Neural Networks

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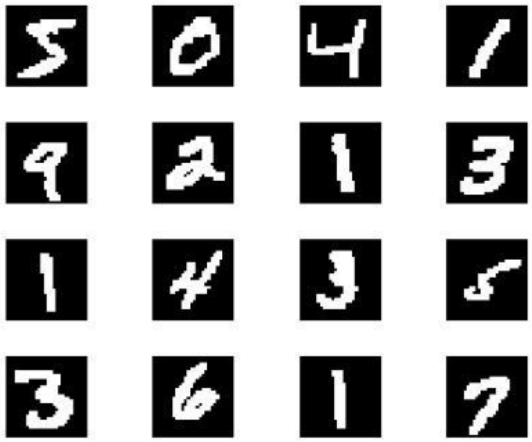
Handwritten Digit Recognition

- 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)



Digits from the MNIST data set

Neural Networks

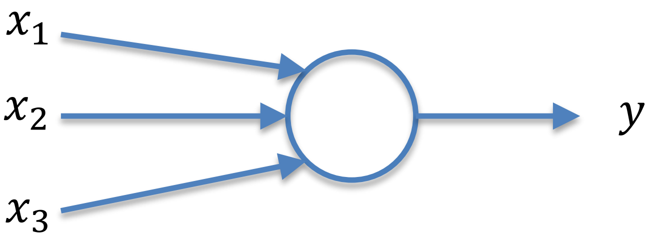
- The basis of neural networks was developed in the 1940s -1960s
  - The idea was to build mathematical models that might “compute” in the same way that neurons in the brain do
  - As a result, neural networks are biologically inspired, though many of the algorithms developed for them are not biologically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

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

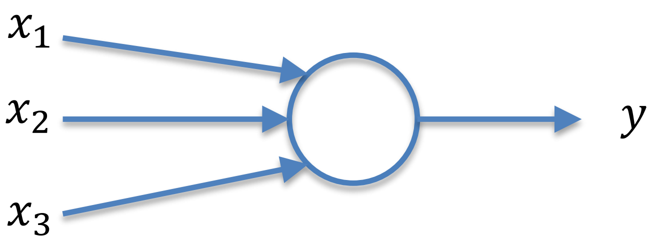
- A perceptron is an artificial neuron that takes a collection of binary inputs and produces a binary output
  - The output of the perceptron is determined by summing up the weighted inputs and thresholding the result: if the weighted sum is larger than the threshold, the output is one (and zero otherwise)



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

Perceptrons

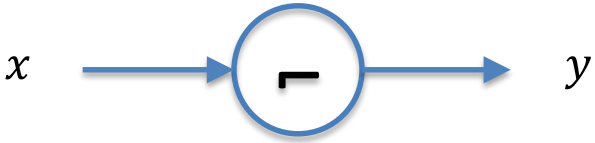
- Perceptrons are usually expressed in terms of a collection of input weights and a bias b (which is the negative threshold)



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

- A single node perceptron is just a linear classifier
- This is actually where the “perceptron algorithm” comes from

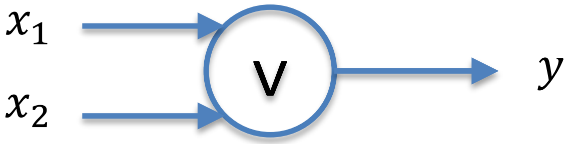
Perceptron for NOT



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

Perceptron for OR

Perceptron for OR

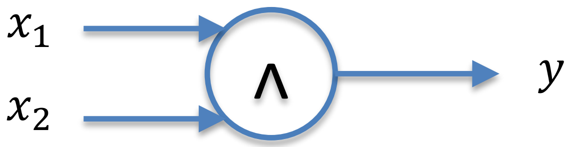


- Choose $w_1 = w_2 = 1$, threshold $= 0$

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

Perceptron for AND

Perceptron for AND

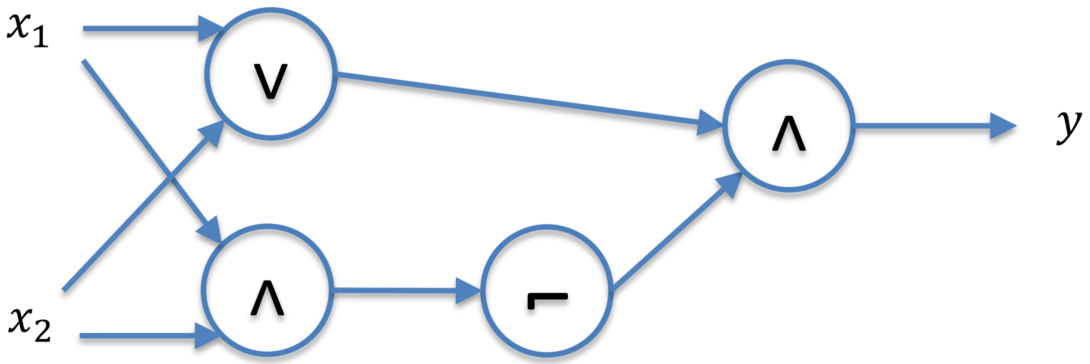


- Choose $w_1 = w_2 = 1$, threshold $= 1.5$
- $y = \begin{cases} 1 & x_1 + x_2 > 1.5 \\ 0 & x_1 + x_2 \leq 1.5 \end{cases}$

Perceptron for XOR

Perceptron for XOR

- Need more than one perceptron!

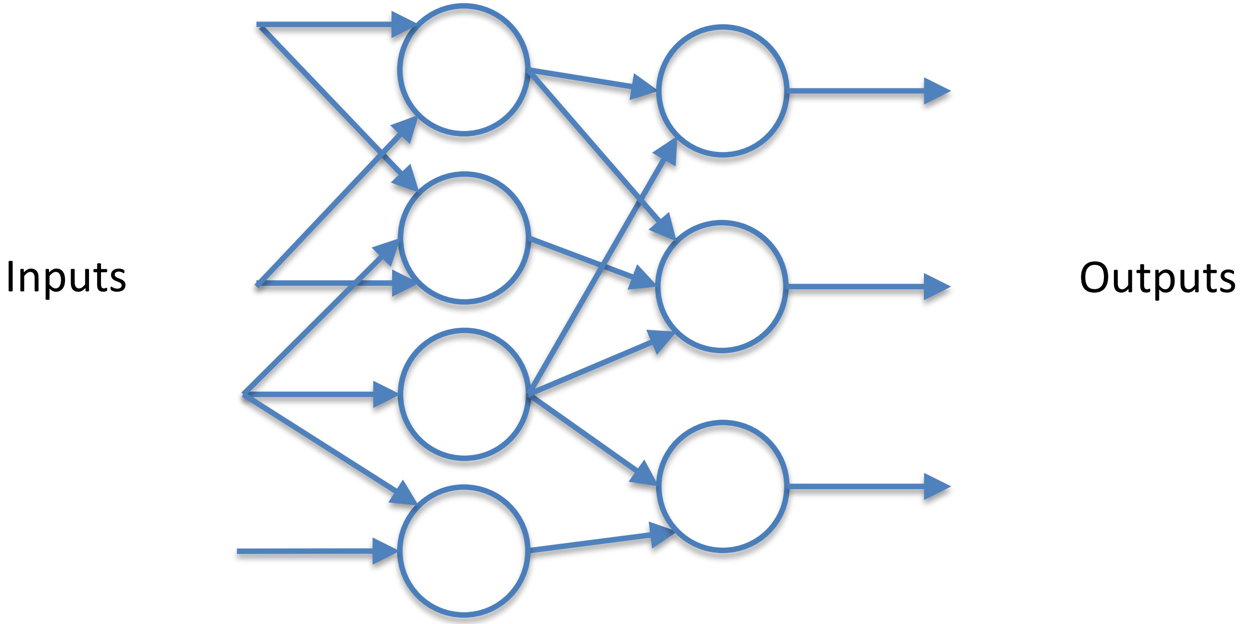


- Weights for incoming edges are chosen as before
- Networks of perceptrons can encode any circuit!

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

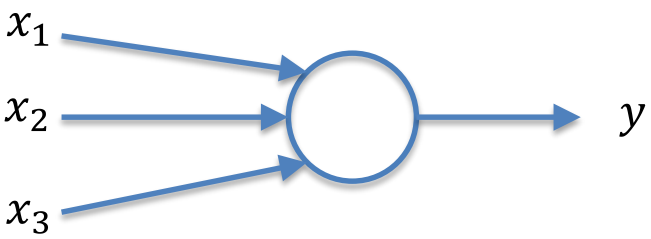


Beyond Perceptrons

- 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

- 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



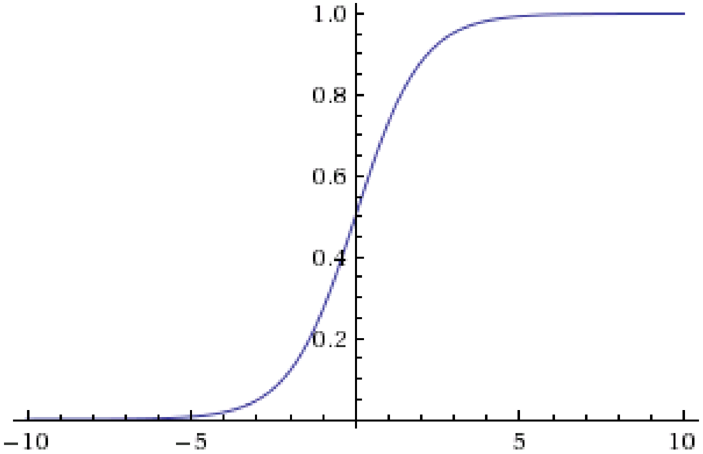
$$y = \sigma(w_1 x_1 + w_2 x_2 + w_3 x_3 + b)$$

where σ is the sigmoid function

The Sigmoid Function

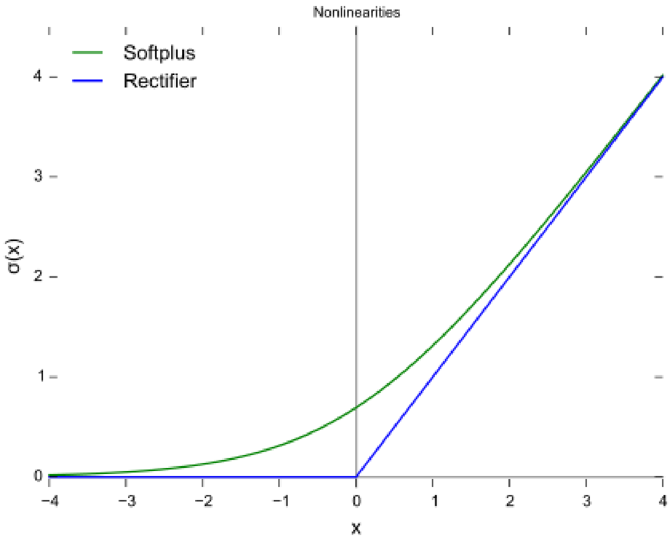
- The sigmoid function is a continuous function that approximates a step function

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



Rectified Linear Units

- 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 $\ln(1 + e^x)$



Softmax

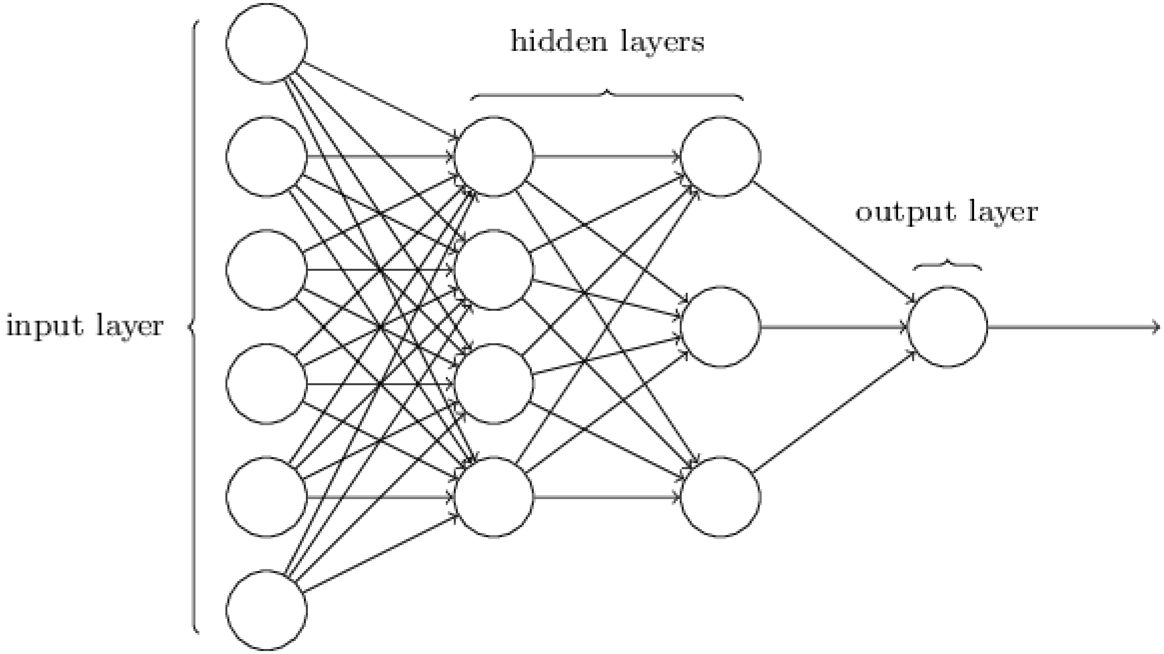
- The softmax function maps a vector of real numbers to a vector of probabilities as

$$\text{softmax}(z)_j = \frac{e^{z_j}}{\sum_k e^{z_k}}$$

- 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

Multilayer Neural Networks



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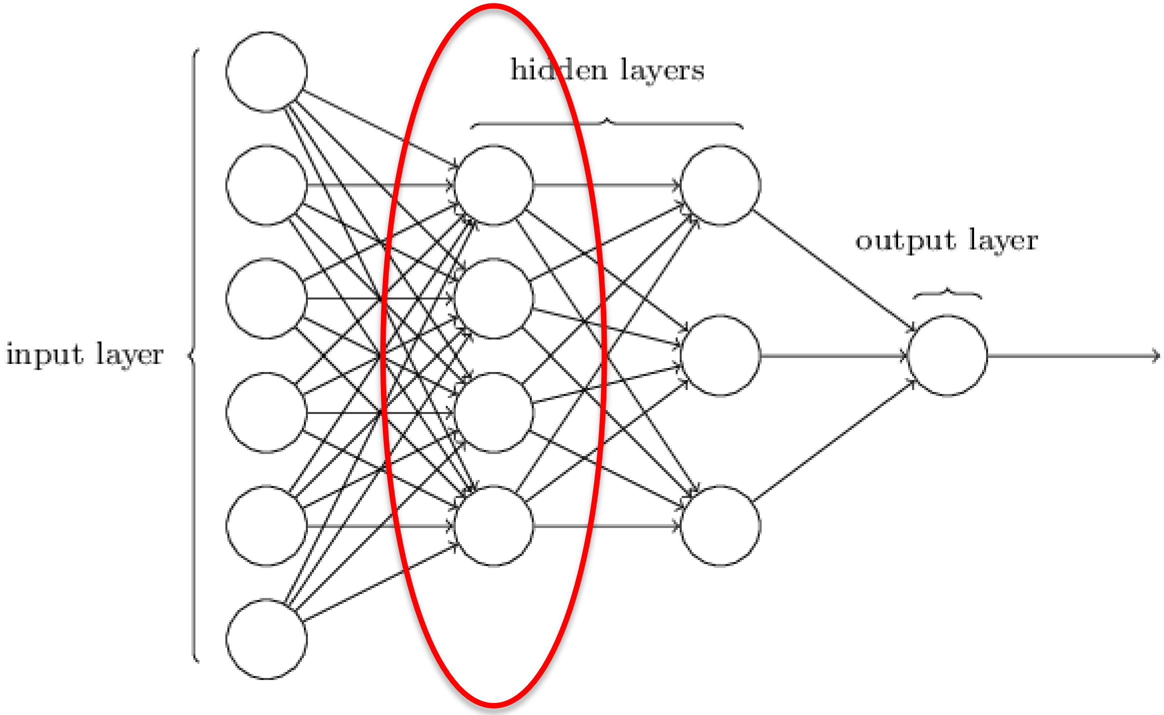
Multilayer Neural Networks

NO intralayer connections



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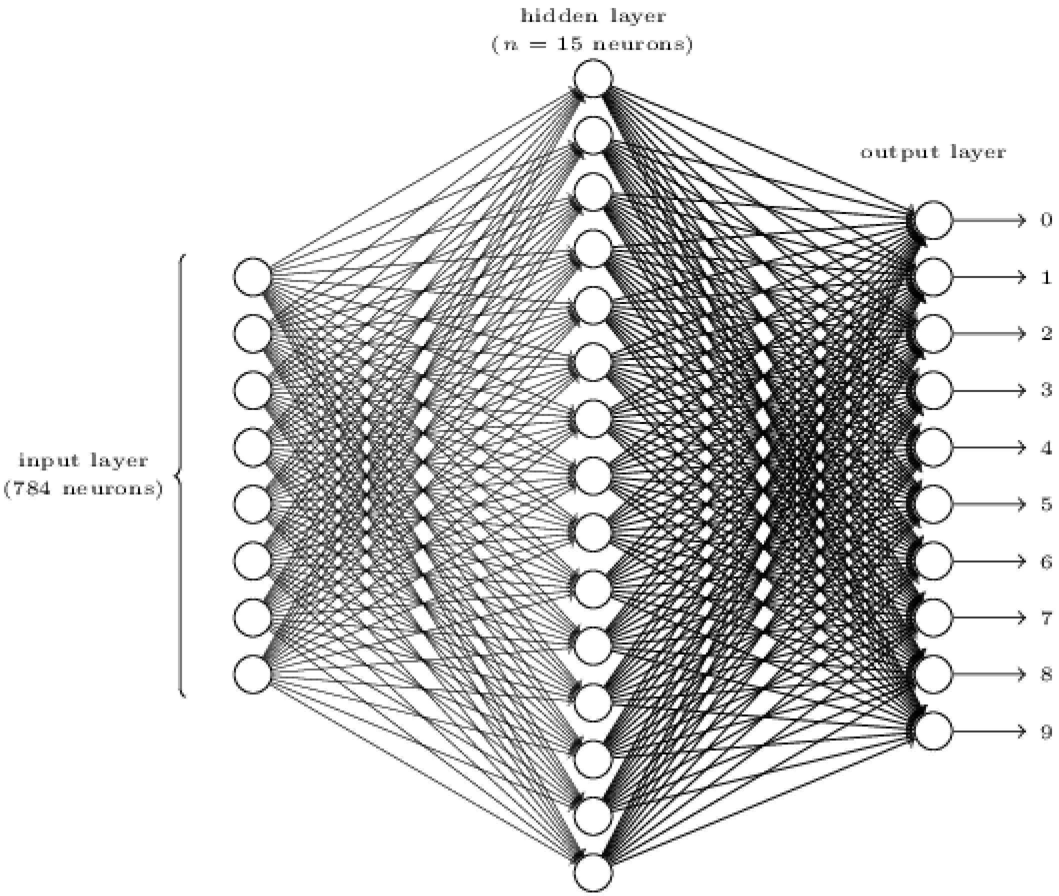
Neural Network for Digit Classification



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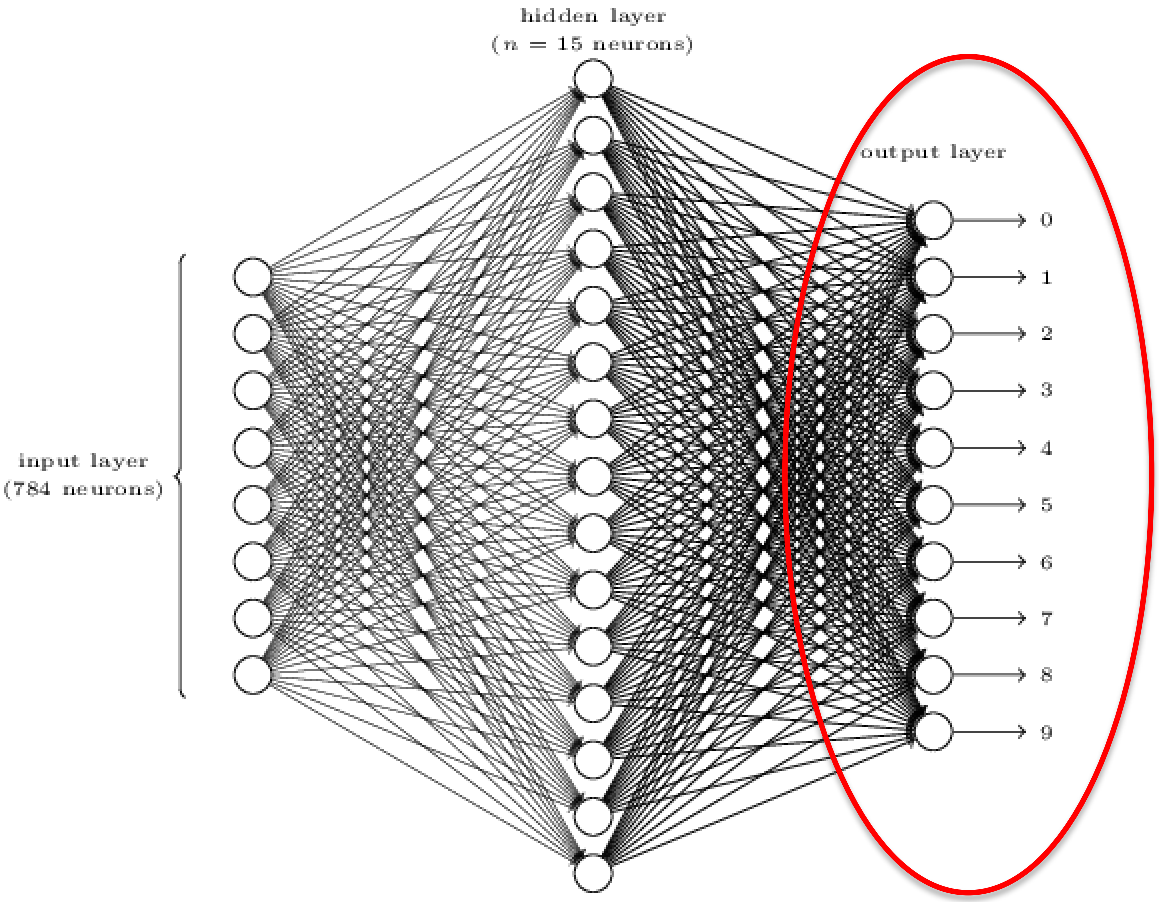
Neural Network for Digit Classification



Why 10 instead of 4?

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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

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

- 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
- w and b are the weights and biases

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

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

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

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

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

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

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

Computing the Gradient

For the output layer, we have the following partial derivative

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

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

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

$$= \delta_j^L$$

- 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

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

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

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

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

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

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

Computing the Gradient

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

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

where $\sigma(z^{L-1})$ 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

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

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

- 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

- 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

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

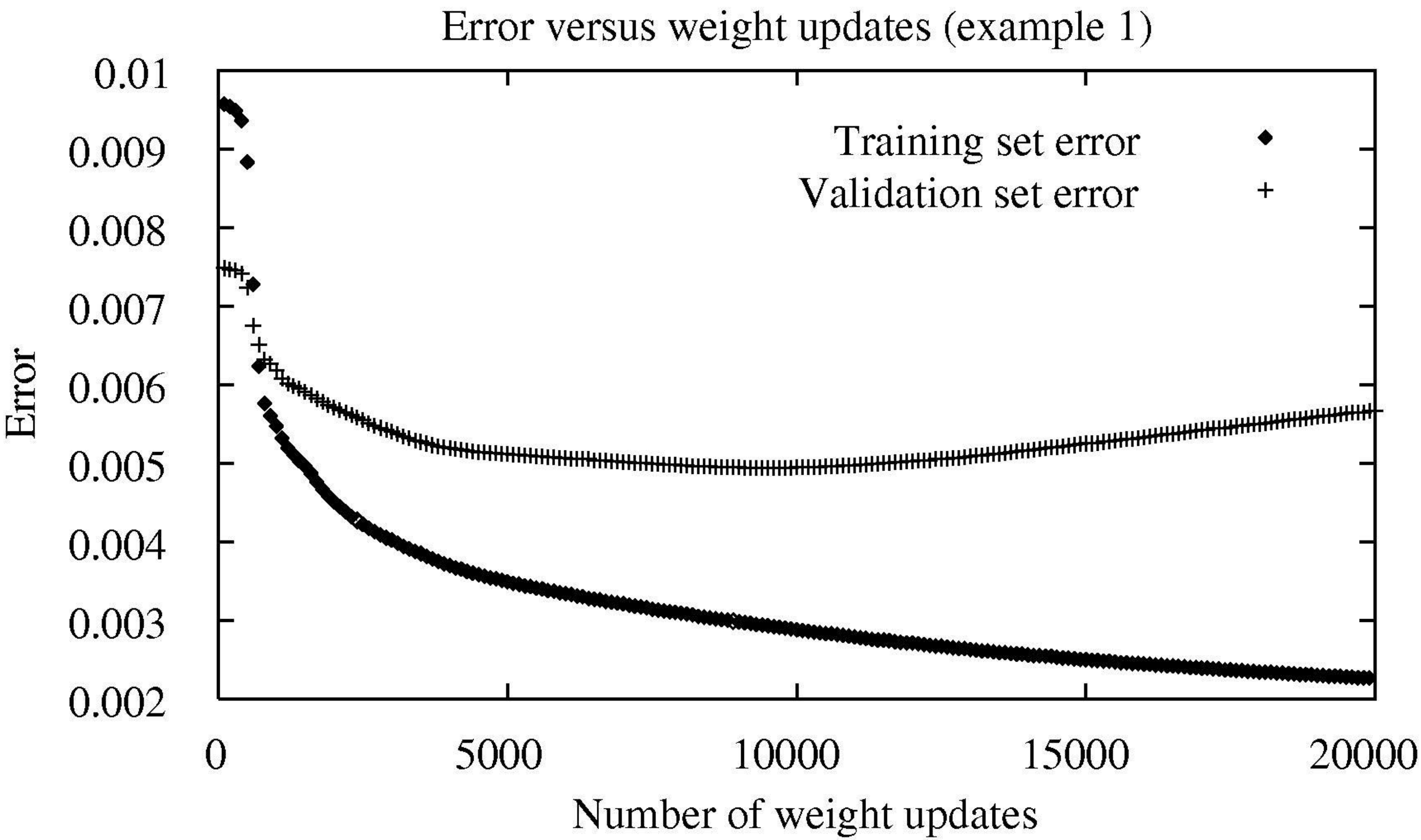
$$w_{jk}^l = w_{jk}^l - \gamma \cdot \delta_j^l a_k^{l-1}$$

Backpropagation

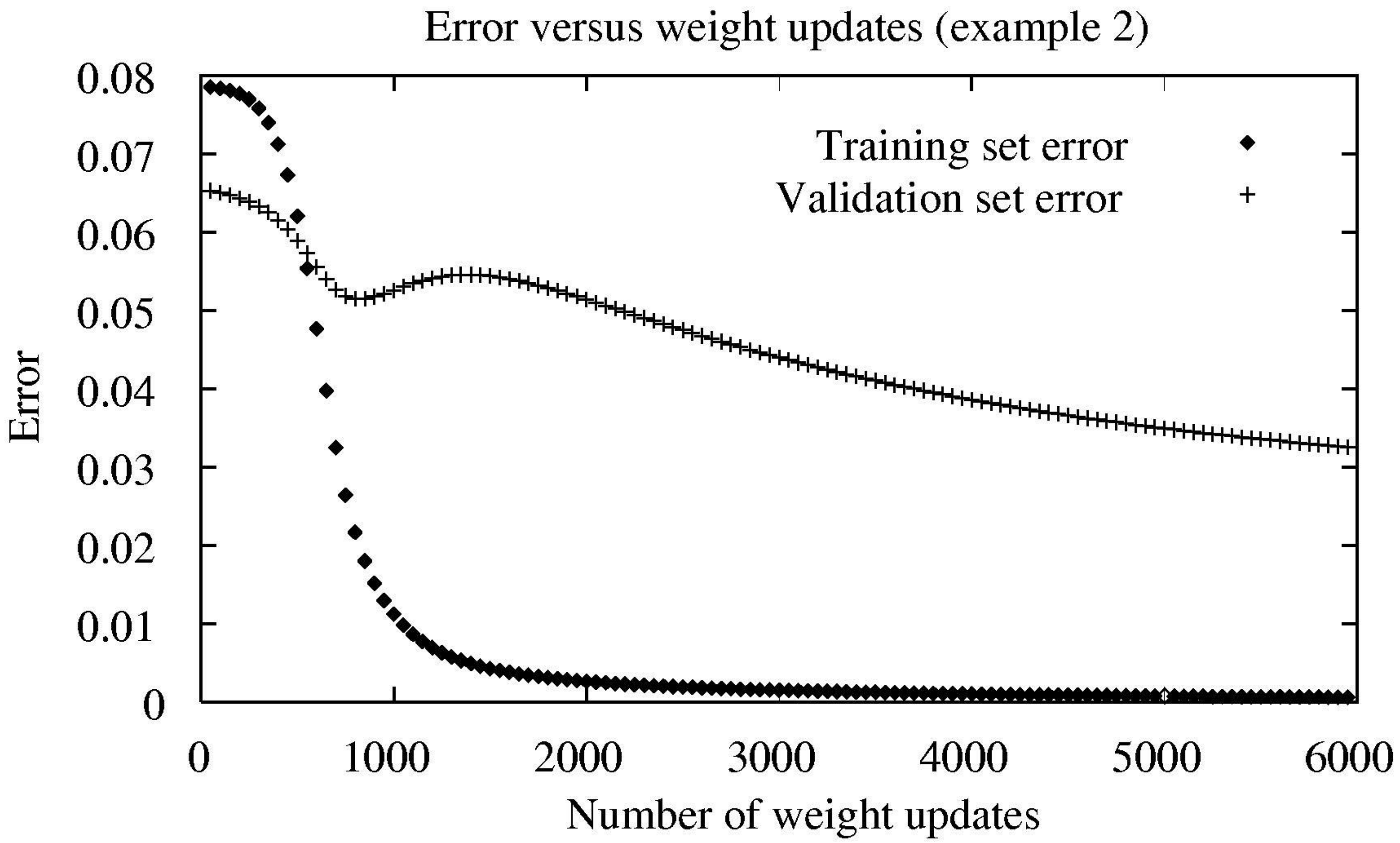
- Backpropagation converges to a local minimum (loss is not convex in the weights and biases)
  - Like EM, can just run it several times with different initializations
  - Training can take a very long time (even with stochastic gradient descent)
  - Prediction after learning is fast
  - Sometimes include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



Overfitting



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

Regularized Loss

- Penalize learning large weights

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

- 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