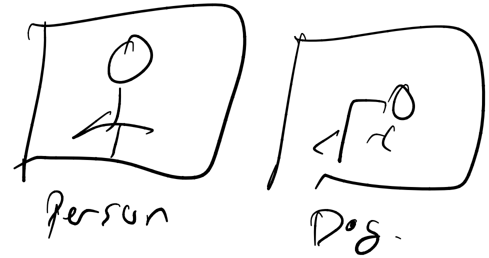
Neural Networks

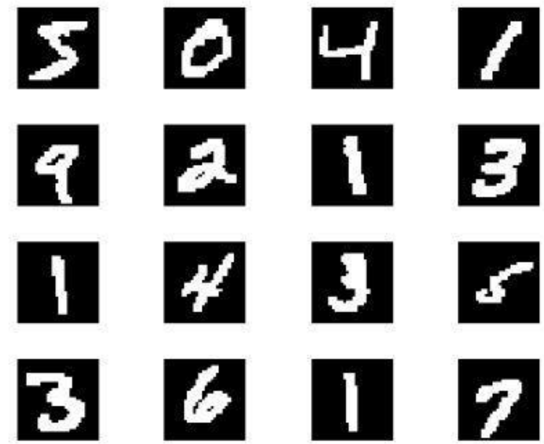
Rishabh Iyer
University of Texas at Dallas

Thanks to Nick Rouzzi for sharing these slides

Handwritten Digit Recognition

- Given a collection of handwritten digits and their corresponding labels, we'd like to be able to correctly classify handwritten digits
  - A simple algorithmic technique can solve this problem with 95% accuracy
    - State-of-the-art methods can achieve near 99% accuracy (you've probably seen these in action if you've deposited a check recently)





10 Class

Digits from the MNIST data set

Natural Images → LR (20-40%, Random 10%)
[CIFAR-10] DNN (≈ 95%+)

Pre Deep learning (2012 –)

Input → Black box feat Ext → ML SVM/LR/.. → Classify

Image
speech
text
⋮

80-90%

Vision / Speech / NLP

↑ CIFAR-10
[70-80%]

Input → NN Arch. → Classify ← CIFAR-10
[95+%]

[95% Vision papers use Deep Learning]

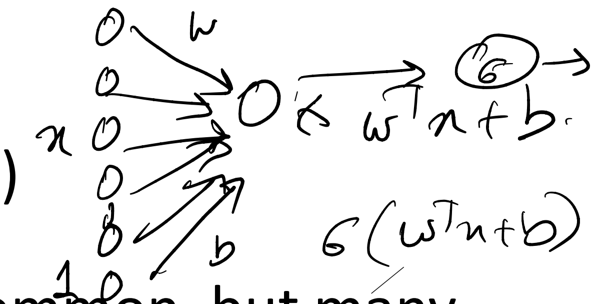
Neural Networks

- The basis of neural networks was developed in the 1940s -1960s
  - The idea was to build mathematical models that might "compute" in the same way that neurons in the brain do
  - As a result, neural networks are biologically inspired, though many of the algorithms developed for them are not biologically plausible
  - Perform surprisingly well for the handwritten digit recognition task (and many others)

[Vision / NLP / Speech].

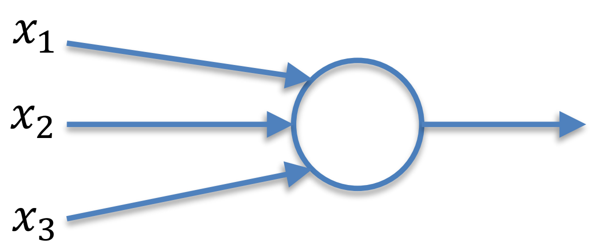
Neural Networks

- Neural networks consist of a collection of artificial neurons
- There are different types of neuron models that are commonly studied
  - The perceptron (one of the first studied)
  - The sigmoid neuron (one of the most common, but many more)
  - Rectified linear units
- A neural network is a directed graph consisting of a collection of neurons (the nodes), directed edges (each with an associated weight), and a collection of fixed binary inputs



The Perceptron

- A perceptron is an artificial neuron that takes a collection of binary inputs and produces a binary output
  - The output of the perceptron is determined by summing up the weighted inputs and thresholding the result: if the weighted sum is larger than the threshold, the output is one (and zero otherwise)



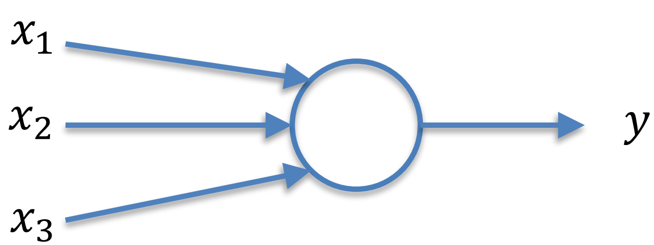
$y = \mathbb{1}(w^T x + b > 0)$

$$y = \begin{cases} 1 & w_1x_1 + w_2x_2 + w_3x_3 > threshold \\ 0 & otherwise \end{cases}$$

$w^T x + b > 0$

Perceptrons

- Perceptrons are usually expressed in terms of a collection of input weights and a bias b (which is the negative threshold)

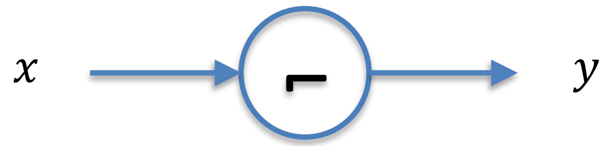


$$y = \begin{cases} 1 & w_1x_1 + w_2x_2 + w_3x_3 + b > 0 \\ 0 & otherwise \end{cases}$$

- A single node perceptron is just a linear classifier

- This is actually where the “perceptron algorithm” comes from

Perceptron for NOT



- Choose $w = -1$, threshold $= -.5$

- $y = \begin{cases} 1 & -x > -.5 \\ 0 & -x \leq -.5 \end{cases}$

$x < 0.5$

$x \geq 0.5$

$w^T x + b$

$-x + 0.5 > 0$

$w = -1$

$b = 0.5$

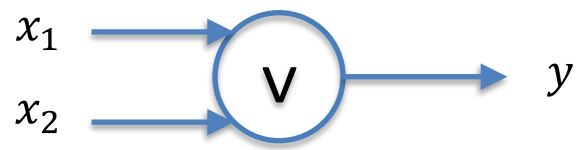
Perceptron for OR

$$x_1, x_2 \rightarrow \text{OR} \rightarrow y$$

$$x_1 + x_2 > 0$$

$$\mathbb{I}(w^T x + b > 0)$$

Perceptron for OR



$y = x_1$ OR x_2

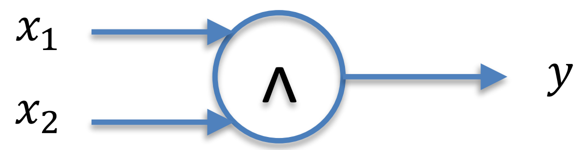
- Choose $w_1 = w_2 = 1$, threshold $= 0$

- $y = \begin{cases} 1 & x_1 + x_2 > 0 \\ 0 & x_1 + x_2 \le 0 \end{cases}$

$w = \begin{bmatrix} 1 \\ 1 \end{bmatrix}, \ b = 0$

Perceptron for AND

Perceptron for AND



$y = x_1$ AND x_2.

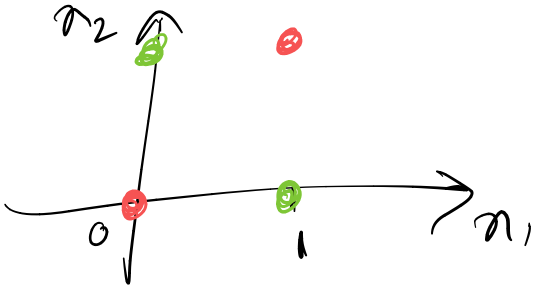
x_1	x_2	y
0	0	0
0	1	0
1	0	0
1	1	1

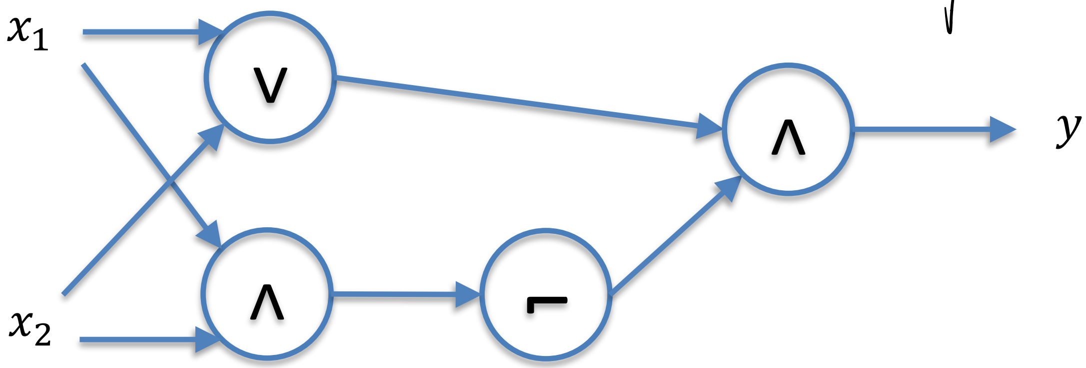
- Choose $w_1 = w_2 = 1$, threshold $= 1.5$
- $y = \begin{cases} 1 & x_1 + x_2 > 1.5 \\ 0 & x_1 + x_2 \le 1.5 \end{cases}$

Perceptron for XOR

Perceptron for XOR

- Need more than one perceptron!





- Weights for incoming edges are chosen as before

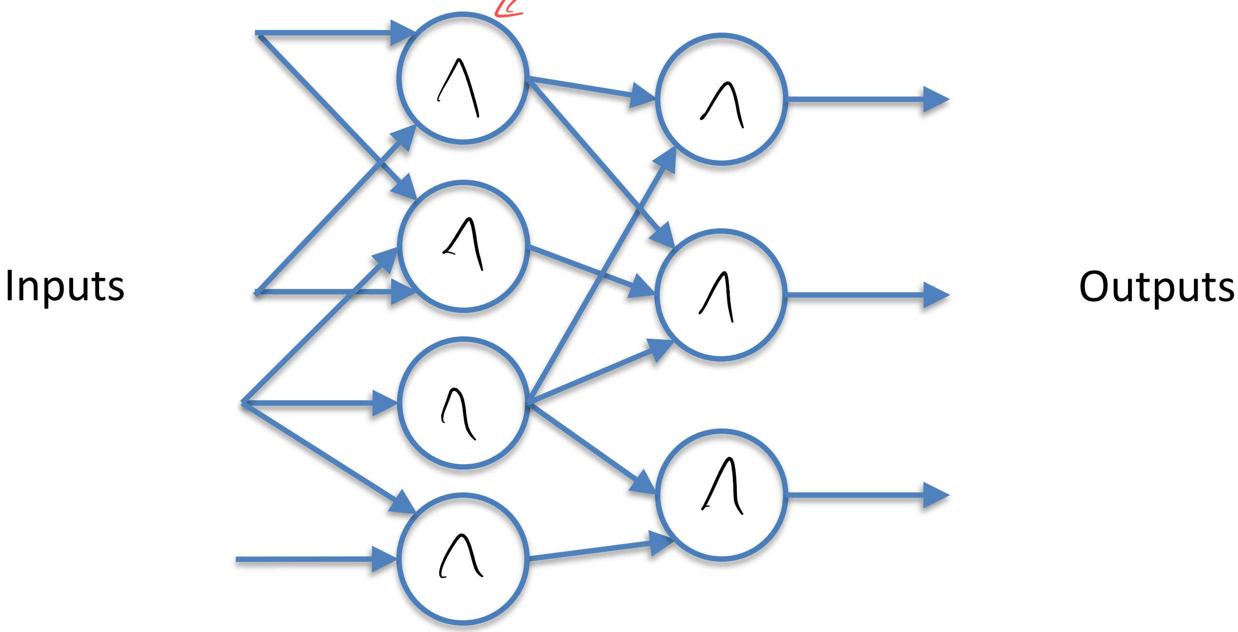
- Networks of perceptrons can encode any circuit!

Neural Networks

- Gluing a bunch of perceptrons together gives us a neural network

- In general, neural nets have a collection of binary inputs and a collection of binary outputs

$1(w^T x + b > 0)$

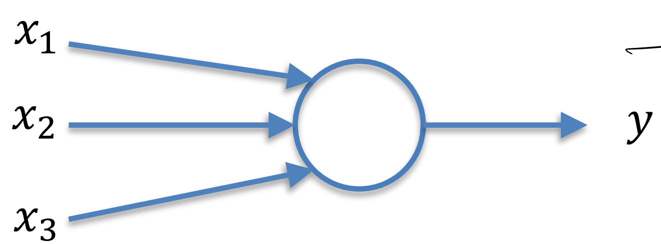


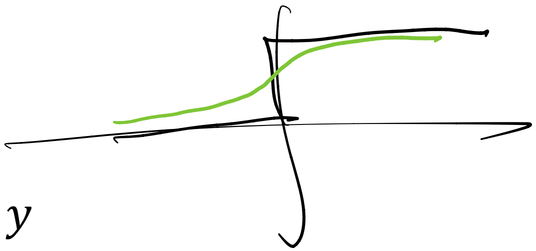
Beyond Perceptrons

- Given a collection of input-output pairs, we'd like to learn the weights of the neural network so that we can correctly predict the output of an unseen input
  - We could try learning via gradient descent (e.g., by minimizing the Hamming loss)
    - This approach doesn't work so well: small changes in the weights can cause dramatic changes in the output
    - This is a consequence of the discontinuity of sharp thresholding (same problem we saw with perceptron alg.)

The Sigmoid Neuron [Logistic Regression]

- A sigmoid neuron is an artificial neuron that takes a collection of real inputs and produces an output in the interval [0,1]
  - The output is determined by summing up the weighted inputs plus the bias and applying the sigmoid function to the result





$$y = \sigma(w_1x_1 + w_2x_2 + w_3x_3 + b)$$

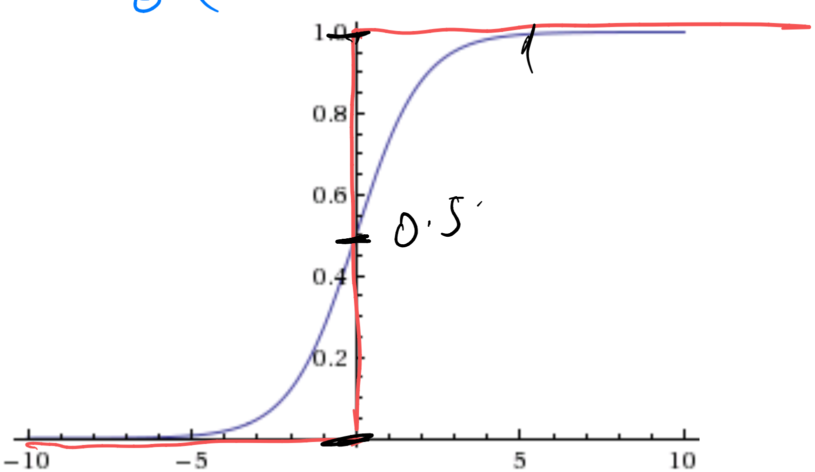
where σ is the sigmoid function

The Sigmoid Function

- The sigmoid function is a continuous function that approximates a step function

$= 1(w^T x + b)$

$= \sigma(w^T x + b)$



$w^T x + b$

$$\underbrace{\sigma(z)} = \frac{1}{1 + e^{-z}}$$

$$p(y=1|x) = \sigma(w^T x + b)$$

$$= \frac{1}{1 + e^{-(w^T x + b)}}$$

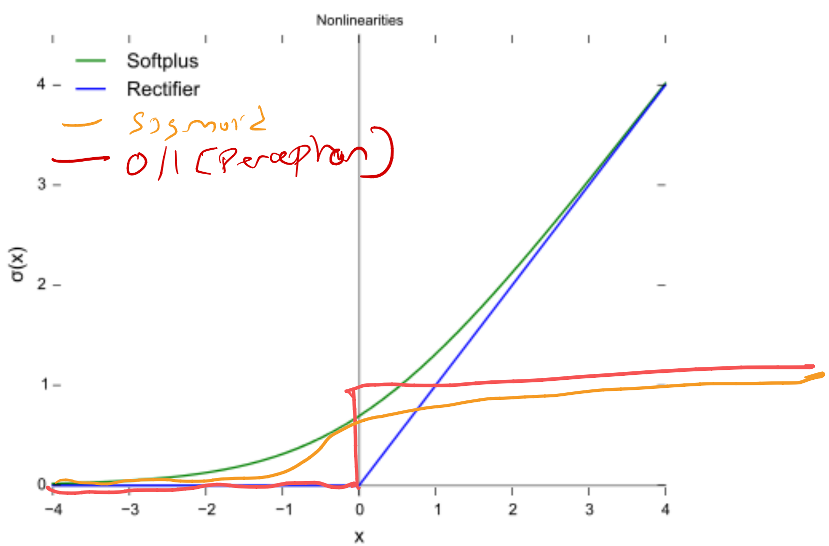
$$p(y=1|x) > 0.5$$

$$\Rightarrow w^T x + b > 0$$

Rectified Linear Units ← Perceptron Loss fn

- The sigmoid neuron approximates a step function as a smooth function

- The relu is given by $\max(0, x)$ which can be approximated as a smooth continuous function $\ln(1 + e^{x})$ $\approx \max(0,x)$



Softmax

- The softmax function maps a vector of real numbers to a vector of probabilities as

$$\begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix} \leftarrow \text{largest } z \qquad \mathrm{softmax}(z)_j = \frac{e^{z_j}}{\sum_k e^{z_k}} \approx \mathbb{1}\left(j == \operatorname{argmax}_k z_k\right)$$

- If there is a dominant value in z, then it will become one under the softmax

- Often used as the final layer of a neural network

Multi-class Classification

$$z = \begin{bmatrix} 1 \\ 2 \\ 3 \\ 4 \end{bmatrix}$$

Non-Linearities

$$\xrightarrow{w^T x + b} F \longrightarrow y = F(w^T x + b)$$

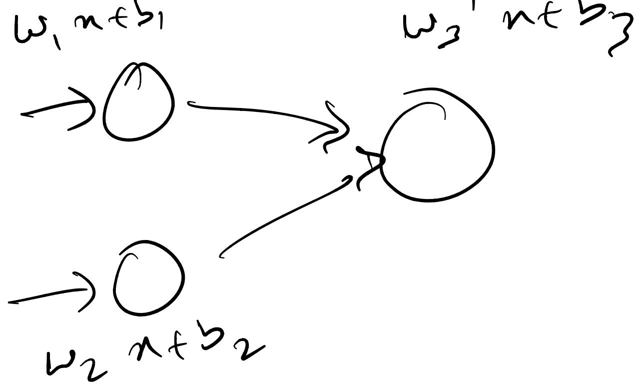
1. $F(z) = \sigma(z) = \dfrac{1}{1+e^{-z}}$

2. $F(z) = \mathrm{RELU}(z) = \max(0, z)$

3. $F(z) = \text{SOFT-PLUS}(z) = \log(1+e^{z})$

4. $F(z) = \text{SOFT-MAX}(z) = \dfrac{e^{z_j}}{\sum_k e^{z_k}}$ for class j

What if we dont have non-linearity?

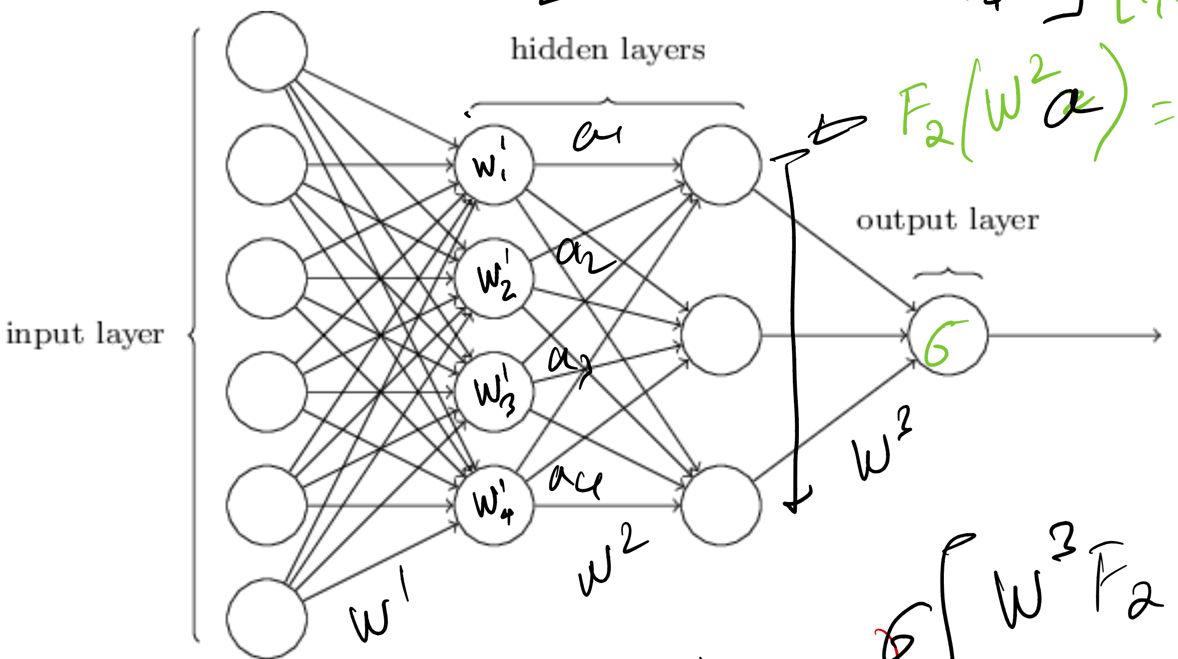


$$w_3^1(w_1 x + b_1) + w_3^2(w_2 x + b_2) + b_3$$

$$\underbrace{(w_3^1 w_1 + w_3^2 w_2)}_{w} x + \underbrace{w_3^1 b_1 + w_3^2 b_2 + b_3}_{b}$$

Multilayer Neural Networks

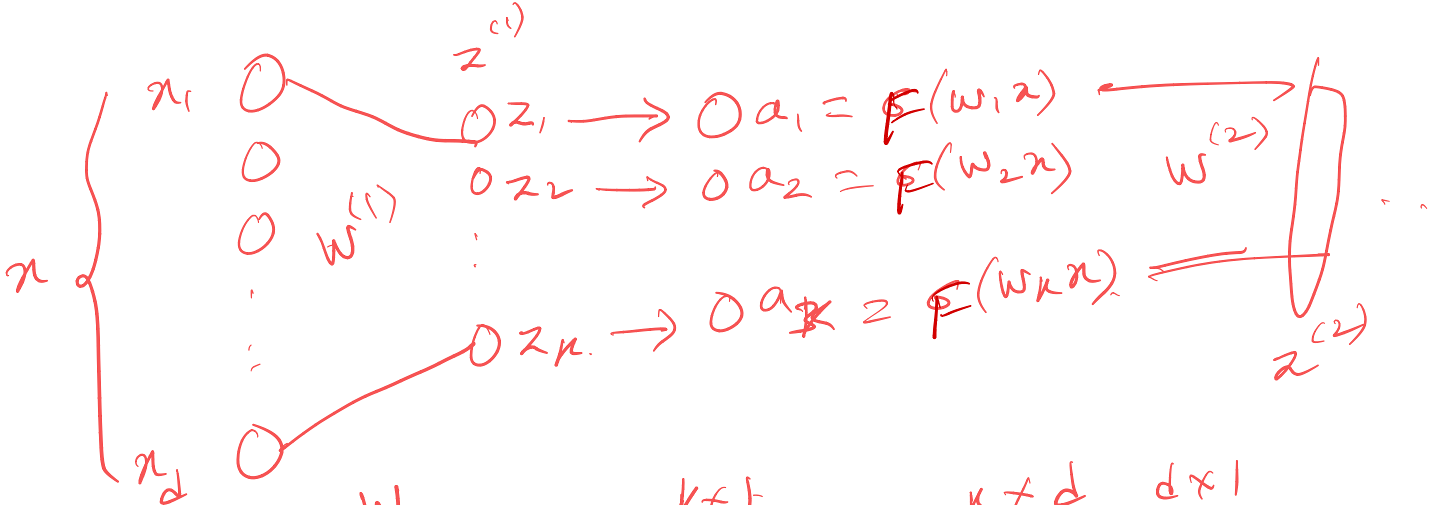
$$F_1(W^1 x) = F_1\left(\begin{bmatrix} w_1^1 \\ w_2^1 \\ w_3^1 \\ w_4^1 \end{bmatrix} x\right) = F_1\left(\begin{bmatrix} w_1^1 x \\ w_2^1 x \\ w_3^1 x \\ w_4^1 x \end{bmatrix}\right) = \begin{bmatrix} F_1(w_1^1 x) \\ F_1(w_2^1 x) \\ F_1(w_3^1 x) \\ F_1(w_4^1 x) \end{bmatrix} = \begin{bmatrix} a_1 \\ a_2 \\ a_3 \\ a_4 \end{bmatrix}$$



$$\Rightarrow F_2(W^2 a) = F_2\left[W^2 F_1(W^1 x)\right]$$

$$p(y=1 \mid a) = \sigma\left[W^3 F_2\left(W^2 F_1(W^1 x)\right)\right]$$

from Neural Networks and Deep Learning by Michael Nielson



x $\quad W \qquad k \times 1 \qquad k \times d \qquad d \times 1$

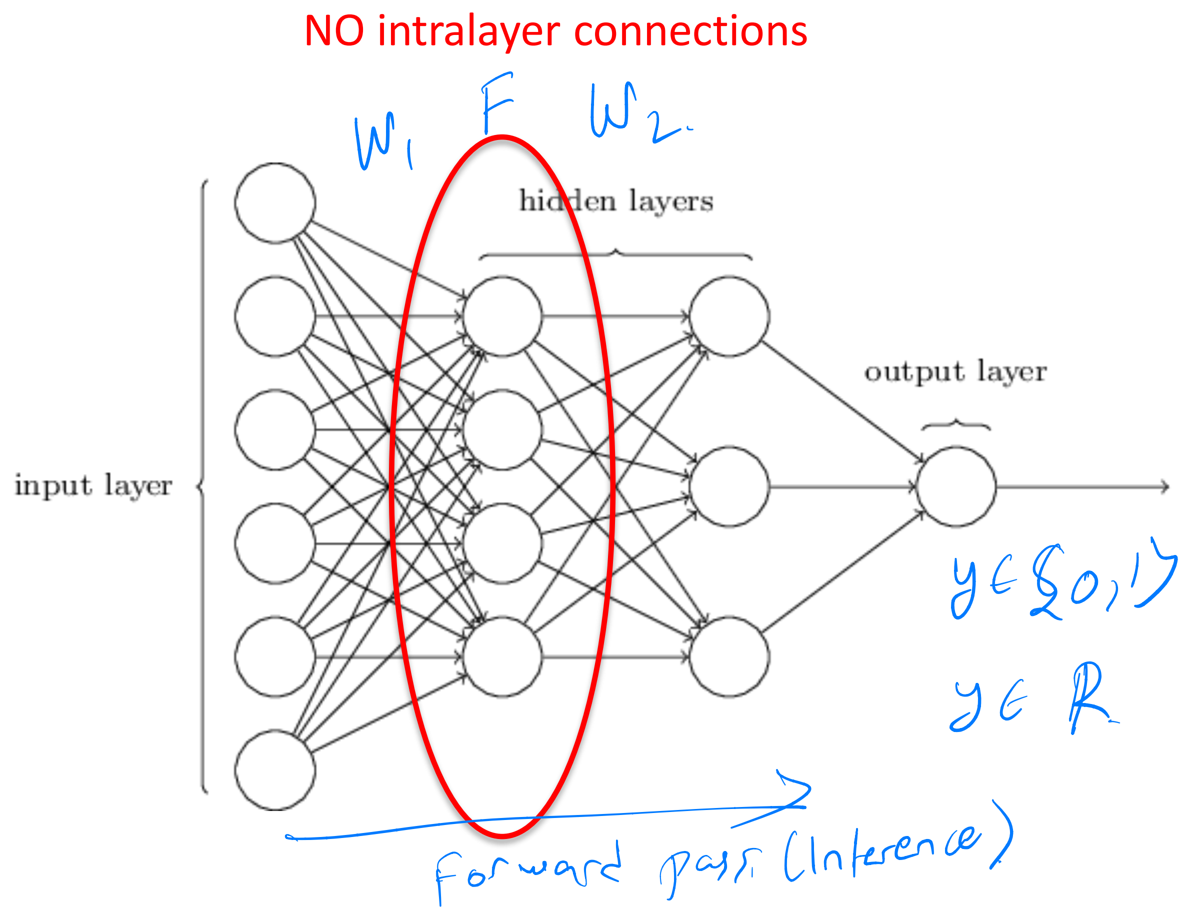
$$z_1 = w_1 x$$
$$z_2 = w_2 x$$
$$\vdots$$
$$z_k = w_k x$$

$$\Rightarrow \begin{bmatrix} z \end{bmatrix} = \underbrace{\begin{bmatrix} w_1 \\ w_2 \\ \vdots \\ w_k \end{bmatrix}}_{W} x$$

$$W \in \mathbb{R}^{k \times d}$$

$$z = Wx + \underset{\mathbb{R}^d}{b} \quad \text{(with bias)}$$

Multilayer Neural Networks



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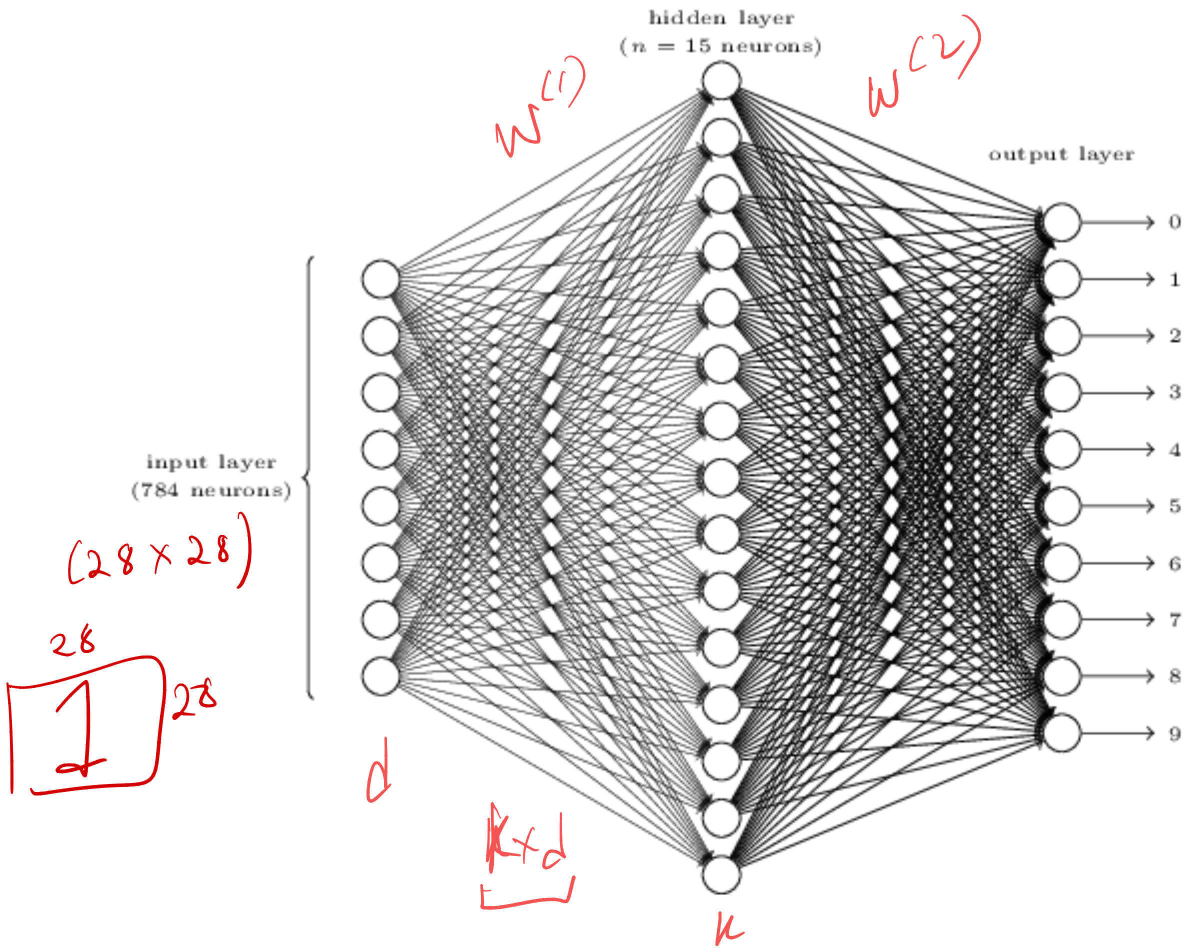
Neural Network for Digit Classification



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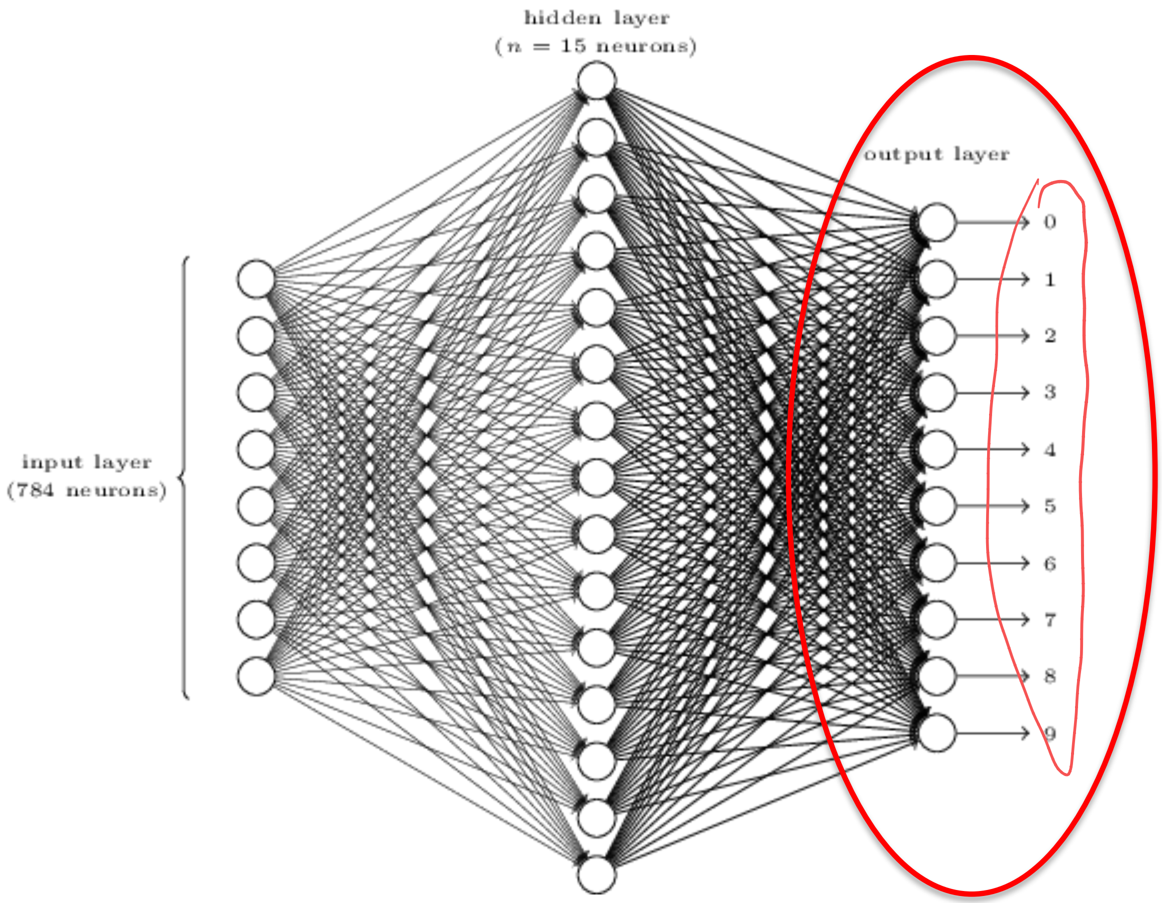
Neural Network for Digit Classification



Why 10 instead of 4?

from Neural Networks and Deep Learning by Michael Nielson

Expressiveness of NNs

- Boolean functions
  - Every Boolean function can be represented by a network with a single hidden layer consisting of possibly exponentially many hidden units
- Continuous functions
  - Every bounded continuous function can be approximated up to arbitrarily small error by a network with one hidden layer
  - Any function can be approximated to arbitrary accuracy with two hidden layers

Expressiveness of NNs

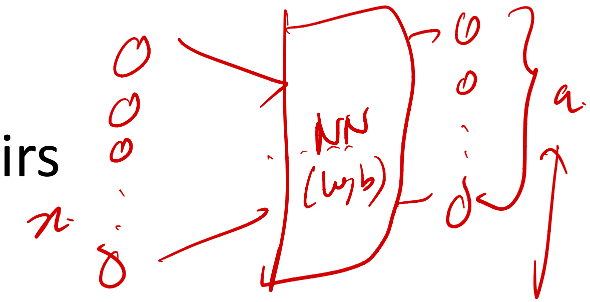
- **Theorem [Zhang et al. 2016]:** There exists a two-layer neural network with ReLU activations and $2n + d$ weights that can represent any function on a sample of size n in d dimensions
  - This should mean that it is very easy to overfit with neural networks
  - Generalization performance of networks is difficult to assess theoretically

Training Neural Networks

- To do the learning, we first need to define a loss function to minimize

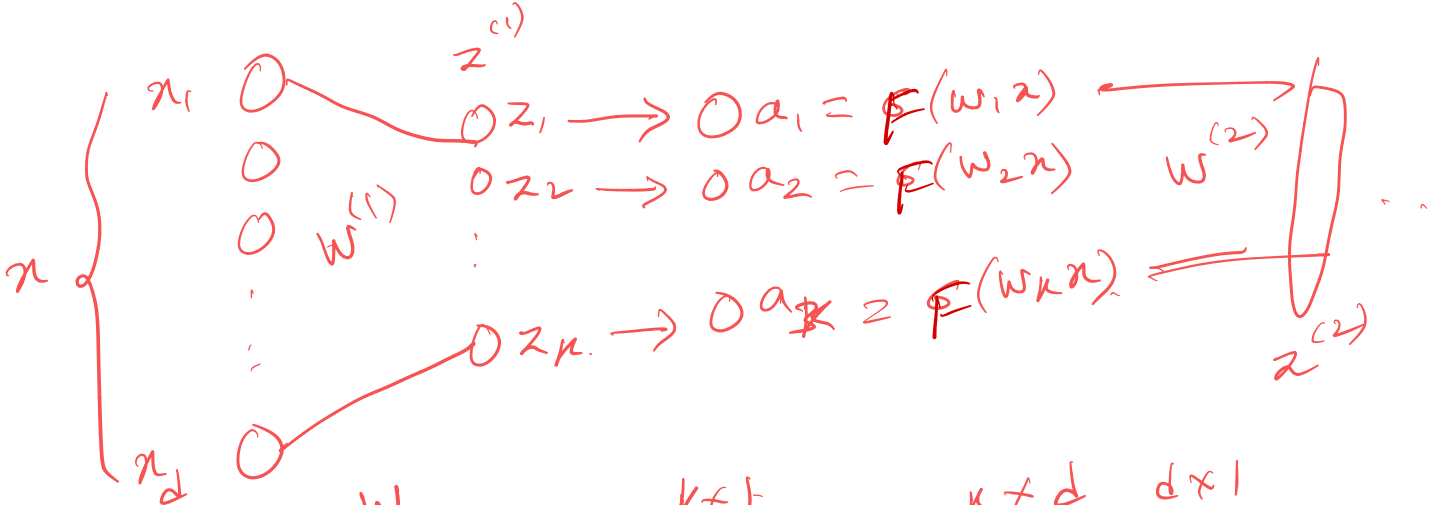
$$C(w,b) = \frac{1}{2M}\sum_{m=1}^{M}\|y^m - a(x^m,w,b)\|^2$$

- The training data consists of input output pairs $(x^1,y^1),\ldots,(x^M,y^M)$



- $a(x^m,w,b)$ is the output of the neural network for the m^{th} sample $a(x,w,b)$

- w and b are the weights and biases



$x \quad W \qquad k \times 1 \qquad k \times d \quad d \times 1$

$$z_1 = w_1 x$$
$$z_2 = w_2 x$$
$$\vdots$$
$$z_k = w_k x$$

$$\Rightarrow \begin{bmatrix} z \end{bmatrix} = \underbrace{\begin{bmatrix} w_1 \\ w_2 \\ \vdots \\ w_k \end{bmatrix}}_{W} x.$$

$$W \in \mathbb{R}^{k \times d}$$

$$z = Wx + \underset{\mathbb{R}^d}{b}. \text{ (with bias)}$$

Gradient of the Loss

- The derivative of the loss function is calculated as follows

$$\frac{\partial C(w,b)}{\partial w_k} = \frac{1}{M}\sum_m [y^m - a(x^m,w,b)]\frac{\partial a(x^m,w,b)}{\partial w_k}$$

  - To compute the derivative of a, use the chain rule and the derivative of the sigmoid function

$$\frac{d\sigma(z)}{dz} = \sigma(z)\cdot(1-\sigma(z))$$

  - This gets complicated quickly with lots of layers of neurons

$$\sigma(z) = \frac{1}{1+e^{-z}}$$

Stochastic Gradient Descent

- To make the training more practical, stochastic gradient descent is used instead of standard gradient descent
- Recall, the idea of stochastic gradient descent is to approximate the gradient of a sum by sampling a few indices and averaging

mini batch of K examples

$$\nabla_x \sum_{i=1}^{n} f_i(x) \approx \frac{1}{K} \sum_{k=1}^{K} \nabla_x f_{i^k}(x)$$

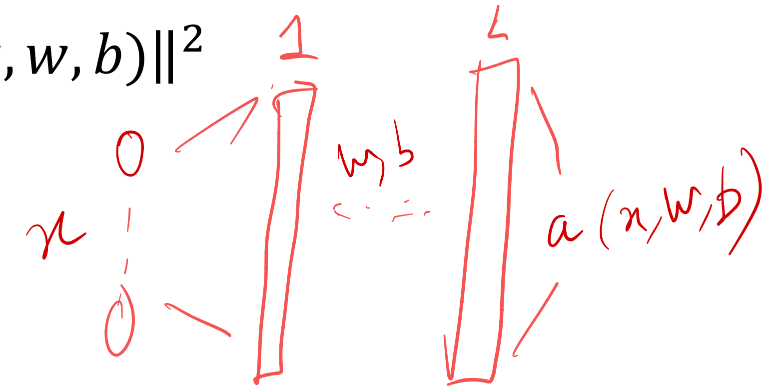
i^k, $k = 1:K$

here, for example, each i^k is sampled uniformly at random from $\{1, \ldots, n\}$

Computing the Gradient

- We'll compute the gradient for a single sample

$$C(w,b) = \frac{1}{2}\|y - a(x,w,b)\|^2$$

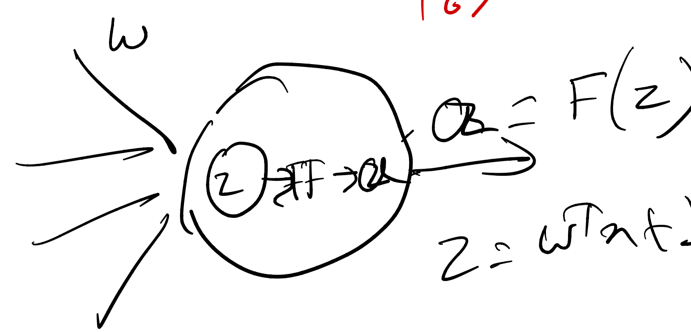


- Some definitions:
  - L is the number of layers
  - a_j^l is the output of the j^{th} neuron on the l^{th} layer
  - z_j^l is the weighted input of the j^{th} neuron on the l^{th} layer

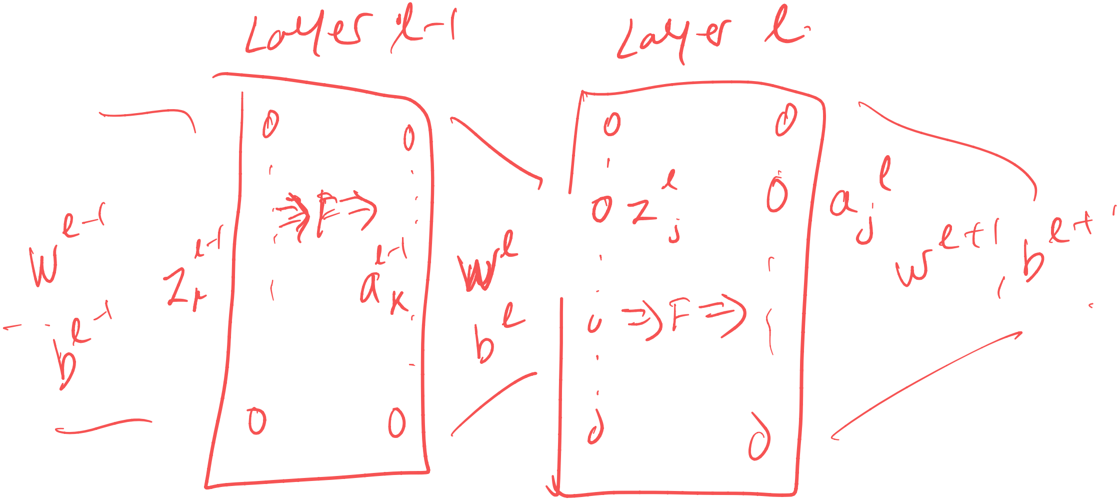
$$z_j^l = \sum_k w_{jk}^l a_k^{l-1} + b_j^l$$

$a_j^l = F(z_j^l)$
(6)

- δ_j^l is defined to be $\frac{\partial C}{\partial z_j^l}$



$z = w^T x + b.$



$$\text{in} \Rightarrow W^1 \Rightarrow W^2 \Rightarrow \cdots W^k \Rightarrow$$

$$o = \underbrace{W^k W^{k-1} \cdots W^1}_{W} \, \text{in}$$

$$z_j^l = \sum_k w_{jk}^l a_k^{l-1} + b_j^l, \quad \forall j$$

$$z^l = W^l a^{l-1} + b^l$$

vector   vector

$$a^l = F(z^l), \Rightarrow a_j^l = F(z_j^l)$$

σ ReLU

Computing the Gradient

For the output layer, we have the following partial derivative

$$C(w,b,x) = \left[y - a^L(w,b,x)\right]^2$$

$$\frac{\partial C}{\partial z_j^L} = -\left(y_j - a_j^L\right)\frac{\partial a_j^L}{\partial z_j^L} \qquad a_j^L = F(z_j^L)$$

$$= -\left(y_j - a_j^L\right)\frac{\partial \sigma\left(z_j^L\right)}{\partial z_j^L} \quad \leftarrow \quad F = \sigma(z)$$

$$= -\left(y_j - a_j^L\right)\sigma\left(z_j^L\right)\left(1 - \sigma\left(z_j^L\right)\right) \qquad \frac{\partial C}{\partial z_j^L} = \frac{\partial C}{\partial a_j^L} \cdot \frac{\partial a_j^L}{\partial z_j^L}$$

$$= \delta_j^L \quad \Rightarrow \quad \delta_j^l, \ \forall\, l$$

- For simplicity, we will denote the vector of all such partials for each node in the l^{th} layer as δ^l

Computing the Gradient

For the $L-1$ layer, we have the following partial derivative

$$\frac{\partial C}{\partial z_k^{L-1}} = \sum_j \underbrace{\left(a_j^L - y_j\right)} \frac{\partial a_j^L}{\partial z_k^{L-1}}$$

$$a_j^L = \sigma(z_j^L)$$

$$= \sum_j \underbrace{\left(a_j^L - y_j\right)} \frac{\partial \sigma\left(z_j^L\right)}{\partial z_k^{L-1}}$$

$$\frac{\partial \sigma(z_j^L)}{\partial z_j^L} \cdot \frac{\partial z_j^L}{\partial z_k^{L-1}}$$

$$\sigma(z_k^{L-1})$$

$$= \sum_j \underbrace{\left(a_j^L - y_j\right)} \sigma\left(z_j^L\right)\left(1 - \sigma\left(z_j^L\right)\right) \frac{\partial z_j^L}{\partial z_k^{L-1}}$$

$$= \sum_j \left(a_j^L - y_j\right) \sigma\left(z_j^L\right)\left(1 - \sigma\left(z_j^L\right)\right) \frac{\partial \sum_{k'} w_{jk'}^L a_{k'}^{L-1} + b_j^L}{\partial z_k^{L-1}}$$

$$= \sum_j \left(a_j^L - y_j\right) \sigma\left(z_j^L\right)\left(1 - \sigma\left(z_j^L\right)\right) \boxed{\sigma\left(z_k^{L-1}\right)\left(1 - \sigma\left(z_k^{L-1}\right)\right) w_{jk}^L}$$

$$= \underbrace{\left(\left(\delta^L\right)^T w_{*k}^L\right)\left(1 - \sigma\left(z_k^{L-1}\right)\right) \sigma\left(z_k^{L-1}\right)}$$

$$\delta^{L-1}$$

$$C = \sum_j \left(a_j^{L-1} - y_j\right)^2$$

$$\frac{\partial a_j^L}{\partial z_k^{L-1}} = \delta^{L-1}$$

$$\frac{\partial C}{\partial z_k^{L-1}}$$

$$z_j^L = \sum_{k'=1}^{K} w_{jk'} a_{k'}^{L-1} + b_j^{L-1}$$

$$a_j^L = \sigma(z_j^L)$$

Computing the Gradient

$$\begin{bmatrix} x_1 \\ \vdots \\ x_n \end{bmatrix} \circ \begin{bmatrix} y_1 \\ \vdots \\ y_n \end{bmatrix} = \begin{bmatrix} x_1 y_1 \\ x_2 y_2 \\ \vdots \\ x_n y_n \end{bmatrix}$$

- We can think of w^l as a matrix
- This allows us to write

$$\delta^{L-1} = \left(\left(\delta^L\right)^T w^L\right)^T \circ \left(1 - \sigma\left(z^{L-1}\right)\right) \circ \sigma\left(z^{L-1}\right)$$

where $\sigma\left(z^{L-1}\right)$ is the vector whose k^{th} component is $\sigma\left(z_k^{L-1}\right)$

- Applying the same strategy, for $l < L$

$$\delta^{l} = \left(\left(\delta^{l+1}\right)^T w^{l+1}\right)^T \circ \left(1 - \sigma\left(z^{l}\right)\right) \circ \sigma\left(z^{l}\right)$$

Computing the Gradient

- Now, for the partial derivatives that we care about

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

$$\frac{\partial C}{\partial b_j^l} = \frac{\partial C}{\partial z_j^l} \cdot \frac{\partial z_j^l}{\partial b_j^l} = \delta_j^l$$

$$z_j^l = \sum_k w_{jk}^l \boxed{a_k^{l-1}} + b_j^l$$

$$\frac{\partial C}{\partial w_{jk}^l} = \frac{\partial C}{\partial z_j^l} \cdot \boxed{\frac{\partial z_j^l}{\partial w_{jk}^l}} = \delta_j^l a_k^{l-1}$$

- We can compute these derivatives one layer at a time!

Backpropagation

- Compute the inputs/outputs for each layer by starting at the input layer and applying the sigmoid functions

$\delta^L, \delta^{L-1}, \ldots, \delta^1$

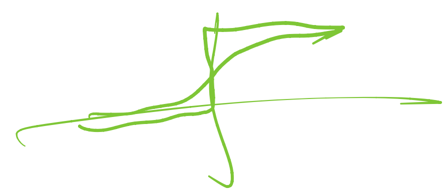
- Compute δ^L for the output layer

$$\delta_j^L = -\left(y_j - a_j^L\right)\sigma\left(z_j^L\right)\left(1 - \sigma\left(z_j^L\right)\right)$$

- Starting from $l = L - 1$ and working backwards, compute

$$\delta^l = \left(\left(\delta^{l+1}\right)^T w^{l+1}\right)^T \circ \sigma\left(z^l\right) \circ \left(1 - \sigma\left(z^l\right)\right)$$

- Perform gradient descent



$$b_j^l = b_j^l - \gamma \cdot \delta_j^l$$

$$w_{jk}^l = w_{jk}^l - \gamma \cdot \delta_j^l a_k^{l-1}$$

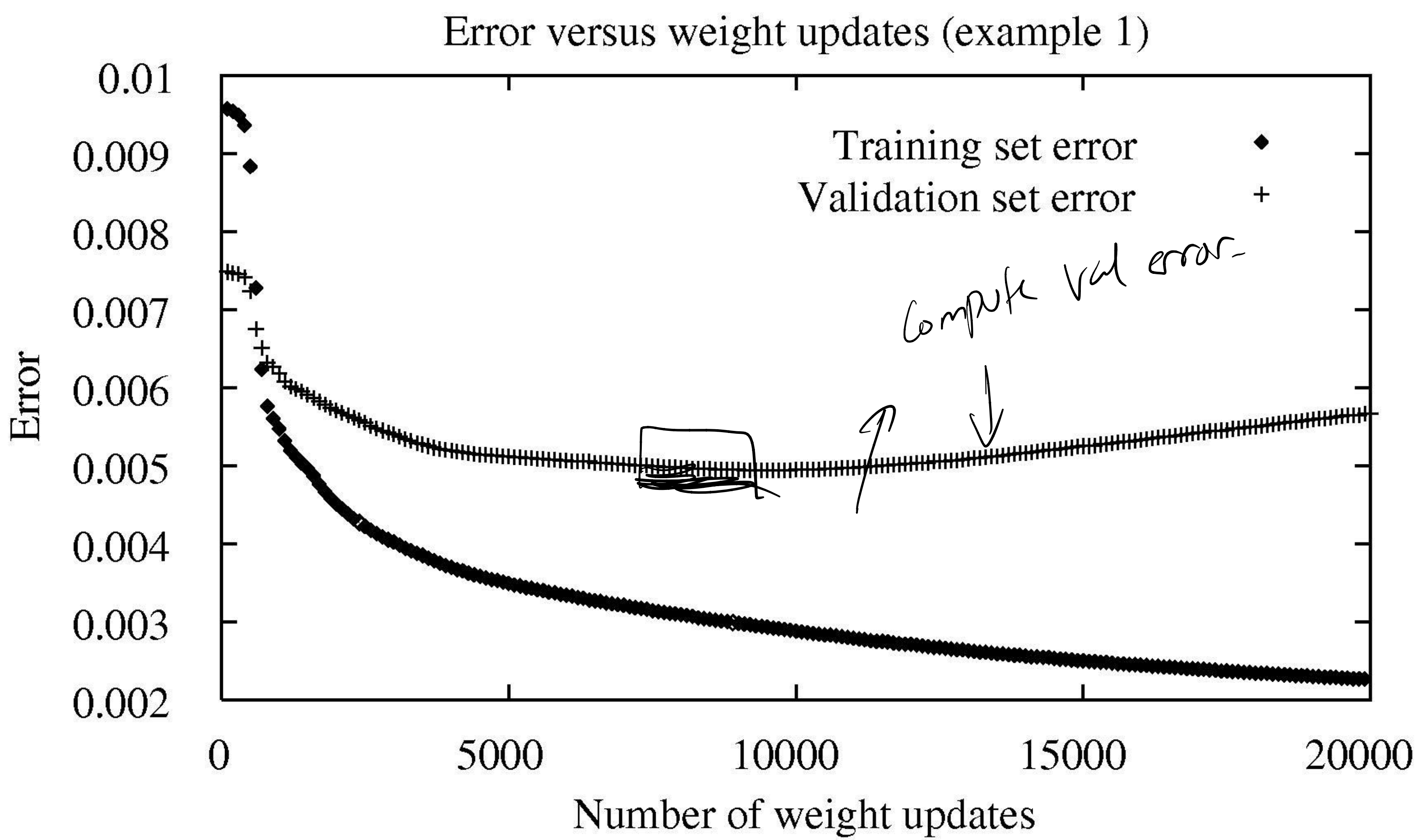
Backpropagation

- Backpropagation converges to a local minimum (loss is not convex in the weights and biases)
  - Like EM, can just run it several times with different initializations
  - Training can take a very long time (even with stochastic gradient descent)
  - Prediction after learning is fast
  - Sometimes include a momentum term α in the gradient update

$$w(t) = w(t-1) - \gamma \cdot \nabla_w C(t-1) + \alpha(-\gamma \cdot \nabla_w C(t-2))$$

Overfitting

Iterations = # mini-batch updates
epochs = # passes through data



Compute val error

Neural Networks in Practice

- Many ways to improve weight learning in NNs
  - Use a regularizer! (better generalization?)
  - Try other loss functions, e.g., the cross entropy

    $$-y \log a(x, w, b) - (1 - y) \log(1 - a(x, w, b))$$

  - Initialize the weights of the network more cleverly
    - Random initializations are likely to be far from optimal
- The learning procedure can have numerical difficulties if there are a large number of layers (and too many sigmoids)

  ↳ Hence ReLus

Regularized Loss

$w^T x^m + b$

- Penalize learning large weights

$$C'^{(w,b)} = \frac{1}{2M}\sum_m \|y^m - a(x^m, w, b)\|^2 + \frac{\lambda}{2}\|\underline{w}\|_2^2$$

- Can still use the backpropagation algorithm in this setting
- ℓ_1 regularization can also be useful
- Regularization can help with convergence, λ should be chosen with a validation set

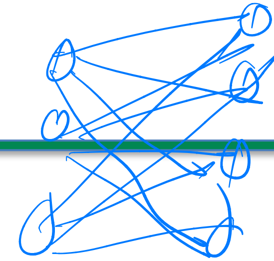
Dropout

- A heuristic bagging-style approach applied to neural networks to counteract overfitting
  - Randomly remove a certain percentage of the neurons from the network and then train only on the remaining neurons
  - The networks are recombined using an approximate averaging technique (keeping around too many networks and doing proper bagging can be costly in practice)

Other Techniques

- Early stopping
  - Stop the learning early in the hopes that this prevents overfitting
- Parameter tying
  - Assume some of the weights in the model are the same to reduce the dimensionality of the learning problem
  - Also a way to learn “simpler” models
  - Can lead to significant compression in neural networks (i.e., >90%)

Other Ideas



- Convolutional neural networks
  - Instead of the output of every neuron at layer l being used as an input to every neuron at layer $l+1$, the edges between layers are chosen more locally
  - Many tied weights and biases (i.e., convolution nets apply the same process to many different local chunks of neurons)
  - Often combined with pooling layers (i.e., layers that, say, half the number of neurons by replacing small regions of neurons with their maximum output)
  - Used extensively for image classification tasks