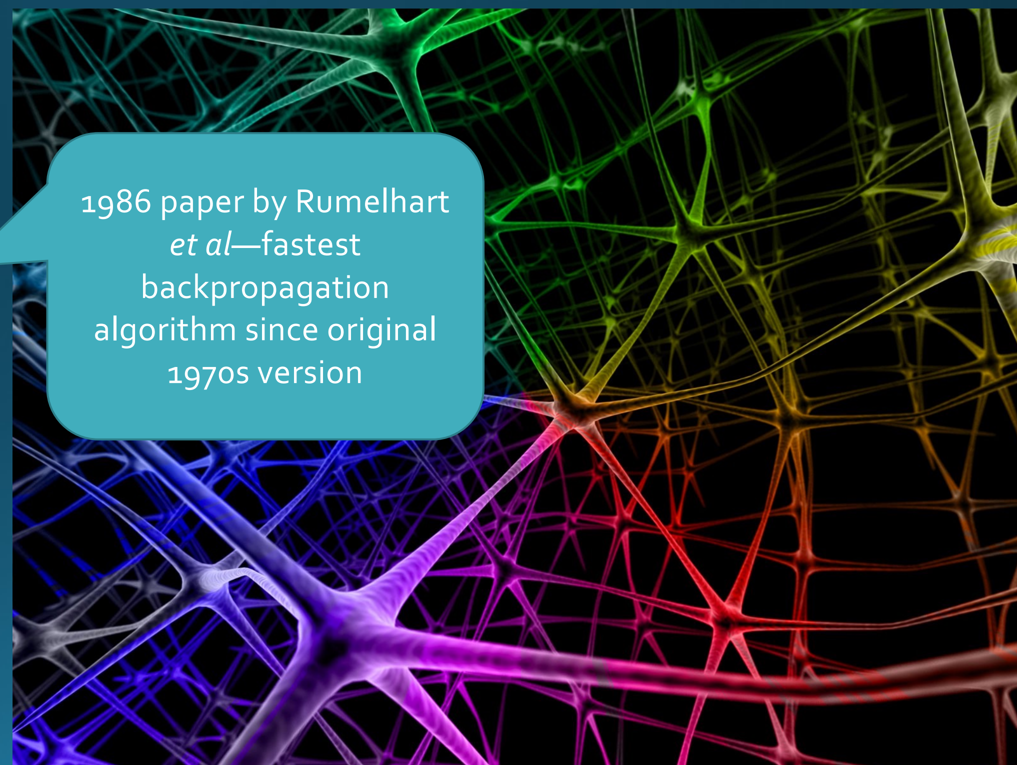
CSCI 4360/6360 Data Science II

Backpropagation

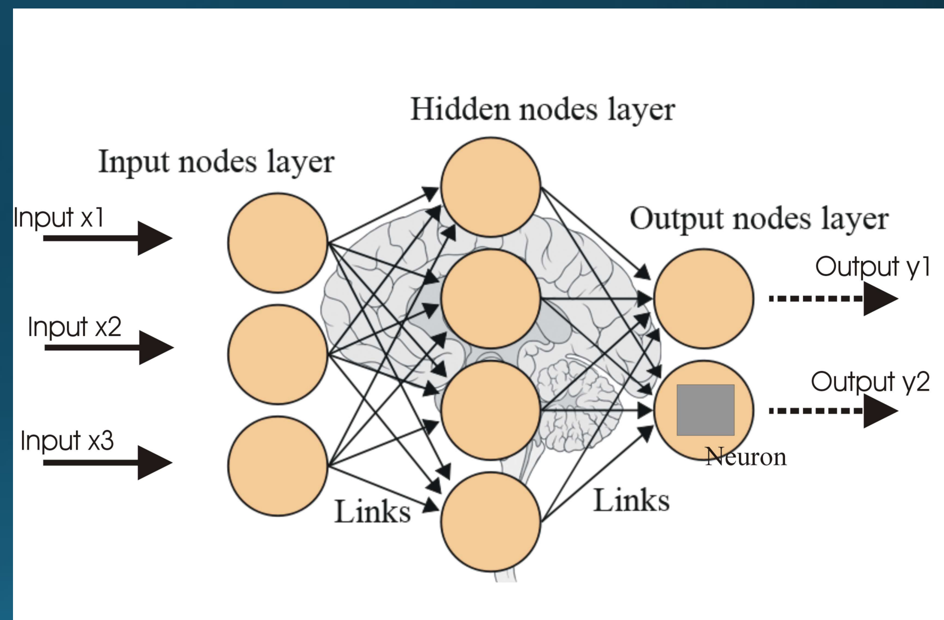
Artificial Neural Networks

- **Not a new concept!**
  - Roots as far back as 1940s work in unsuperivsed learning
  - Took off in 1980s and 1990s
  - Waned in 2000s
- "Biologically-inspired" computing
  - May or may not be true
- **Shift from rule-based to emergent learning**



Multilayer networks

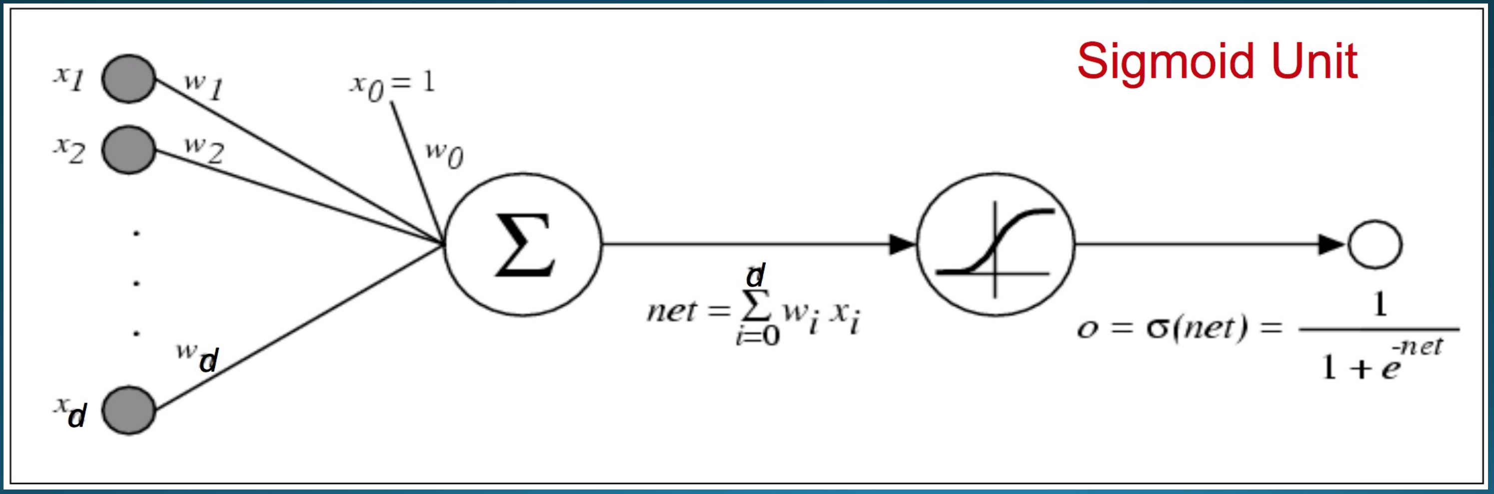
- Simplest case: classifier is a multilayer *network* of *logistic units*
- Each *unit* takes some inputs and produces one output using a logistic classifier
- Output of one unit can be the input of other units



LR as a Graph

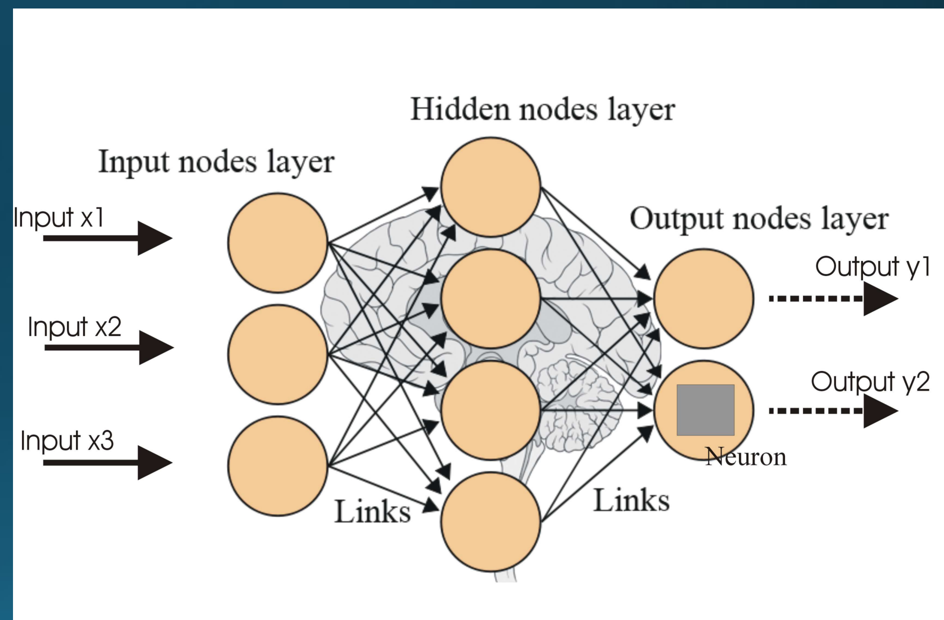
- Define output *o(x)* =

$$\sigma(w_0 + \sum_i w_i X_i) = \frac{1}{1 + \exp(-(w_0 + \sum_i w_i X_i))}$$



Multilayer networks

- Simplest case: classifier is a multilayer *network* of ~~*logistic*~~ *units* ***that perform some differentiable computation***
- Each *unit* takes some inputs and produces one output ~~using a logistic classifier~~
- Output of one unit can be the input of other units

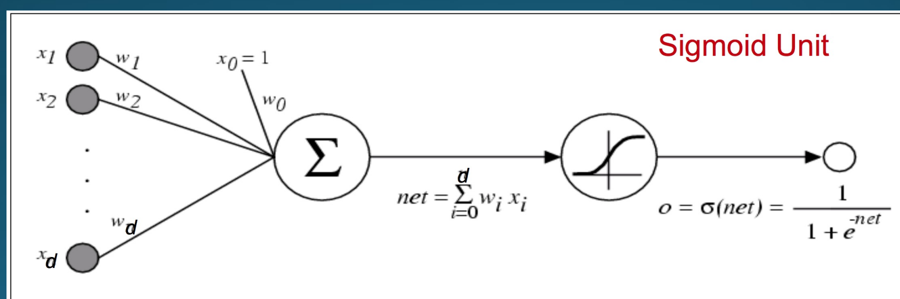


Learning a multilayer network

- Define a loss (simplest case: squared error)
  - But over a network of "units" that do simple computations

$$J_{X,y}(\vec{w}) = \sum_i (y^i - \hat{y}^i)^2$$

- Minimize loss with gradient descent
  - You can do this over complex networks if you can take the *gradient* of each unit: every computation is *differentiable*



ANNs in the 90s

- In the 90s: mostly 2-layer networks (or specialized “deep” networks that were hand-built)
- Worked well, but training was *slow*

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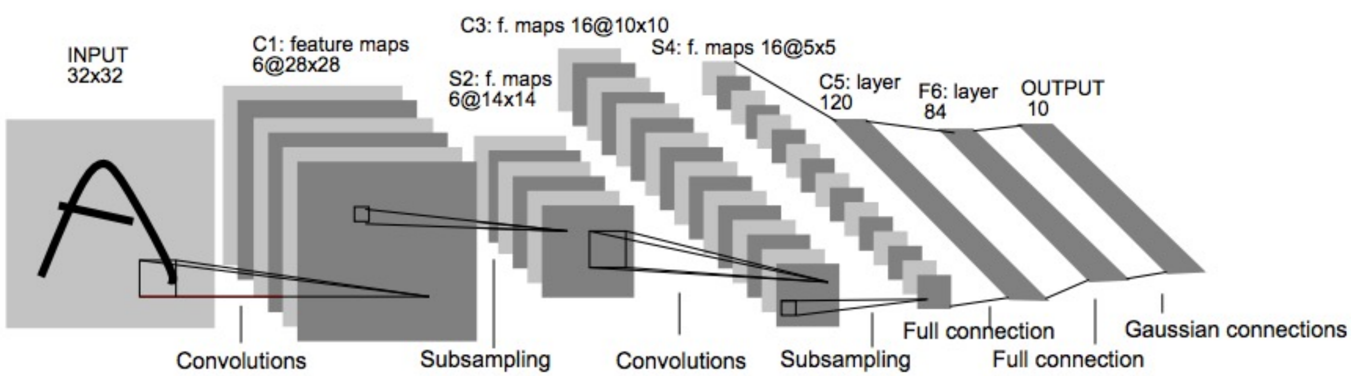
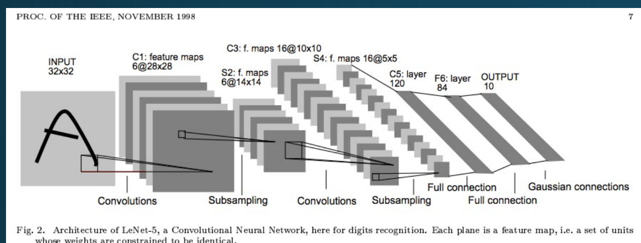
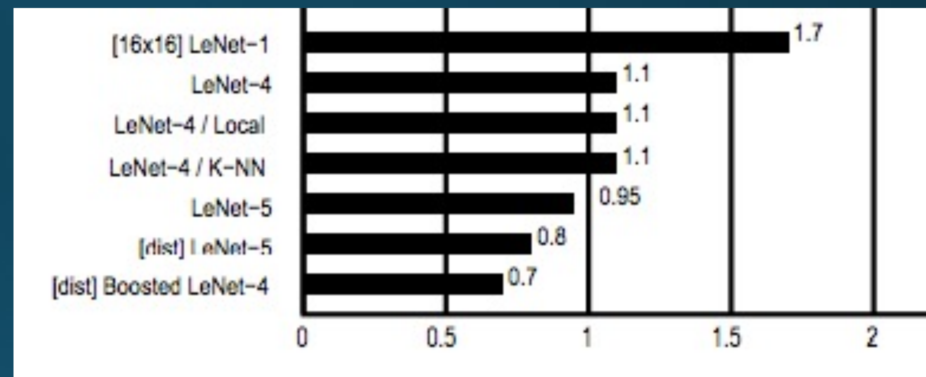


Fig. 2. Architecture of LeNet-5, a Convolutional Neural Network, here for digits recognition. Each plane is a feature map, i.e. a set of units whose weights are constrained to be identical.

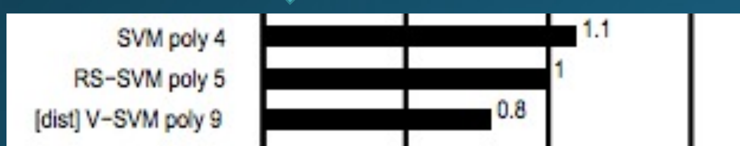
ANNs in the 90's





SVM with polynomial kernel: 98.9 - 99.2% accurate

Custom CNN: 98.3 - 99.3% accurate



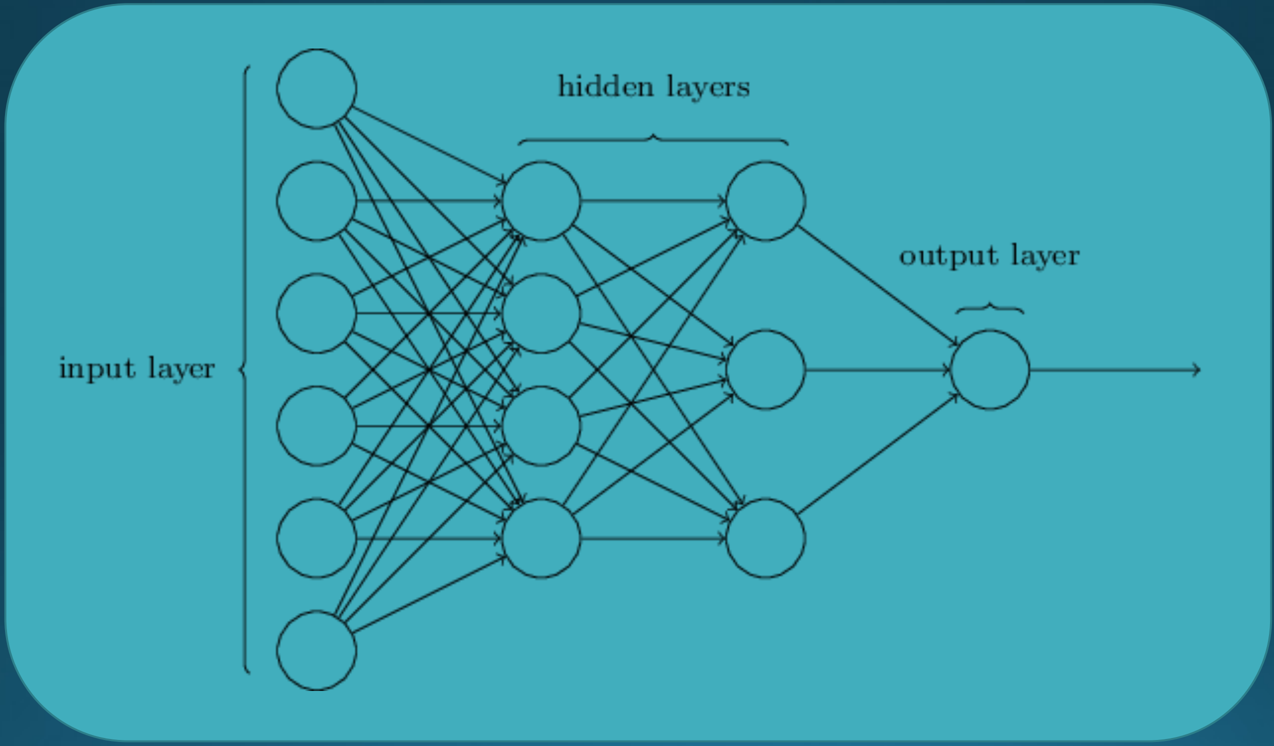
Nomenclature

- *Backpropagation:* refers **only** to the method for computing the gradient of a function
  - Is NOT specific to multilayer neural networks (in principle, can compute gradients for any function)
- *Stochastic gradient descent:* conducts learning using the derived gradient
  - Hence, you can run SGD on gradients you derive manually, or through backprop

Notation

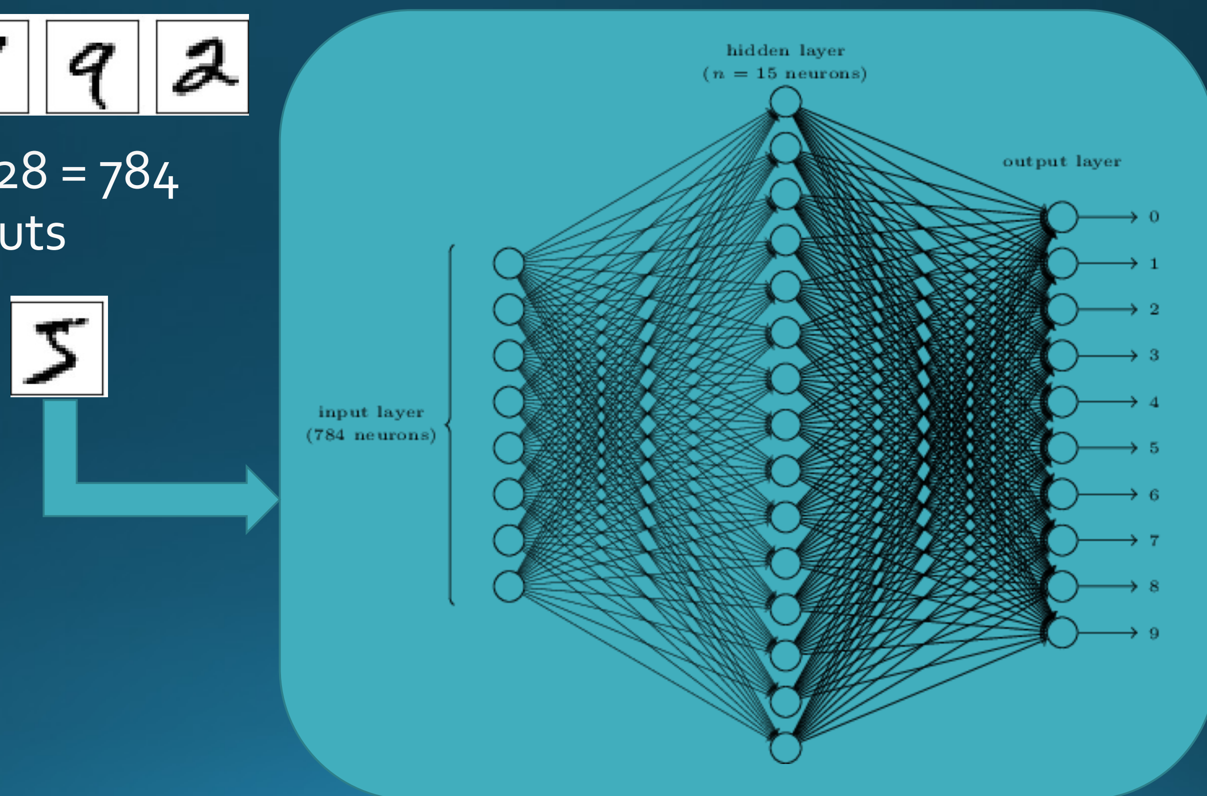
- “Borrowing” from
  - William Cohen at Carnegie Mellon (author of SSL algorithm you implemented in HW4)
  - Michael Nielson of http://neuralnetworksanddeeplearning.com/

Notation



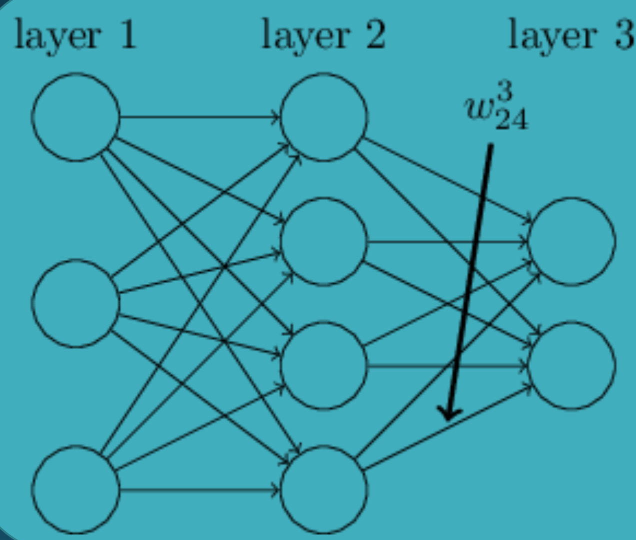
Notation

- Each digit is 28x28 = 784 dimensions / inputs



Notation

Vectorize: w^l is the weight matrix for layer l

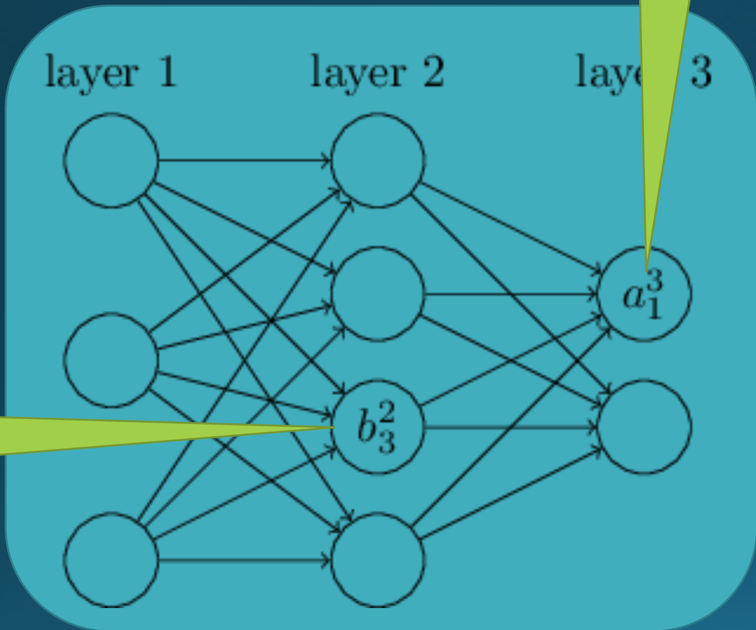


w^l_{jk} is the weight from the k^{th} neuron in the $(l-1)^{\text{th}}$ layer to the j^{th} neuron in the l^{th} layer

Notation

Activation

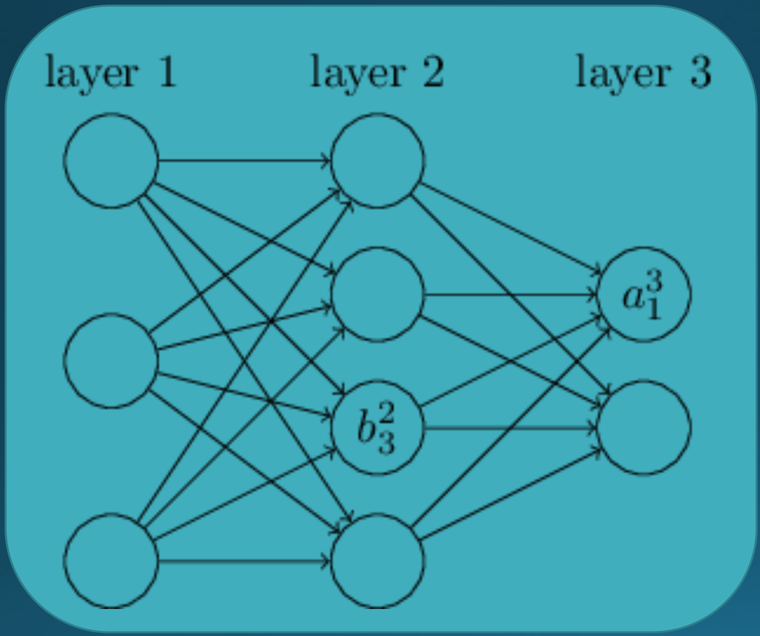
Vectorize: a^l and b^l are activations and bias matrices for layer l



Bias

$$a_j^l = \sigma\left(\sum_k w_{jk}^l a_k^{l-1} + b_j^l\right)$$

Notation

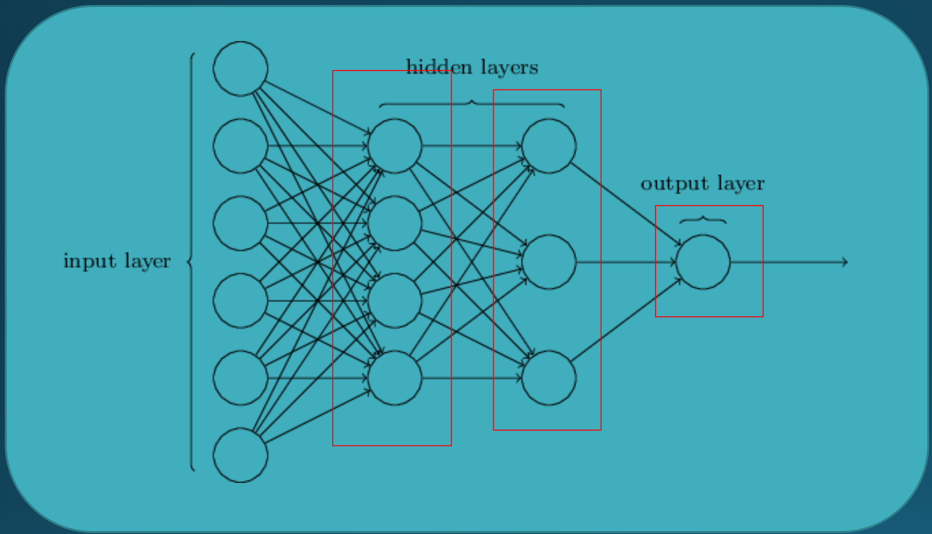


$$a_j^l = \sigma\left(\sum_k w_{jk}^l a_k^{l-1} + b_j^l\right)$$

$$a^l = \sigma(w^l a^{l-1} + b^l).$$

$$z^l \equiv w^l a^{l-1} + b^l$$

Computation is "feedforward"



for *l=1, 2, … L:*

$$a^l = \sigma(w^l a^{l-1} + b^l).$$

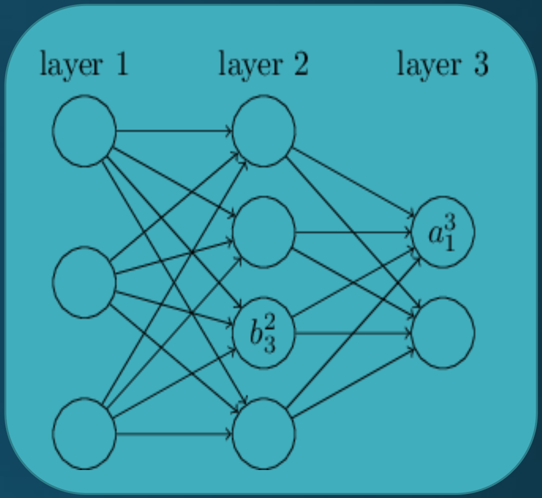
Notation

- Set up a cost function, *C*

$$C = \frac{1}{2n}\sum_x ||y(x) - a^L(x)||^2$$

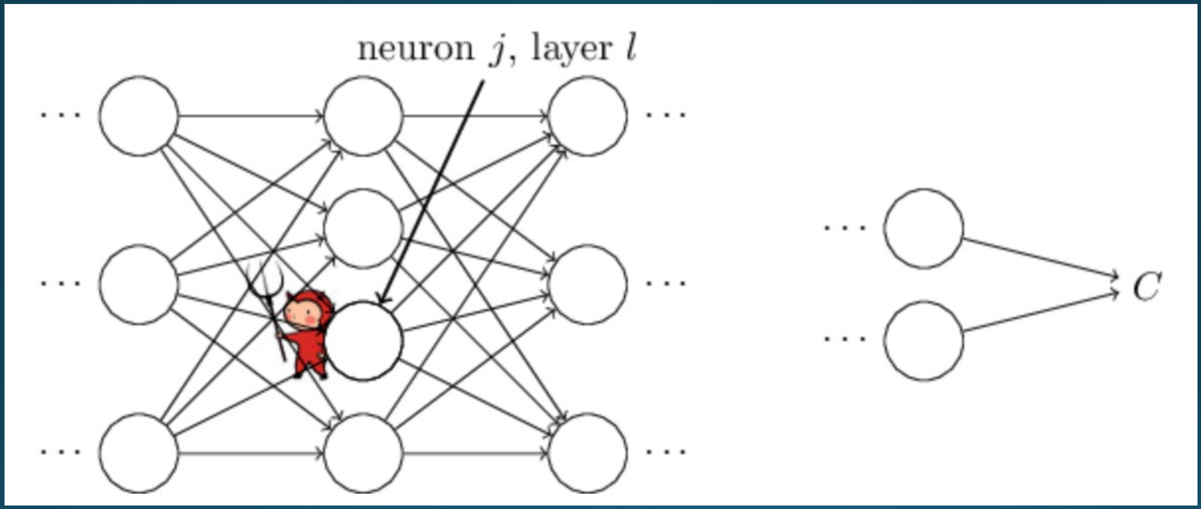
- Rewrite as an average

$$C = \frac{1}{n}\sum_x C_x \quad \text{where} \quad C_x = \frac{1}{2}||y - a^L||^2$$



Allows us to compute partial derivatives *dC_x/dw* and *dC_x/db* for single training examples, then recover *dC/dw* and *dC/db* by averaging over training examples.

Notation



Error in j^{th} neuron at the l^{th} layer

$$\delta_j^l \equiv \frac{\partial C}{\partial z_j^l}.$$

BackProp: last layer

$$\delta_j^L = \frac{\partial C}{\partial a_j^L} \sigma'(z_j^L).$$

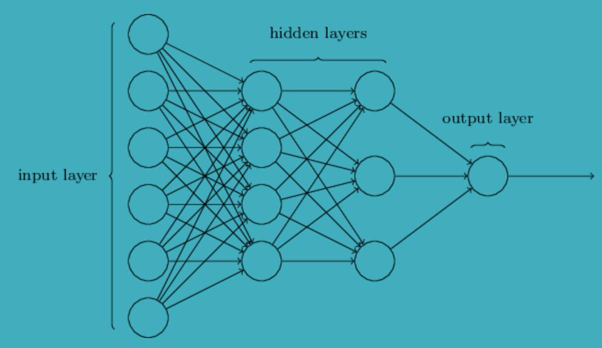
Matrix form:

$$\delta^L = \nabla_a C \odot \sigma'(z^L).$$

components are $\frac{\partial C}{\partial a_j^L}$

components are $\sigma'(z_j^L)$

The Hadamard Product: just element-wise multiplication



Level *l* for *l=1,…,L*
Matrix: w^l
Vectors:

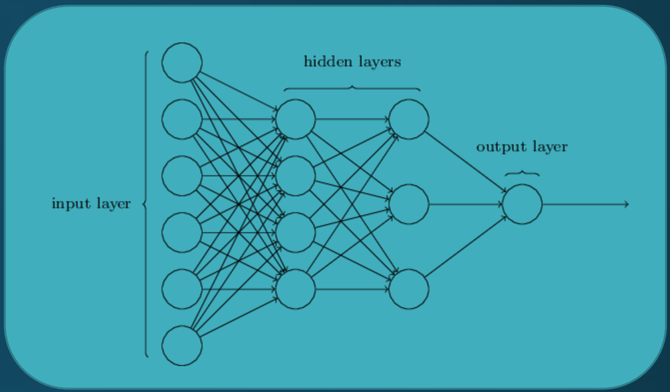
- bias b^l
- activation a^l
- pre-sigmoid activ: z^l
- target output *y*
- "local error" δ^l

BackProp: last layer

$$\delta_j^L = \frac{\partial C}{\partial a_j^L} \sigma'(z_j^L).$$

Matrix form for square loss:

$$\delta^L = (a^L - y) \odot \sigma'(z^L).$$



Level *l* for *l=1,…,L*
Matrix: w^l
Vectors:

- bias b^l
- activation a^l
- pre-sigmoid activ: z^l
- target output y
- "local error" δ^l

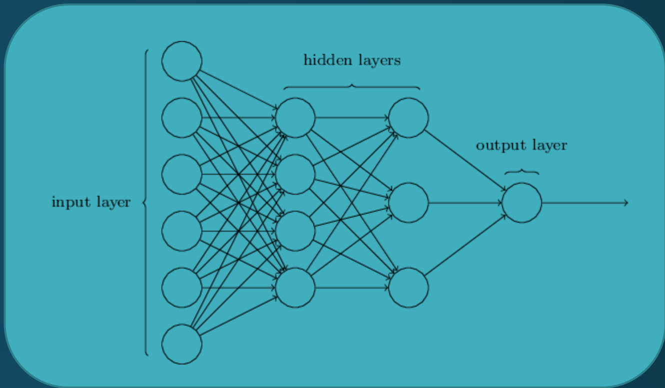
BackProp: error at level *l* in terms of error at level *l+1*

$$\delta^l = ((w^{l+1})^T \delta^{l+1}) \odot \sigma'(z^l)$$

which we can use to compute

$$\frac{\partial C}{\partial b^l_j} = \delta^l_j \quad \Rightarrow \quad \frac{\partial C}{\partial b} = \delta,$$

$$\frac{\partial C}{\partial w^l_{jk}} = a^{l-1}_k \delta^l_j. \quad \Rightarrow \quad \frac{\partial C}{\partial w} = a_{\rm in}\delta_{\rm out}$$



Level *l* for *l=1,…,L*
Matrix: w^l
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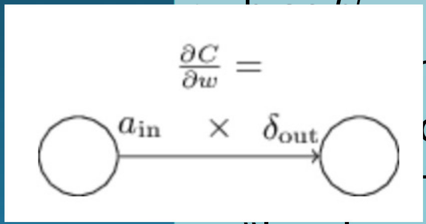


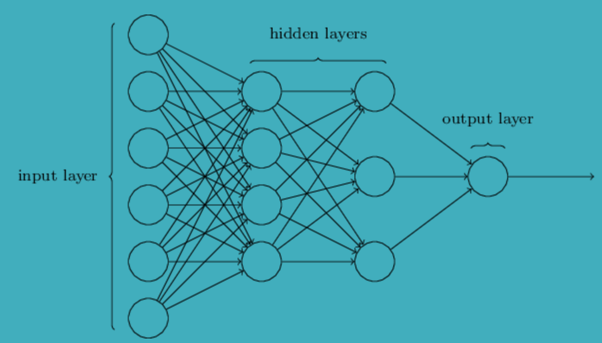
BackProp: Summary

$$\delta^L = \nabla_a C \odot \sigma'(z^L)$$

$$\delta^l = ((w^{l+1})^T \delta^{l+1}) \odot \sigma'(z^l)$$

$$\frac{\partial C}{\partial b^l_j} = \delta^l_j$$

$$\frac{\partial C}{\partial w^l_{jk}} = a^{l-1}_k \delta^l_j$$



Level *l* for *l=1,…,L*
Matrix: w^l
Vectors*:*
- bias b^l
- activation a^l
- pre-sigmoid activ: z^l
- target output *y*
- "local error" δ^l

Full Backpropagation

1. **Input x:** Set the corresponding activation a^1 for the input layer.

2. **Feedforward:** For each $l = 2, 3, \ldots, L$ compute $z^l = w^l a^{l-1} + b^l$ and $a^l = \sigma(z^l)$.

3. **Output error δ^L:** Compute the vector $\delta^L = \nabla_a C \odot \sigma'(z^L)$.

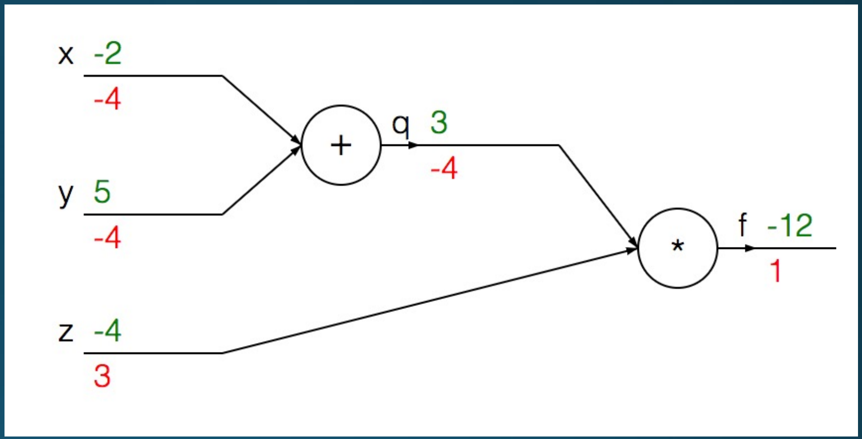
4. **Backpropagate the error:** For each $l = L-1, L-2, \ldots, 2$ compute $\delta^l = ((w^{l+1})^T \delta^{l+1}) \odot \sigma'(z^l)$.

5. **Output:** The gradient of the cost function is given by $\frac{\partial C}{\partial w^l_{jk}} = a^{l-1}_k \delta^l_j$ and $\frac{\partial C}{\partial b^l_j} = \delta^l_j$.

Use SGD to update the weights according to the gradients

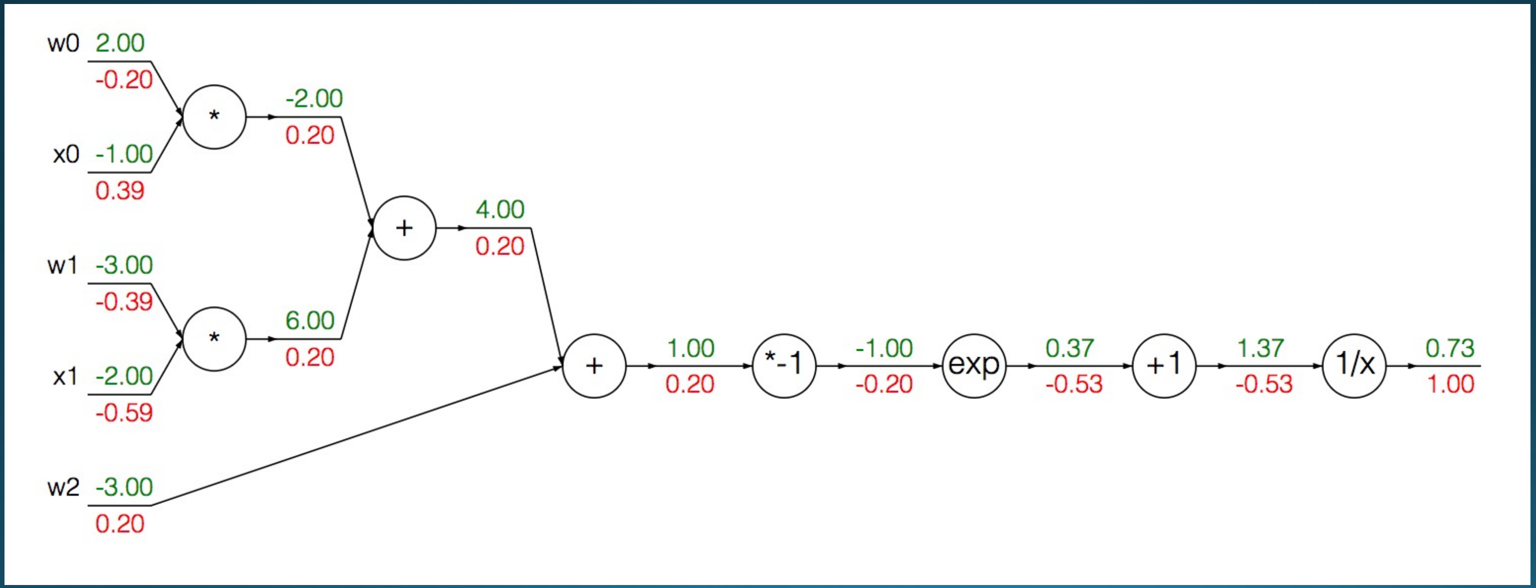
Example

- Simple equation
  $$f(x, y, z) = (x + y)z$$
- Some example inputs
  - x = -2
  - y = 5
  - z = -4



[slightly less simple] Example

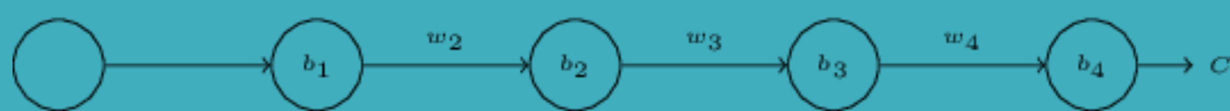
- 2D Logistic Regression, with a bias term $P(Y=1|X) = \frac{1}{1+\exp(-(w_0 + \sum_i w_i X_i))}$



Weight updates for multilayer ANN

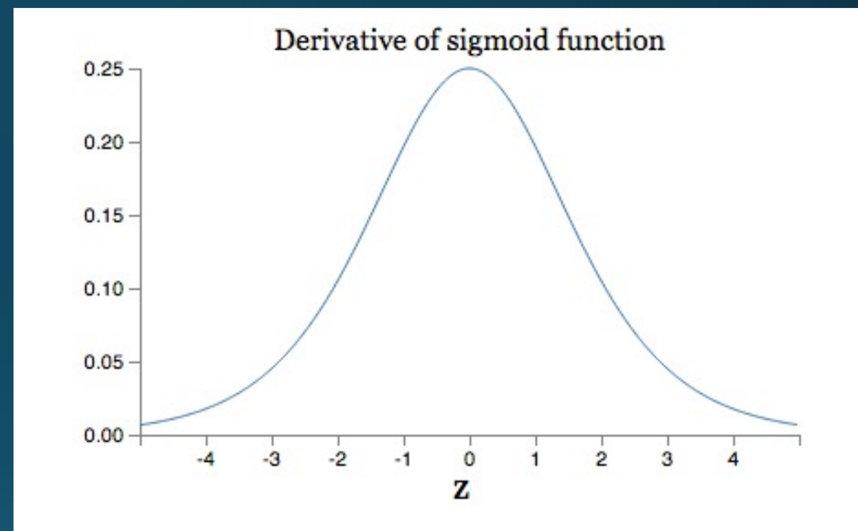
- For nodes *k* in output layer *L*: $$\delta_k^L = (t_k - a_k)a_k(1 - a_k)$$
- For nodes *j* in hidden layer *h*: $$\delta_j^h = \sum_k (\delta_j^{h+1} w_{kj})a_j(1 - a_j)$$
- What happens as the layers get further and further from the output layer?

$$\frac{\partial C}{\partial b_1} = \sigma'(z_1) \times w_2 \times \sigma'(z_2) \times w_3 \times \sigma'(z_3) \times w_4 \times \sigma'(z_4) \times \frac{\partial C}{\partial a_4}$$



Gradients are unstable

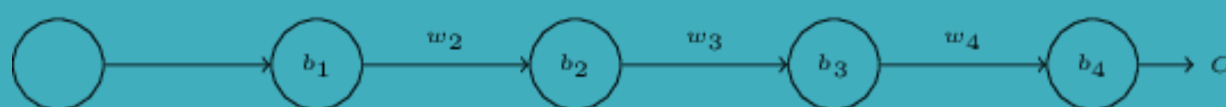
Max at 1/4



- If weights are usually < 1, and we are multiplying by many, *many* such numbers…

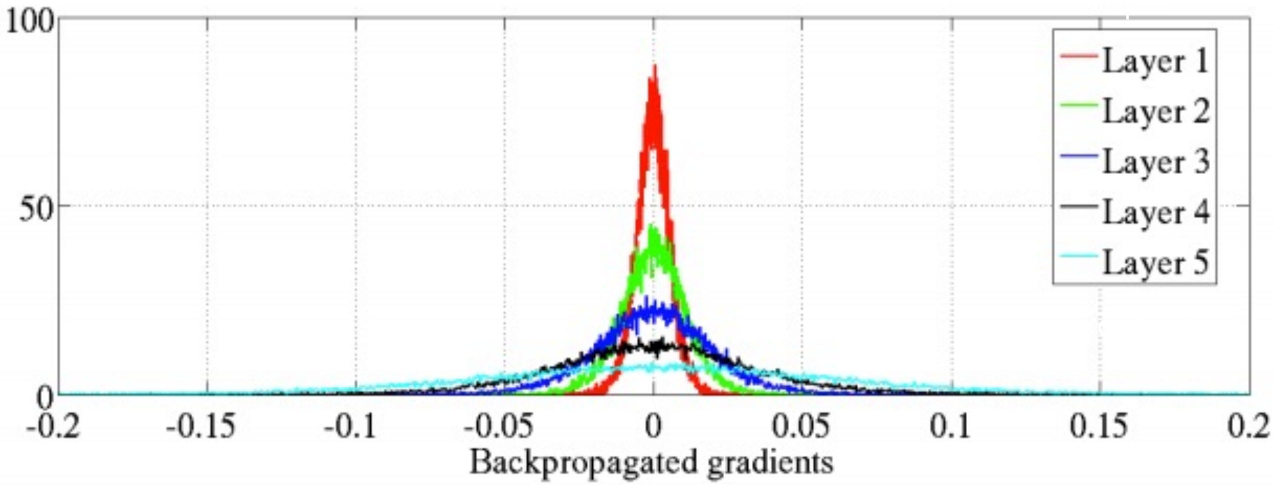
The Amazing Vanishing Gradient!

$$\frac{\partial C}{\partial b_1} = \sigma'(z_1) \times w_2 \times \sigma'(z_2) \times w_3 \times \sigma'(z_3) \times w_4 \times \sigma'(z_4) \times \frac{\partial C}{\partial a_4}$$



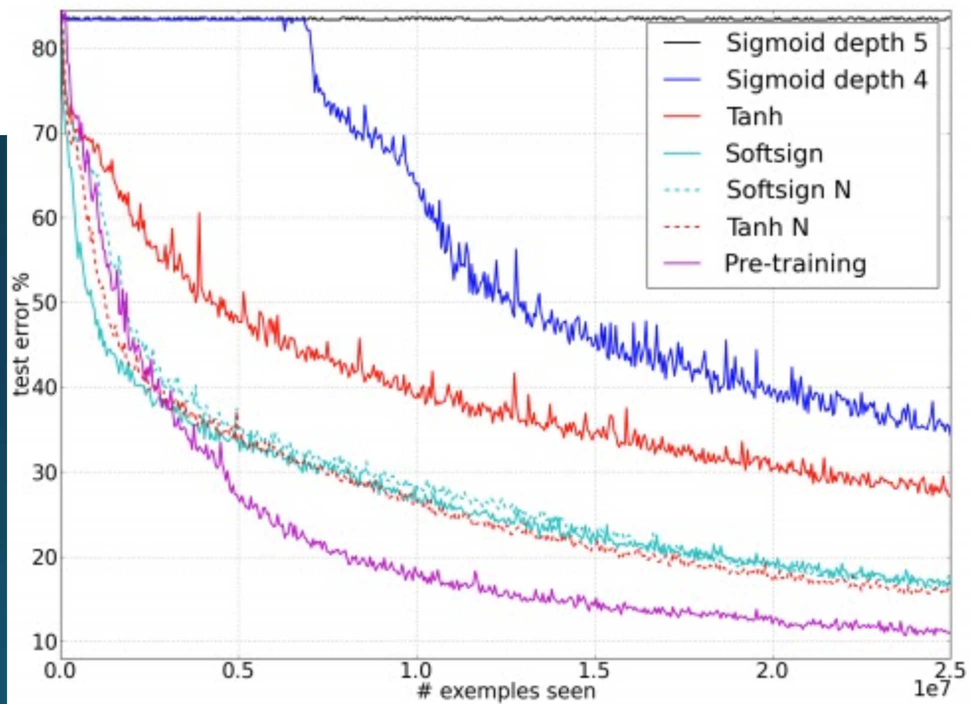
Understanding the difficulty of training deep feedforward neural networks

Xavier Glorot **Yoshua Bengio**
DIRO, Université de Montréal, Montréal, Québec, Canada

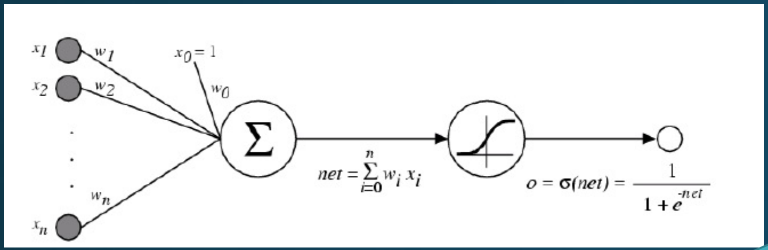


Histogram of gradients in a 5-layer network for an artificial image recognition task

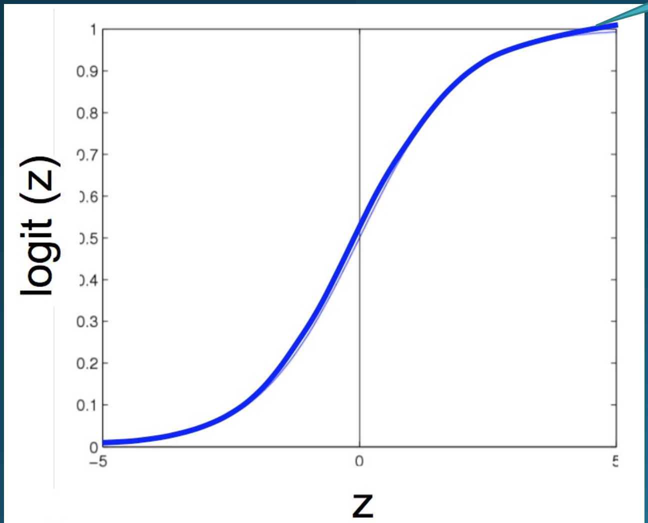
Understanding the difficulty of training deep feedforward neural networks

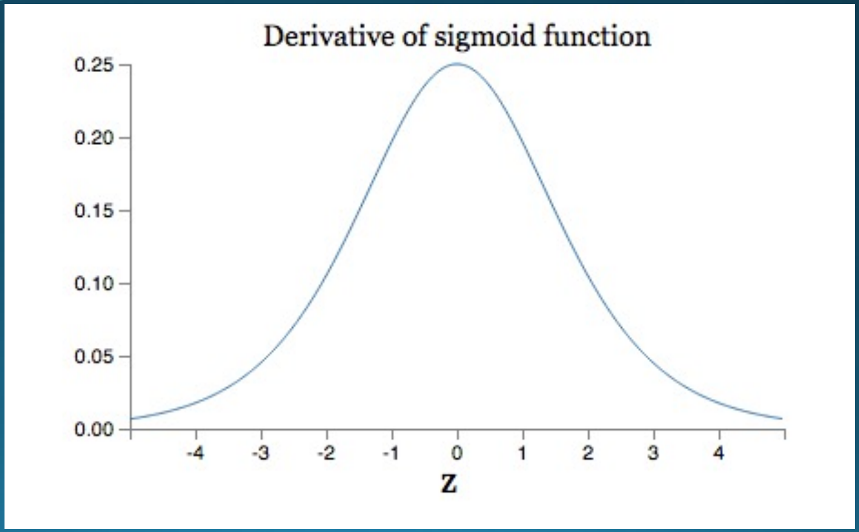


It's easy for sigmoid units to saturate



Learning rate approaches zero, and neuron gets "stuck"





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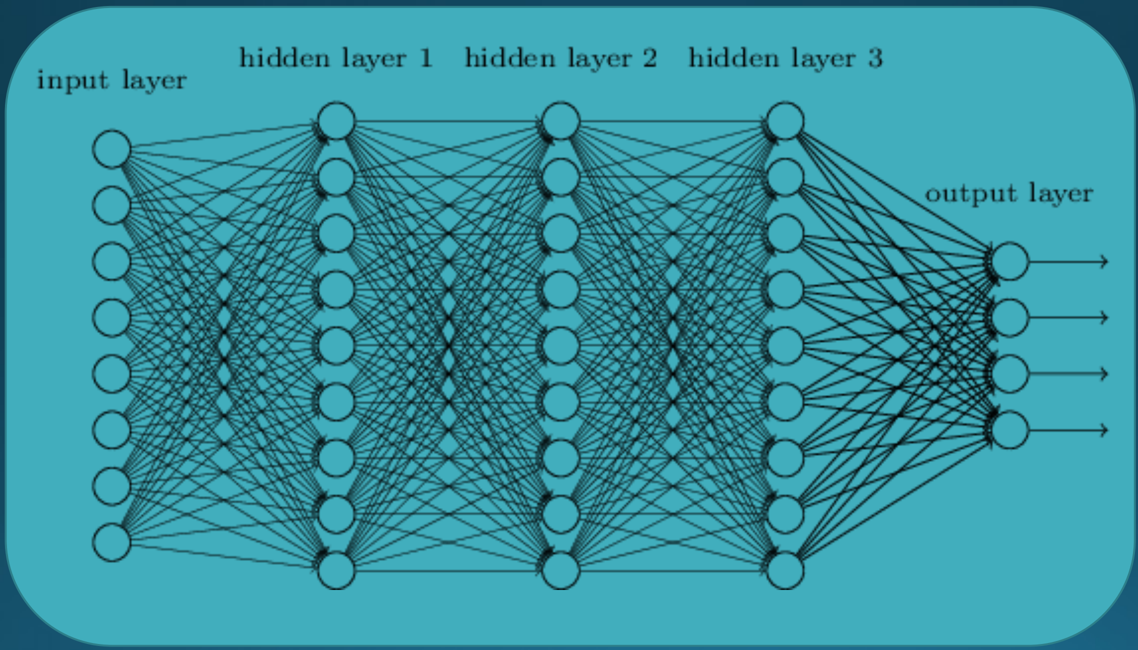
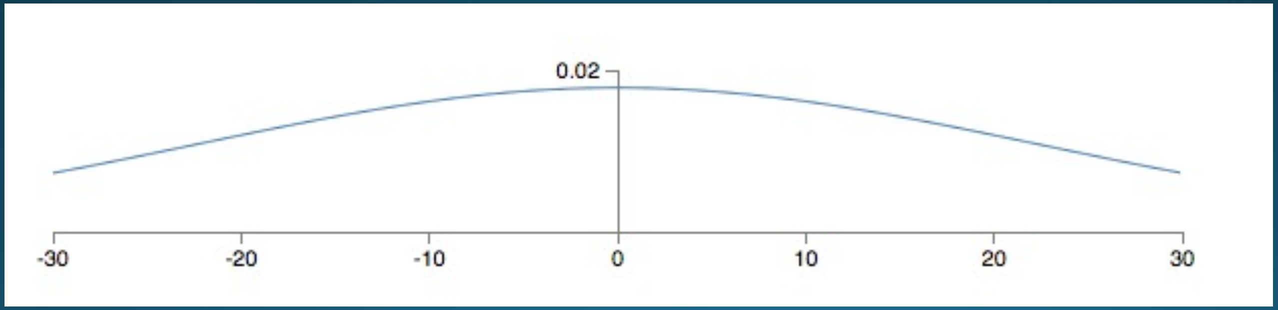


It’s easy for sigmoid units to saturate

- If there are 500 non-zero inputs initialized with a Gaussian ~N(0,1) then the SD is $\sqrt{500} \approx 22.4$



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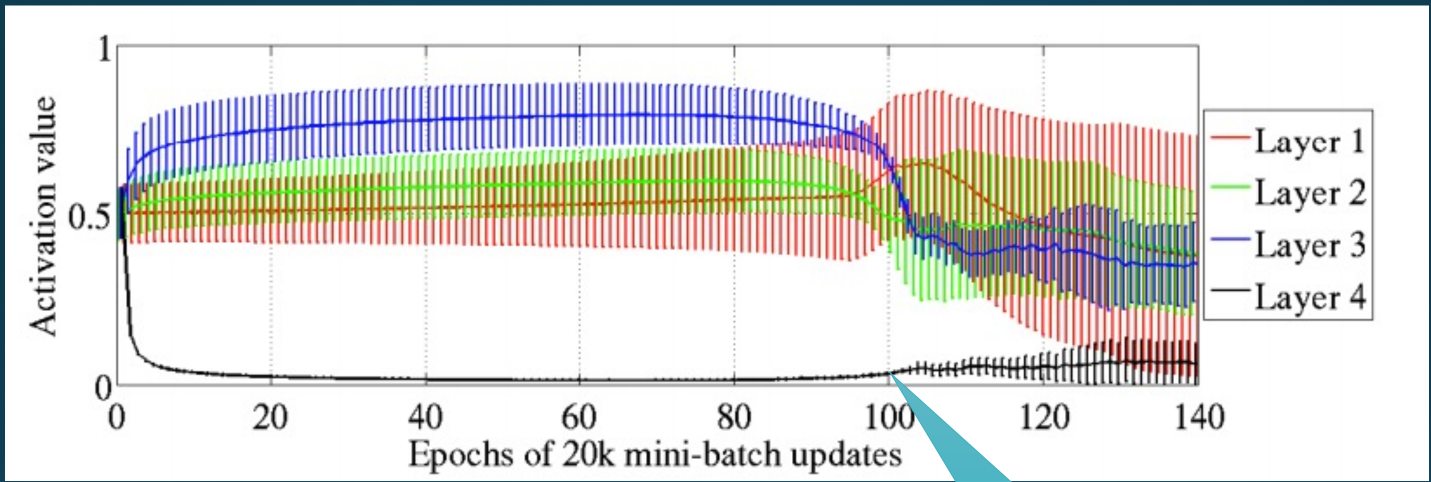


- Saturation visualization from Glorot & Bengio 2010 -- using a smarter initialization scheme

Bottom layer still stuck for first 100 epochs

What's Different About Modern ANNs?

Some key differences

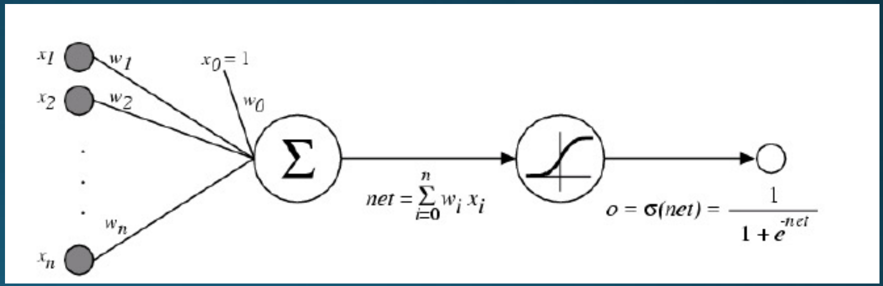
- **Use of softmax and entropic loss instead of quadratic loss**
- Use of alternate non-linearities
  - reLU and hyperbolic tangent
- Better understanding of weight initialization
- Data augmentation
  - Especially for image data
- Ability to explore architectures rapidly

Cross-entropy loss

$$C = -\frac{1}{n}\sum_x [y \ln a + (1-y)\ln(1-a)]$$

$$\frac{\partial C}{\partial w_j} = \frac{1}{n}\sum_x x_j(\sigma(z) - y)$$

$$\frac{\partial C}{\partial w} = \sigma(z) - y$$



Cross-entropy loss

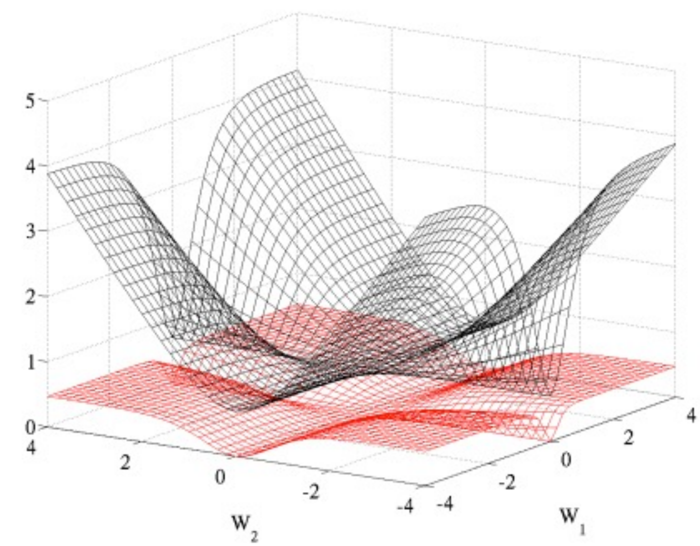
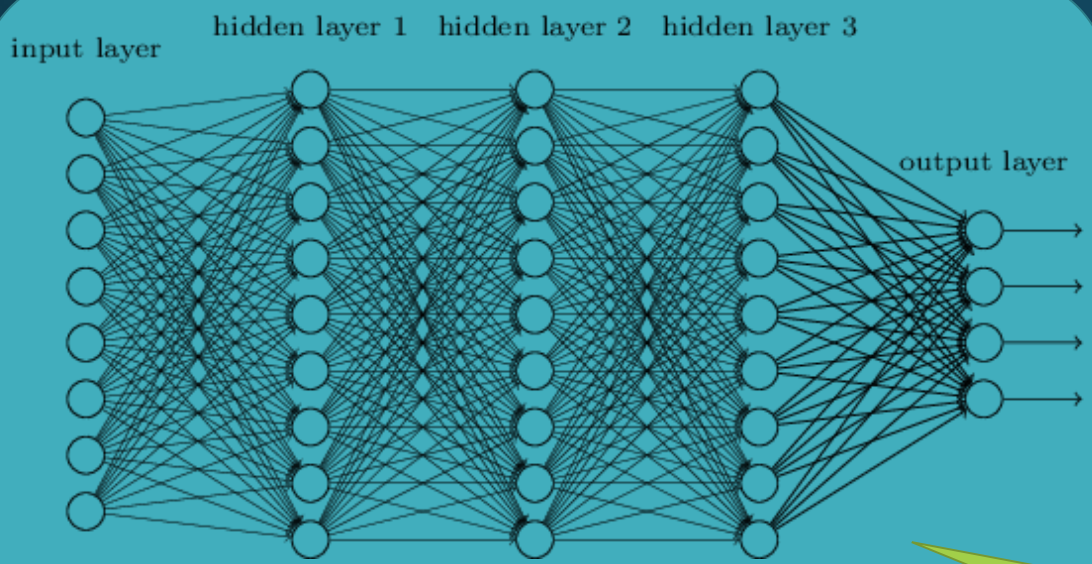


Figure 5: *Cross entropy (black, surface on top) and quadratic (red, bottom surface) cost as a function of two weights (one at each layer) of a network with two layers, W_1 respectively on the first layer and W_2 on the second, output layer.*

Softmax output layer

Cross-entropy loss after a softmax layer gives a very simple, numerically stable gradient: (y - a^L)



$$a_j^L = \frac{e^{z_j^L}}{\sum_k e^{z_k^L}}$$

$\Delta w_{ij} = (y_i - z_i) y_j$

Network outputs a probability distribution!

Some key differences

- Use of softmax and entropic loss instead of quadratic loss.
  - **Often learning is faster and more stable as well as getting better accuracies in the limit**
- Use of alternate non-linearities
- Better understanding of weight initialization
- Data augmentation
  - Especially for image data
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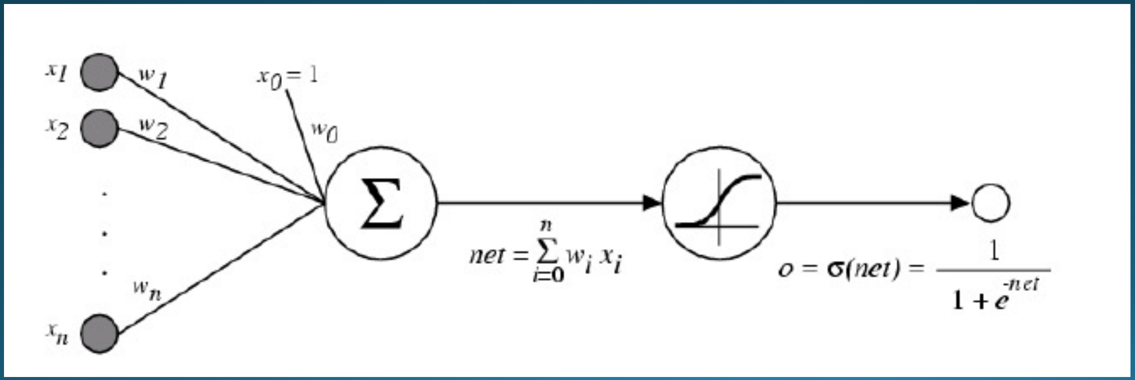
Alternative non-linearities

- Changes so far
  - Changed the **loss** from square error to cross-entropy (no effect at test time)
  - Proposed adding another output layer (softmax)
- A new change: modifying the nonlinearity
  - The logistic is not widely used in modern ANNs



Alternative non-linearities

- A new change: modifying the nonlinearity
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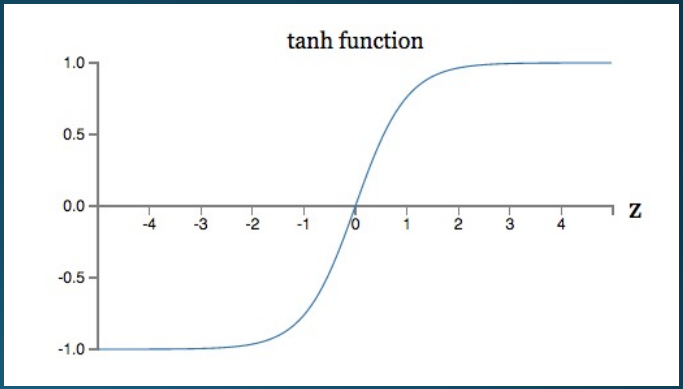
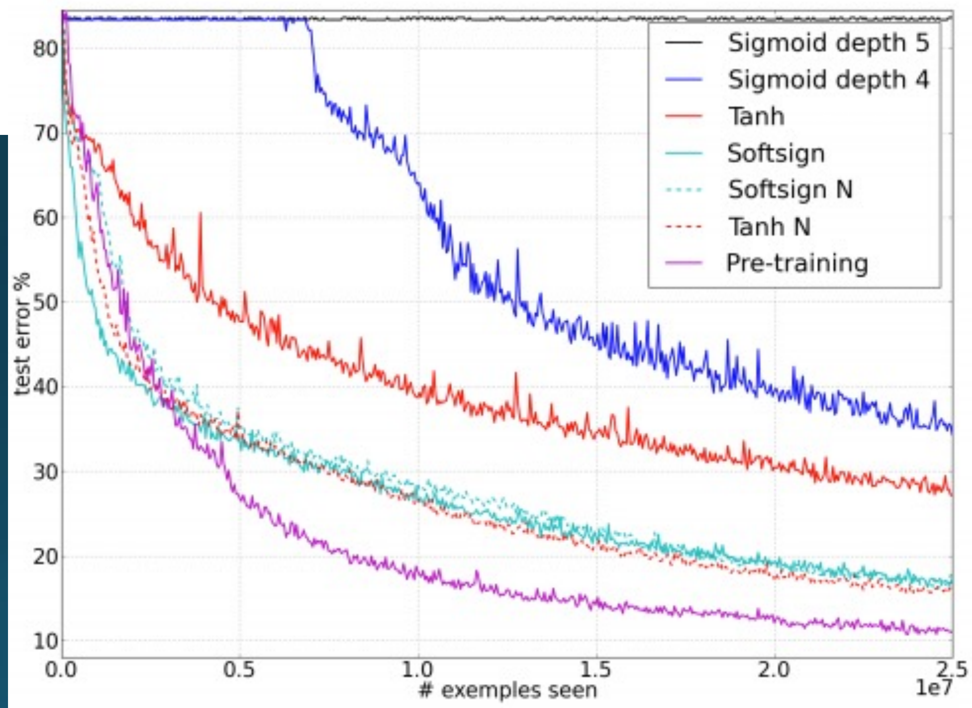
- Alternative #1: tanh
  - Like logistic, but shifted to range [-1, +1]



Understanding the difficulty of training deep feedforward neural networks



Alternative non-linearities

- A new change: modifying the nonlinearity
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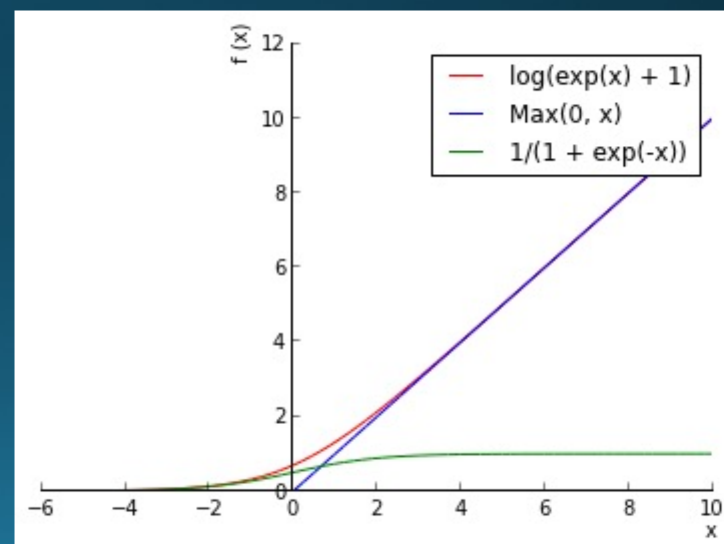
- Alternative #1: tanh
  - Like logistic, but shifted to range [-1, +1]
- Alternative #2: ReLU
  - Linear with cut-off at zero
- Alternative #2.5: "Soft" ReLU
  - Doesn't saturate (at one end)
  - Sparsifies outputs
  - Helps with vanishing gradient



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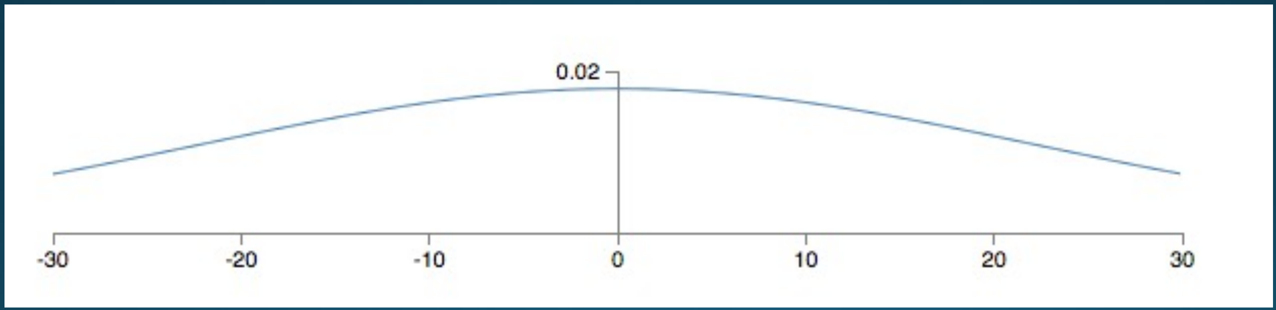
It’s easy for sigmoid units to saturate

- If there are 500 non-zero inputs initialized with a Gaussian ~N(0,1) then the SD is $\sqrt{500} \approx 22.4$



- Common heuristics for initializing weights

$$N\left(0, \frac{1}{\sqrt{\#\text{ of inputs}}}\right) \quad U\left(\frac{-1}{\sqrt{\#\text{ of inputs}}}, \frac{1}{\sqrt{\#\text{ of inputs}}}\right)$$

Initializing to avoid saturation

- In Glorot and Bengio (2010) they suggest weights if level *j* (with n_j inputs) from

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

TYPE	Shapeset	MNIST	CIFAR-10	ImageNet
Softsign	**16.27**	**1.64**	55.78	**69.14**
Softsign N	**16.06**	**1.72**	**53.8**	**68.13**
Tanh	27.15	**1.76**	55.9	70.58
Tanh N	**15.60**	**1.64**	**52.92**	**68.57**

First breakthrough deep learning results were based on clever pre-training initialization schemes, where deep networks were seeded with weights learned from unsupervised strategies

This is not always the solution – but good initialization is very important for deep nets!

Summary

- Backpropagation makes training deep neural networks possible
  - Known since 1970s, understood since 1980s, used since 1990s, tractable since 2010s
- Feed-forward versus backward propagation
  - Feed-forward evaluates the network's current configuration, J()
  - Backpropagation assigns error in J() to individual weights
- Each layer considered a function of its inputs
  - Differentiable activation functions strung together
  - Chain rule of calculus
- Modern deep architectures made possible due to logistical tweaks
  - Vanishing / Exploding gradient and new activation functions

References

- "A gentle introduction to backpropagation", http://numericinsight.com/uploads/A_Gentle_Introduction_to_Backpropagation.pdf
- "Deep Feed-Forward Networks", Chapter 6, *Deep Learning Book*, http://www.deeplearningbook.org/contents/mlp.html
- "Backpropagation, Intuitions", CS231n "CNNs for Visual Recognition", https://cs231n.github.io/optimization-2/
- "How the Backpropagation Algorithm works", Chapter 2, *Neural Networks and Deep Learning*, http://neuralnetworksanddeeplearning.com/