
Introduction to Neural Networks

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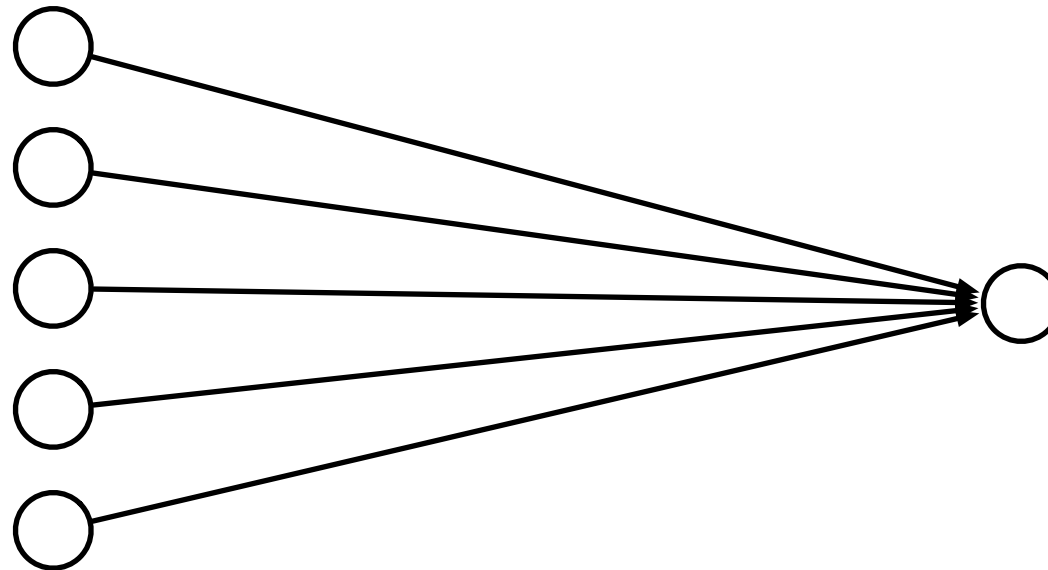
24 September 2020



- We used before weighted linear combination of feature values h_j and weights λ_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

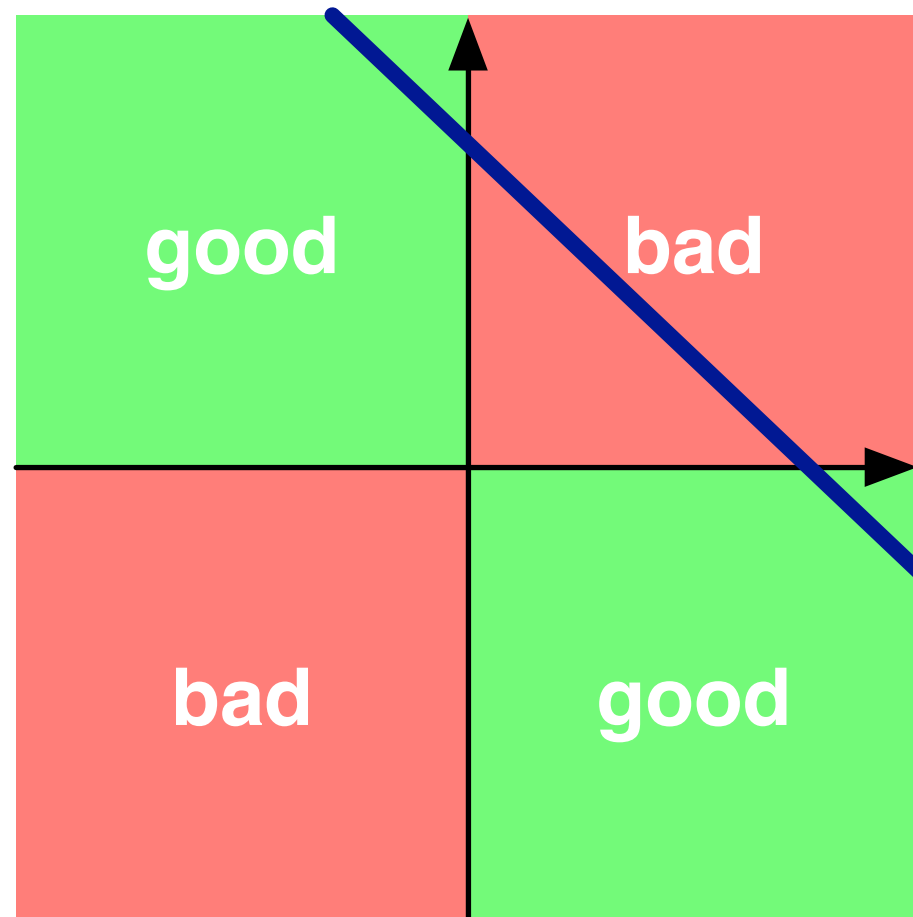


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- We can give each feature a weight
- But not more complex value relationships, e.g.,
 - any value in the range $[0;5]$ is equally good
 - values over 8 are bad
 - higher than 10 is not worse

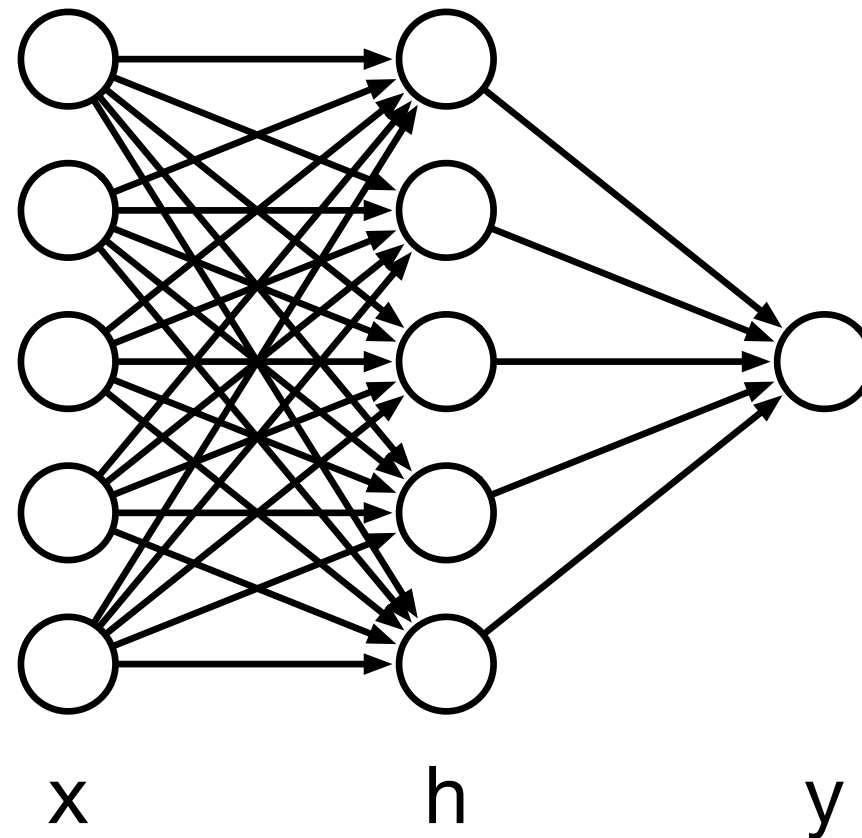
XOR

- 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

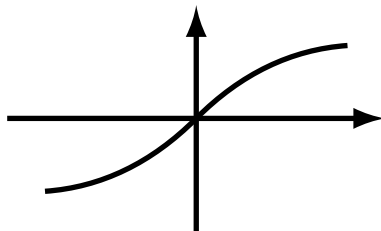
$$\text{score}(\lambda, \mathbf{d}_i) = \sum_j \lambda_j h_j(\mathbf{d}_i)$$

- Add a non-linear function

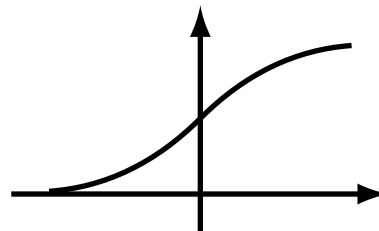
$$\text{score}(\lambda, \mathbf{d}_i) = f\left(\sum_j \lambda_j h_j(\mathbf{d}_i)\right)$$

- Popular choices

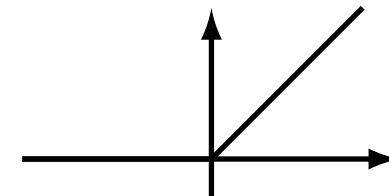
$\tanh(x)$



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



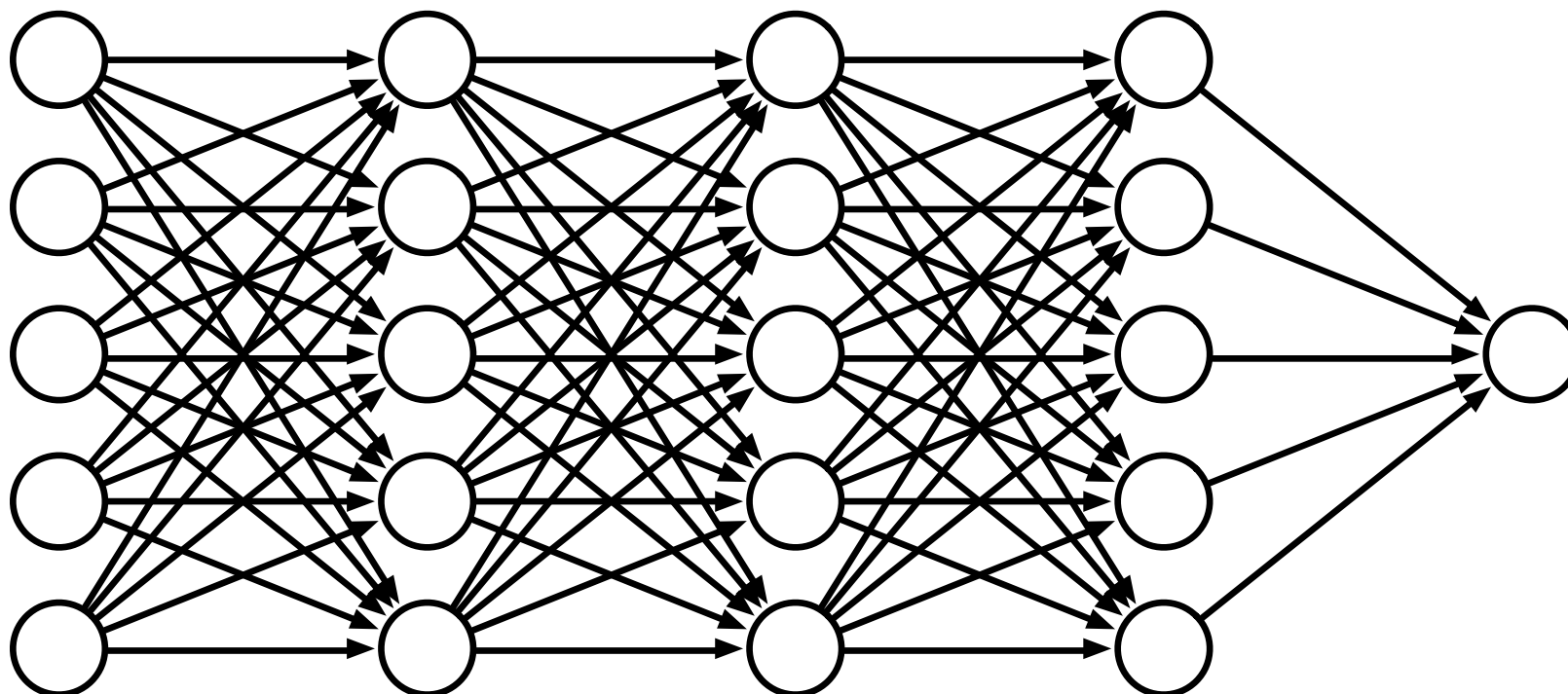
$\text{relu}(x) = \max(0, x)$



(sigmoid is also called the "logistic function")

Deep Learning

- More layers = deep learning



What Depths Holds

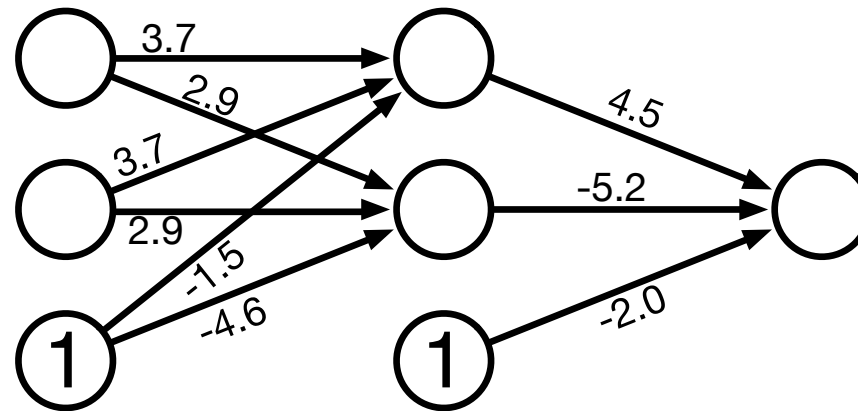


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- Each layer is a processing step
- Having multiple processing steps allows complex functions
- Metaphor: NN and computing circuits
 - computer = sequence of Boolean gates
 - neural computer = sequence of layers
- Deep neural networks can implement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

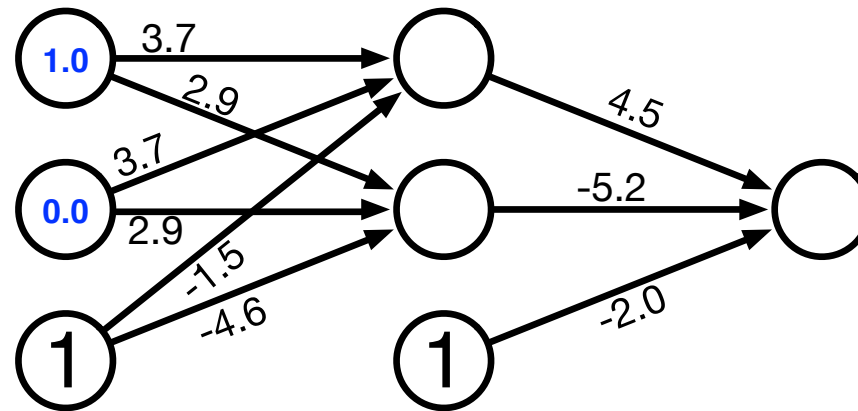
example

Simple Neural Network



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

Sample Input

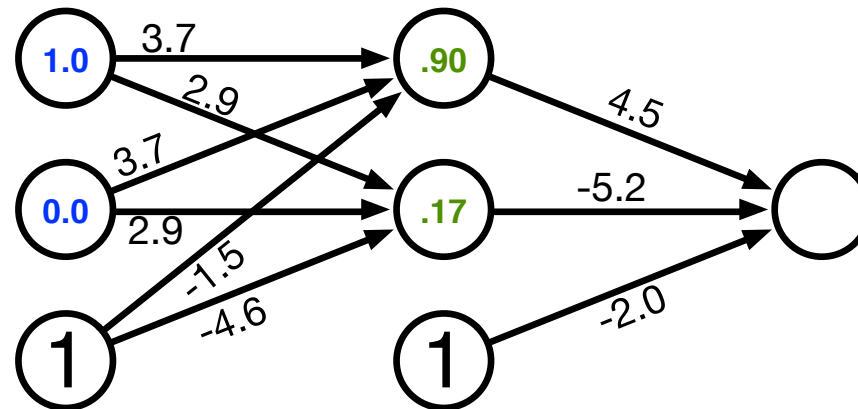


- Try out two input values
- Hidden unit computation

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

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

Computed Hidden

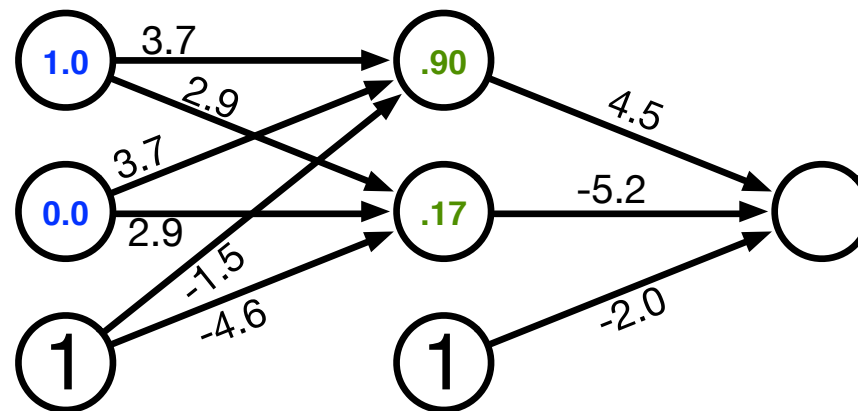


- Try out two input values
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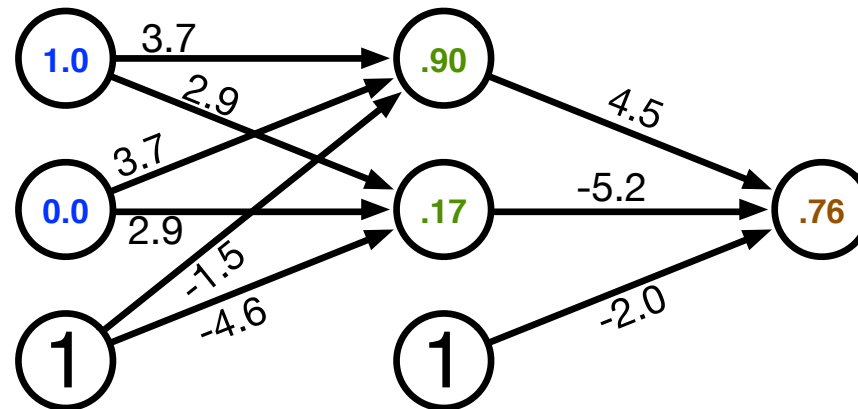
Compute Output



- 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

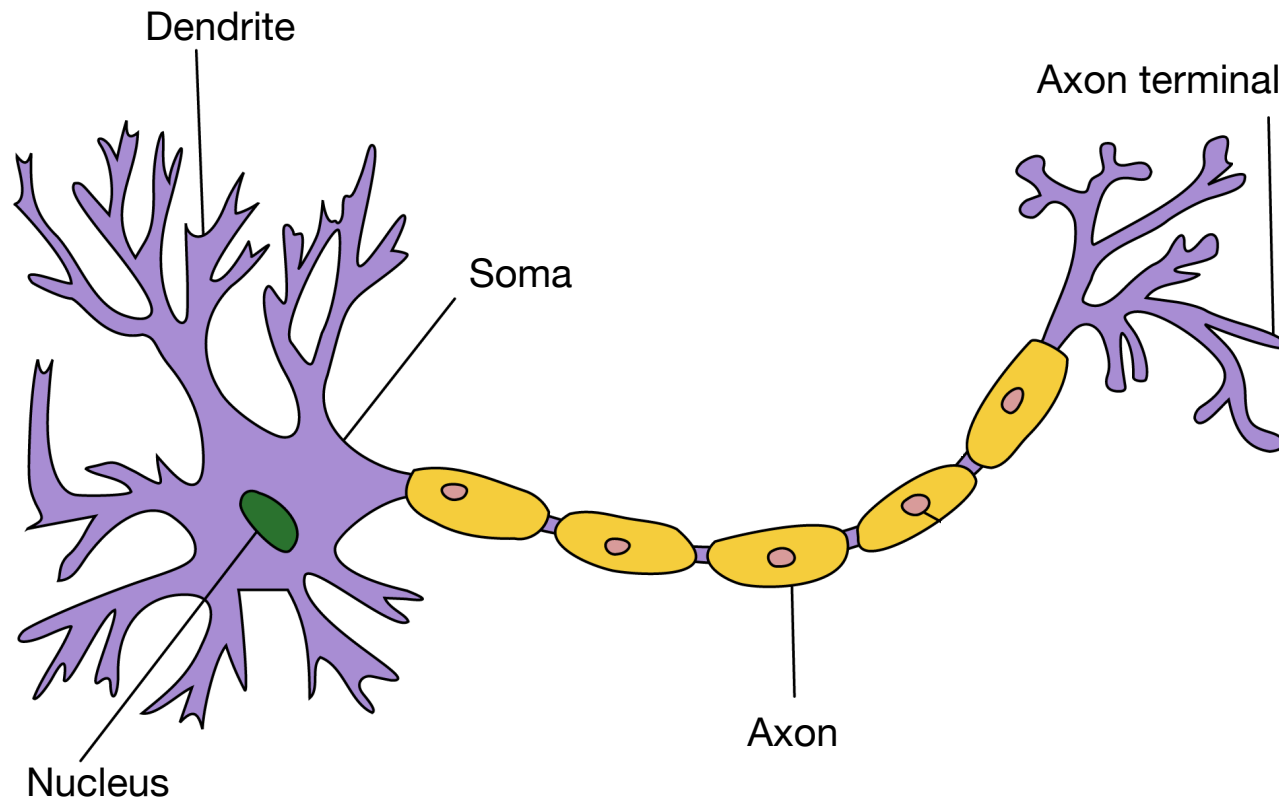
Input x_0	Input x_1	Hidden h_0	Hidden h_1	Output y_0
0	0	0.12	0.02	$0.18 \rightarrow 0$
0	1	0.88	0.27	$0.74 \rightarrow 1$
1	0	0.73	0.12	$0.74 \rightarrow 1$
1	1	0.99	0.73	$0.33 \rightarrow 0$

- 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

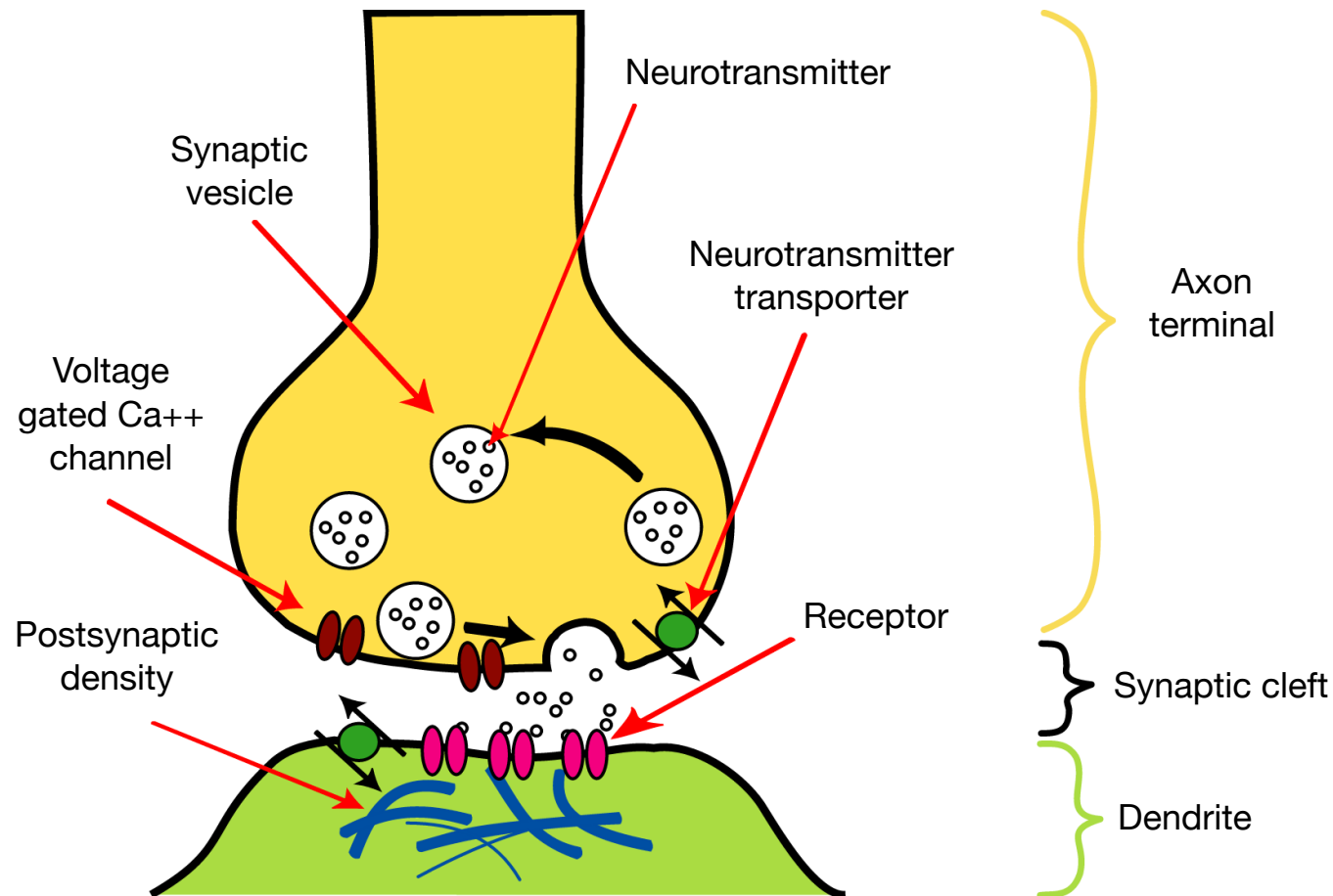
- The human brain is made up of about 100 billion neurons



- 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

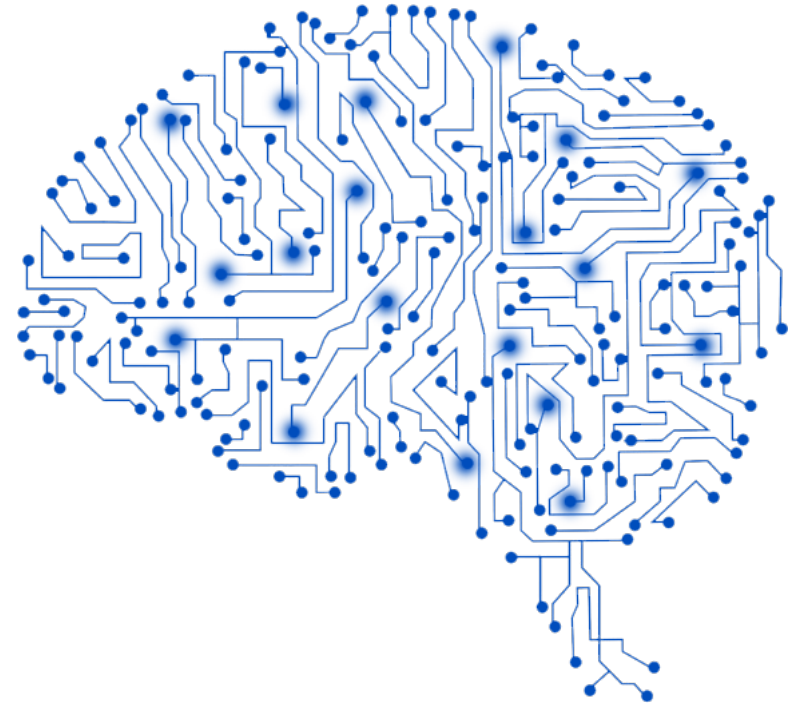


The Brain vs. Artificial Neural Networks

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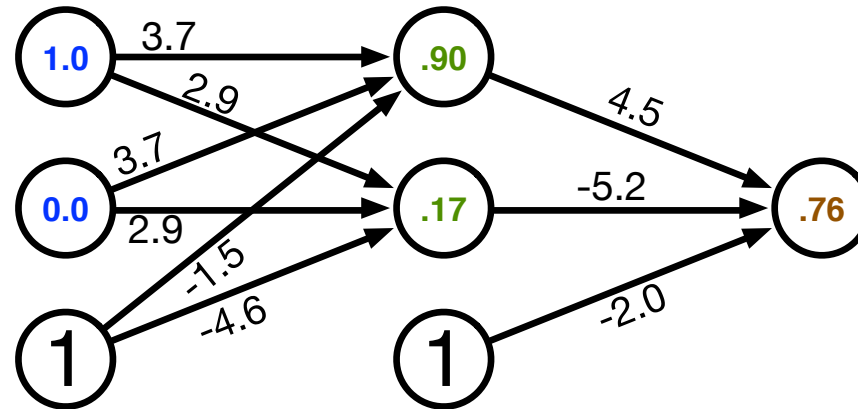


- Similarities
 - Neurons, connections between neurons
 - Learning = change of connections, not change of neurons
 - Massive parallel processing
- But artificial neural networks are much simpler
 - computation within neuron vastly simplified
 - discrete time steps
 - typically some form of supervised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



back-propagation training

Error



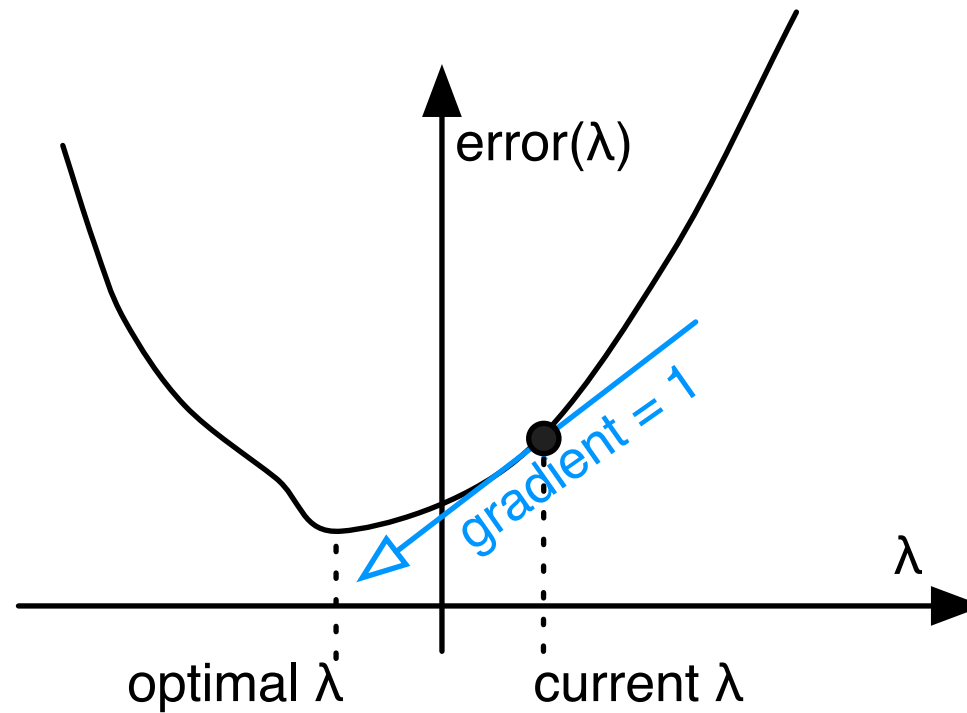
- Computed output: $y = .76$
- Correct output: $t = 1.0$

⇒ How do we adjust the weights?

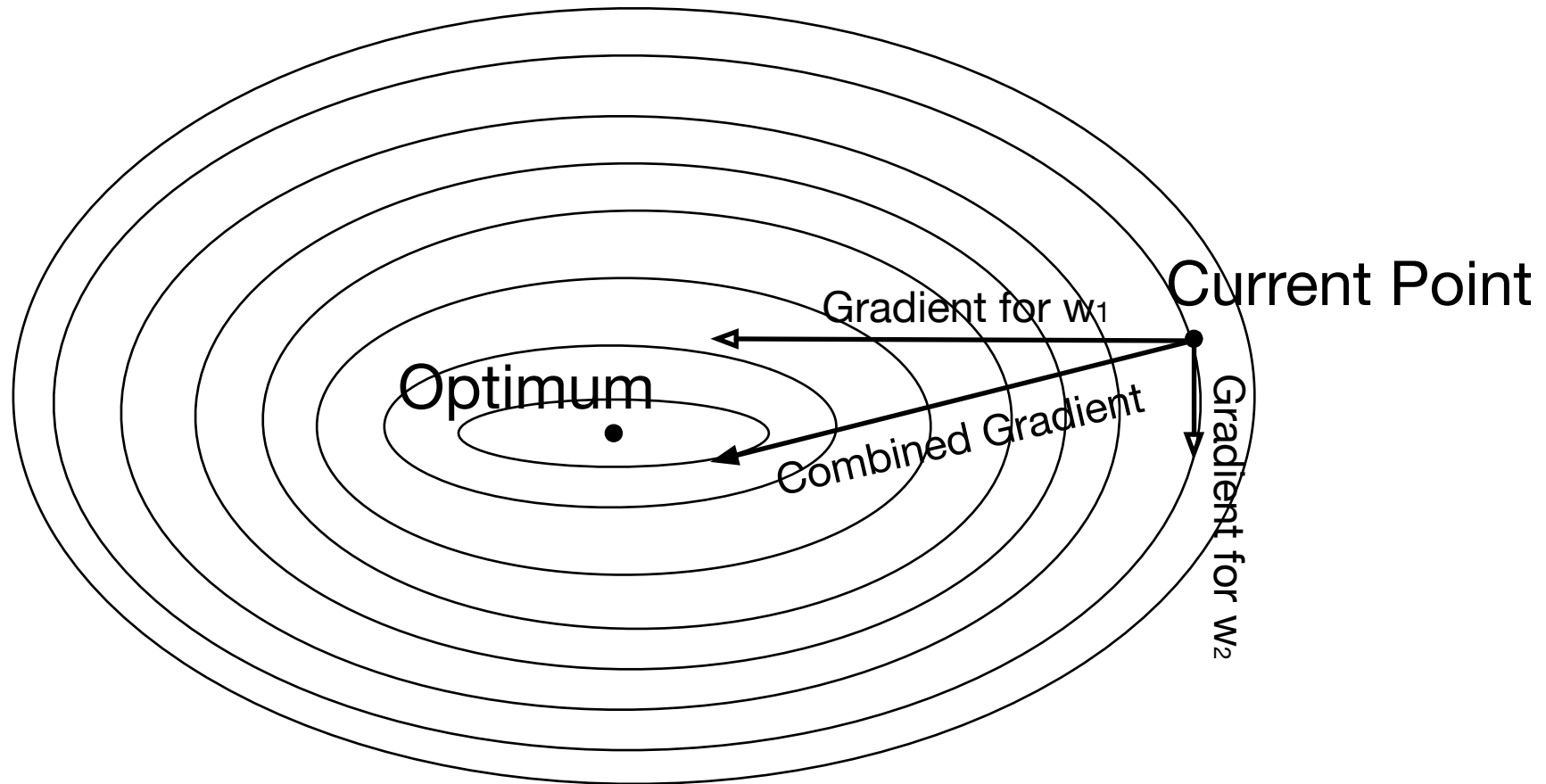
Key Concepts

- 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 μ

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

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

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

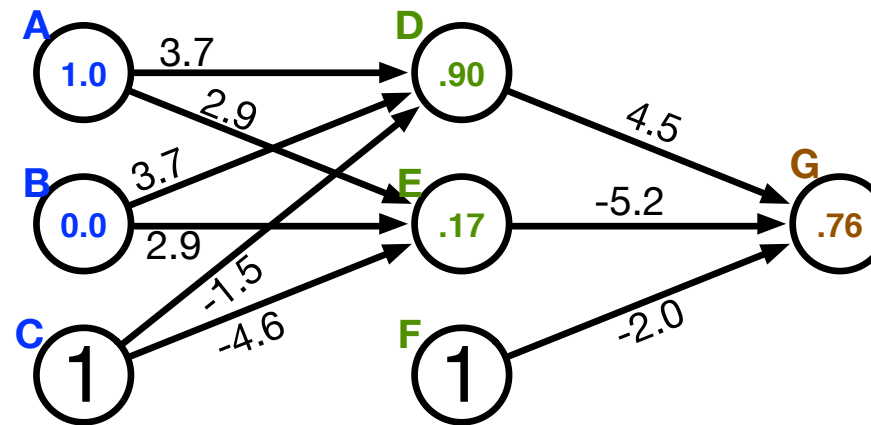
- Back-propagate the error term
(why this way? there is math to back it up...)

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

- Universal update formula

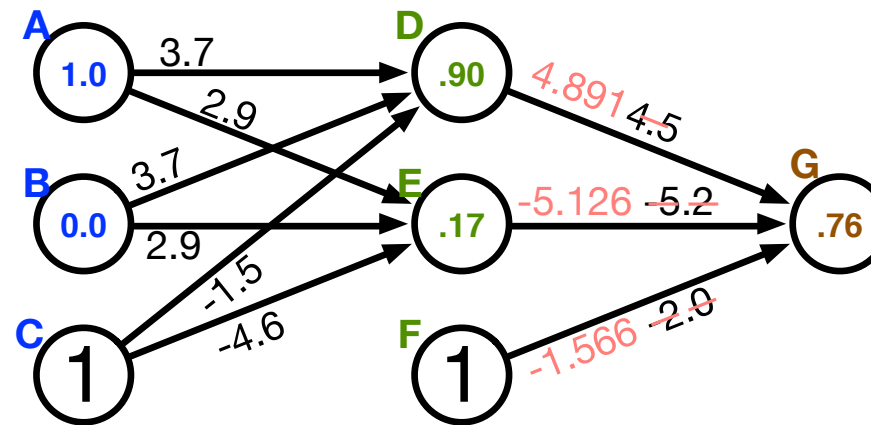
$$\Delta w_{j \leftarrow k} = \mu \delta_j h_k$$

Our Example



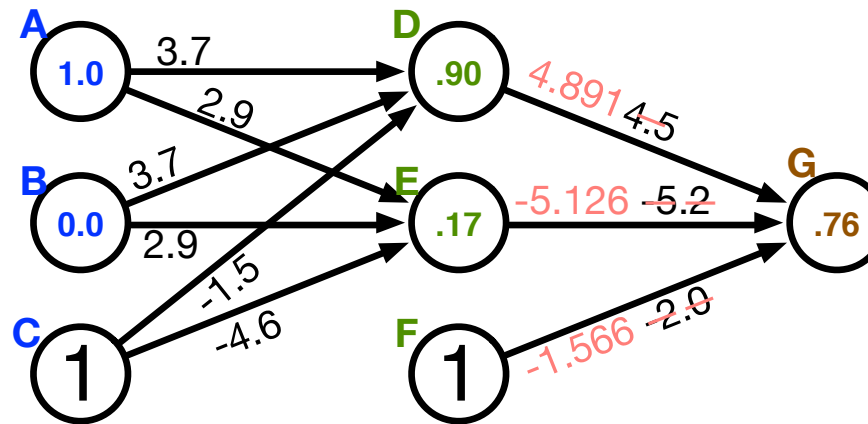
- Computed output: $y = .76$
- Correct output: $t = 1.0$
- Final layer weight updates (learning rate $\mu = 10$)
 - $\delta_G = (t - y) y' = (1 - .76) 0.181 = .0434$
 - $\Delta w_{GD} = \mu \delta_G h_D = 10 \times .0434 \times .90 = .391$
 - $\Delta w_{GE} = \mu \delta_G h_E = 10 \times .0434 \times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

Our Example



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

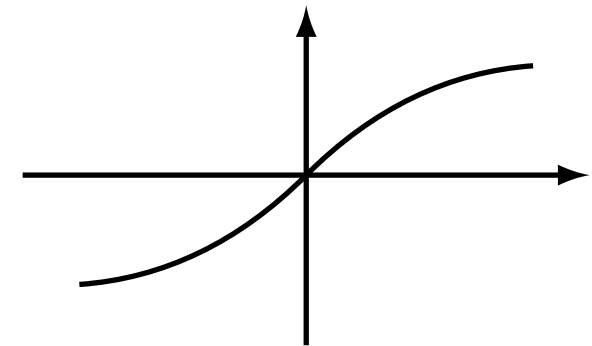
some additional aspects

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

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

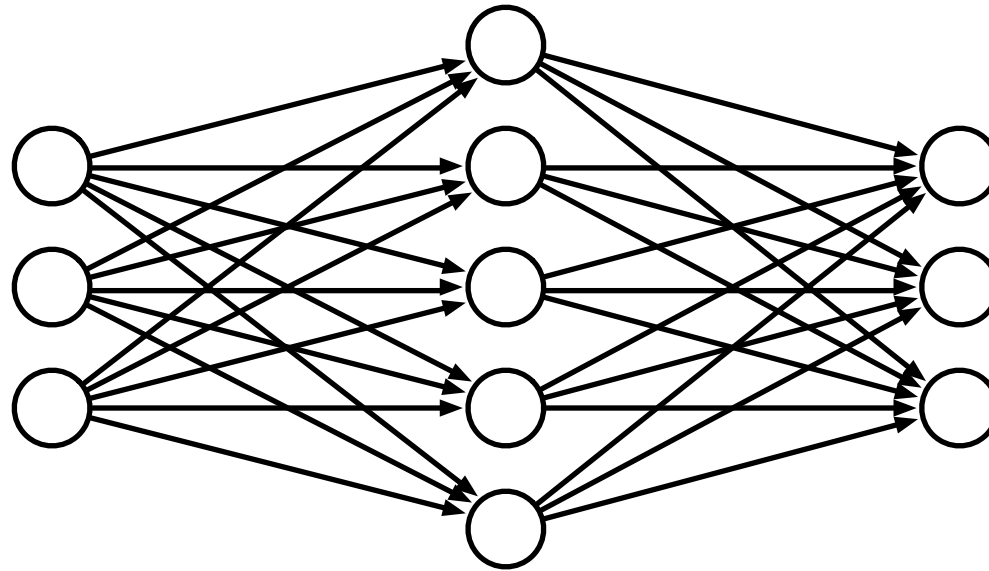
n is the size of the previous layer



- 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

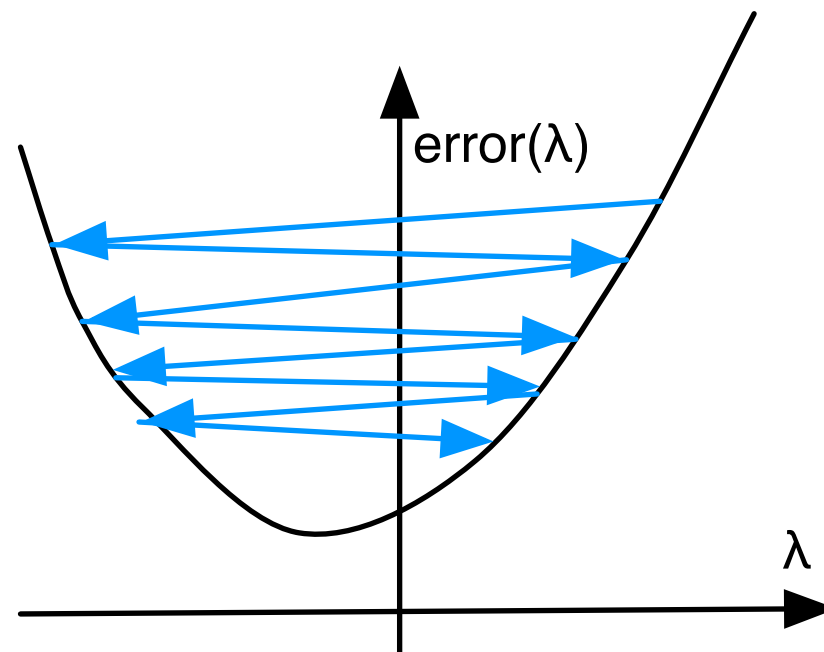


- Predict class: one output node per class
- Training data output: "One-hot vector", e.g., $\vec{y} = (0, 0, 1)^T$
- Prediction
 - predicted class is output node y_i with highest value
 - obtain posterior probability distribution by soft-max

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

Problems with Gradient Descent Training

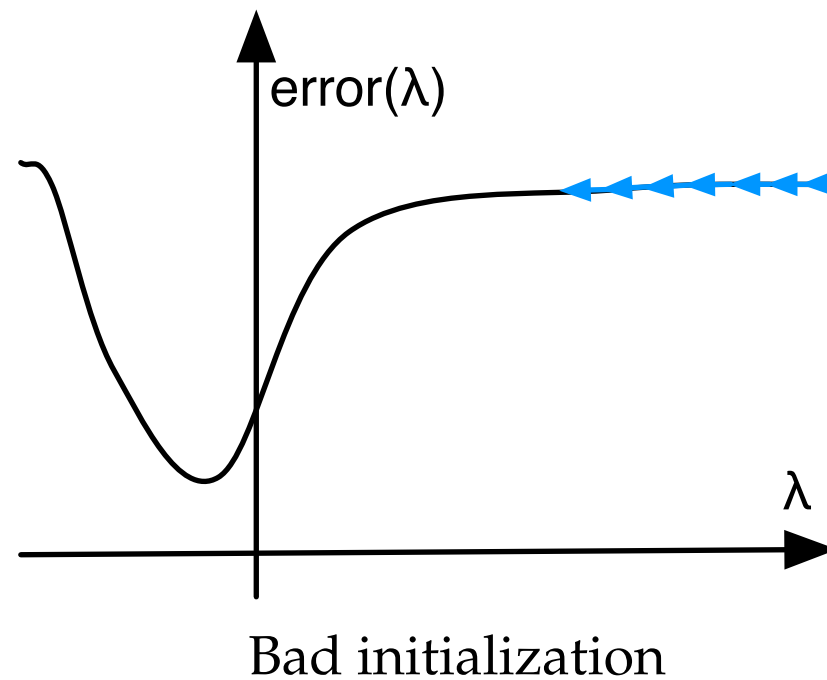
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Too high learning rate

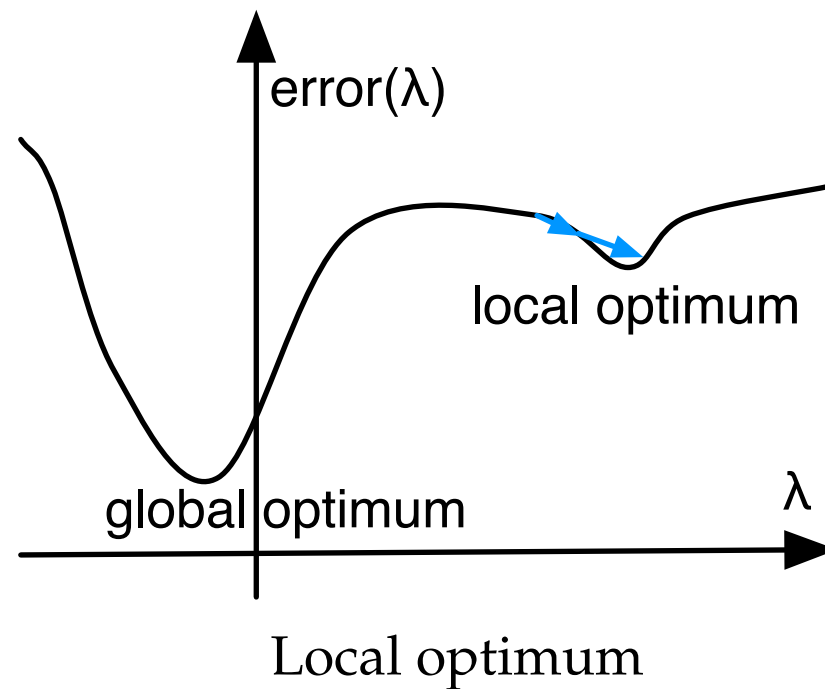
Problems with Gradient Descent Training

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Problems with Gradient Descent Training

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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 ρ)

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

Adagrad

- Typically reduce the learning rate μ 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 $t = g_t = \frac{dE}{dw}$

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

- A general problem of machine learning: overfitting to training data (very good on train, bad on unseen test)
- Solution: **regularization**, e.g., keeping weights from having extreme values
- Dropout: randomly remove some hidden units during training
 - mask: set of hidden units dropped
 - randomly generate, say, 10–20 masks
 - alternate between the masks during training
- Why does that work?
 - bagging, ensemble, ...

Mini Batches

- Each training example yields a set of weight updates Δw_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 Tesla K20c GPU provides 2496 thread processors
- Extensions to C to support programming of GPUs, such as CUDA

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