  is the size of the previous layer



- for deep neural networks

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

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

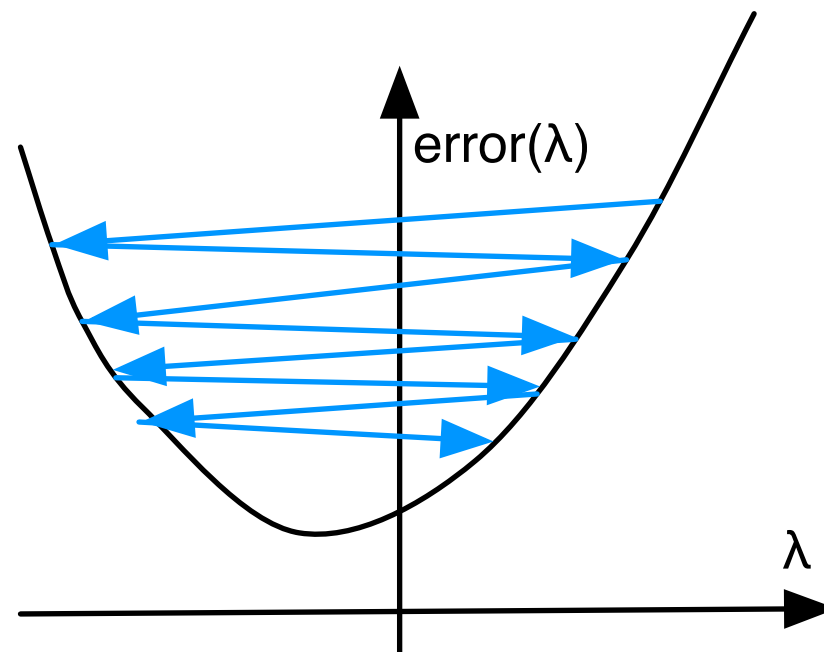


- Predict class: one output node per class
- Training data output: "One-hot vector", e.g.,  $\vec{y} = (0, 0, 1)^T$
- Prediction
  - predicted class is output node  $y_i$  with highest value
  - obtain posterior probability distribution by soft-max

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

# Problems with Gradient Descent Training

39

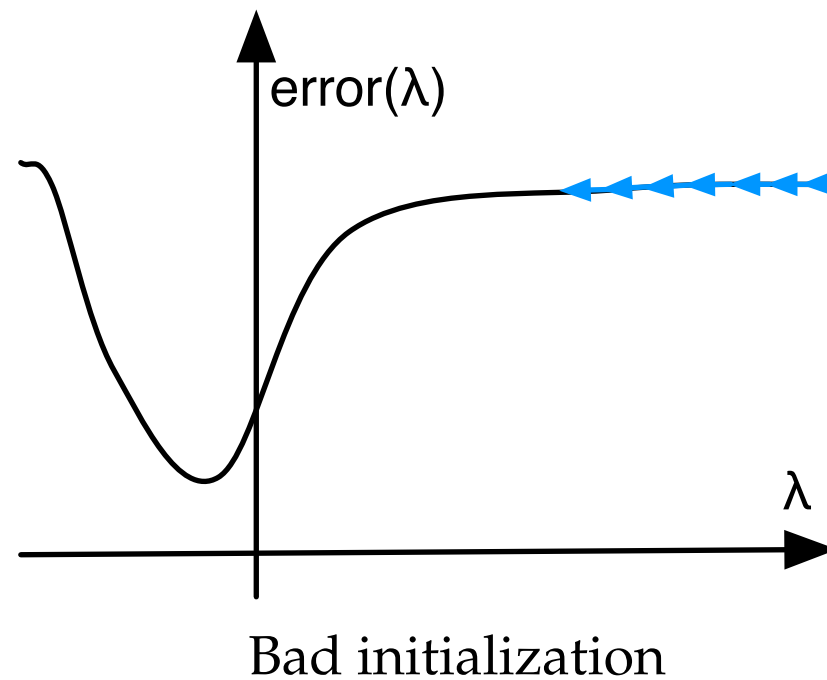


Too high learning rate



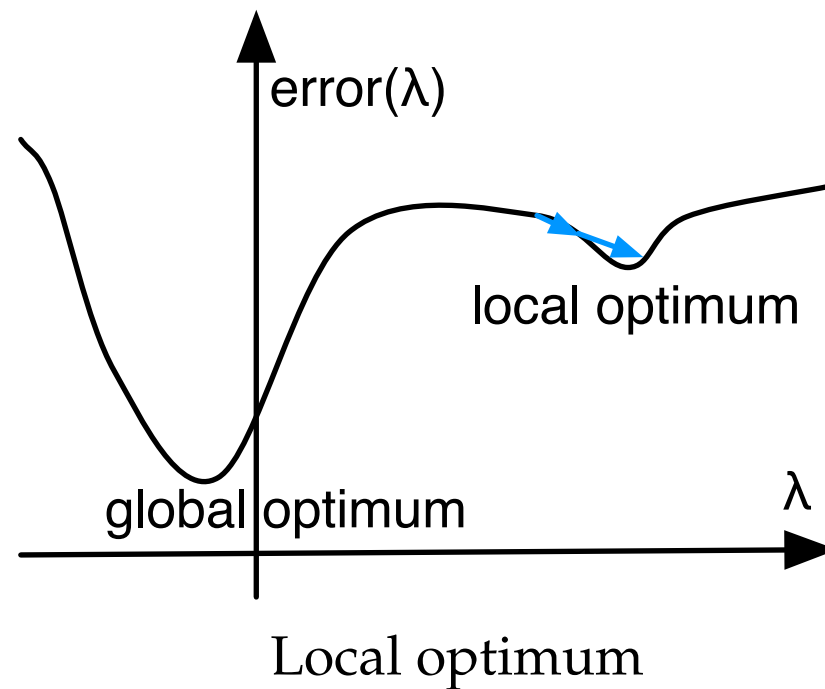
# Problems with Gradient Descent Training

40



# Problems with Gradient Descent Training

41



# 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  $\rho$ )

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

# Adagrad

- Typically reduce the learning rate  $\mu$  over time
  - at the beginning, things have to change a lot
  - later, just fine-tuning
- Adapting learning rate per parameter
- Adagrad update  
based on error  $E$  with respect to the weight  $w$  at time  $t = g_t = \frac{dE}{dw}$

$$\Delta w_t = \frac{\mu}{\sqrt{\sum_{\tau=1}^t g_{\tau}^2}} g_t$$

- Each training example yields a set of weight updates  $\Delta w_i$ .
- Batch up several training examples
  - sum up their updates
  - apply sum to model
- Mostly done for speed reasons

# 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 H100 GPU provides 18,432 CUDA cores
- Extensions to C to support programming of GPUs, such as CUDA



- Theano
- Tensorflow (Google)
- PyTorch (Facebook)
- MXNet (Amazon)
- DyNet