# Neural Networks - Part 2

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Lecture 20

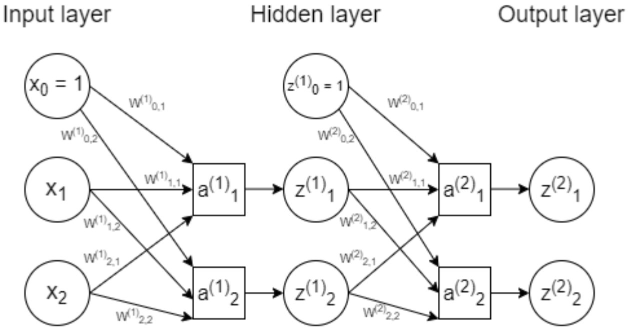
Readings: RN 19.6.2, 21.1, 21.2, PM 7.5, GBC 4.3, 6.5

# Outline

# Learning Goals

- Explain the steps of the gradient descent algorithm.
- Explain how we can modify gradient descent to speed up learning and ensure convergence.
- Describe the back-propagation algorithm including the forward and backward passes.
- Compute the gradient for a weight in a multi-layer feed-forward neural network.
- Describe situations in which it is appropriate to use a neural network or a decision tree.

# A 2-Layer Neural Network



# A 2-Layer Neural Network

Assuming that we want the output of the 2-Layer neural network to be close to certain target value.

Let's assume we are doing spam classification:

The input $x_1$ and $x_2$ are two features: the email length $x_1$ and whether the email is coming from a trusted organization $x_2$.

We have paired training data, $x_1, x_2, y = \{0, 1\}$.

Therefore, we can feed $x_1$ and $x_2$ to the neural network to obtain its output $a_1^{(2)}$ and $a_2^{(2)}$.

# Neural Network Approximation

Let's assume that $a_1^{(2)}$ denotes how likely the email is a spam and $a_2^{(2)}$ denotes how unlikely the email is a spam.

- If an input email is a spam, the desired output should be $[a_1^{(2)}, a_2^{(2)}] = [1, 0]$.
- If an input email is not a spam, the desired output should be $[a_1^{(2)}, a_2^{(2)}] = [0, 1]$.
- If an input email is indistinguishable, the desired output should be $[a_1^{(2)}, a_2^{(2)}] = [0.5, 0.5]$.

# Measuring the Loss Function

Let's assume we want to measure the discrepancy between neural network output and the reference label. The discrepancy is also called loss function $E$. For example, we can have square difference loss as follows:

$$E = \sum_i (a_i^{(2)} - y_i)^2$$

We will be using $E$ as the training signal to perform gradient descent.

# Gradient Descent

*"Walking downhill and always taking a step in the direction that goes down the most."*

- A local search algorithm to find the minimum of a function.
- Steps of the algorithm:
  - Initialize weights randomly.
  - Change each weight in proportion to the negative of the partial derivative of the error with respect to the weight.

$$W := W - \eta \frac{\partial E}{\partial W}$$

  - $\eta$ is the learning rate.
  - Terminate after some number of steps, when the error is small, or when the changes get small.

# Why update the weight proportional to the negative of the partial derivative?

- Suppose that we want to find the minimum of $y = x^2$.

  $\rightarrow$ Think of $x$ as the weight and $y$ as the error.

- Start with $x = x_0$.
- In what direction should we change the value of $x$?

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- In what direction should we change the value of $x$?

  $\rightarrow$ If the gradient is positive, we want to decrease $x_0$. If the gradient is negative, we want to increase $x_0$.

  We want to move in the direction of the negative of the gradient.

# Why update the weight proportional to the negative of the partial derivative?

- By what amount should we change the value of $x$?
  What is the step size?

  $\rightarrow$ If the gradient is large, the curve is steep and we are likely far from the minimum. We can afford to take a larger step. If the gradient is small, the curve is flat and we are likely close to the minimum. We want to take a smaller step.

  Take a step proportional to the gradient.

# How do we update the weights based on the data points?

- Gradient descent updates the weights after sweeping through all the examples.
- To speed up learning, update weights after each example.
  - **Incremental gradient descent** $\rightarrow$ update weights after each example.
  - **Stochastic gradient descent** $\rightarrow$ same as incremental version except each example is chosen randomly.

    $\rightarrow$ With cheaper steps, weights become more accurate more quickly, but not guaranteed to converge as individual examples can move the weights away from the minimum.

# How do we update the weights based on the data points?

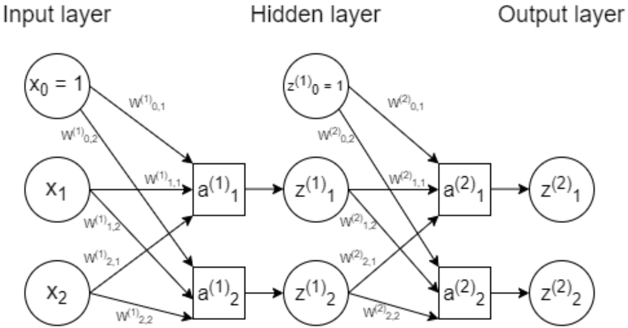
- Trade off learning speed and convergence.
  - **Batched gradient descent**

    $\rightarrow$ update weights after a batch of examples.

    batch = all the examples $\longrightarrow$ gradient descent.

    batch = one example $\longrightarrow$ incremental gradient descent.

# A 2-Layer Neural Network




Let $\hat{y}$ be the output of a network (i.e. prediction).
For this network, $\hat{y} = z^{(2)}$

# The Backpropagation Algorithm

- An efficient method of calculating the gradients in a multi-layer neural network.
- Given training examples $(\vec{x}_n, \vec{y}_n)$ and an error/loss function $E(\hat{y}, y)$. Perform 2 passes.
  - **Forward pass:** compute the error $E$ given the inputs and the weights.
  - **Backward pass:** compute the gradients $\frac{\partial E}{\partial W_{j,k}^{(2)}}$ and $\frac{\partial E}{\partial W_{i,j}^{(1)}}$.
- Update each weight by the sum of the partial derivatives for all the training examples.

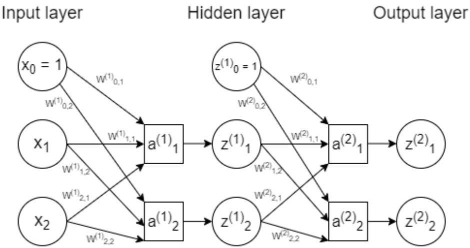
# Forward Pass for a 2-layer Network

Calculate the values of $z_j^{(1)}$ and $z_k^{(2)}$ and $E$.

$$a_j^{(1)} = \sum_i x_i W_{i,j}^{(1)} \qquad z_j^{(1)} = g(a_j^{(1)}) \tag{1}$$

$$a_k^{(2)} = \sum_j z_j^{(1)} W_{j,k}^{(2)} \qquad z_k^{(2)} = g(a_k^{(2)}) \tag{2}$$

$$E(z^{(2)}, y) \tag{3}$$

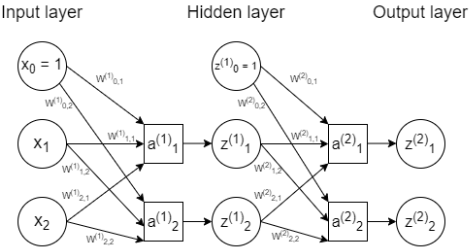


# Backward Pass for a 2-layer Network

Calculate the gradients for $W_{i,j}^{(1)}$ and $W_{j,k}^{(2)}$.

$$\frac{\partial E}{\partial W_{j,k}^{(2)}} = \frac{\partial E}{\partial a_k^{(2)}} z_j^{(1)} = \delta_k^{(2)} z_j^{(1)}, \quad \delta_k^{(2)} = \frac{\partial E}{\partial z_k^{(2)}} g'(a_k^{(2)}) \tag{4}$$

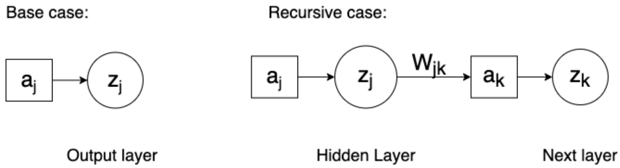
$$\frac{\partial E}{\partial W_{i,j}^{(1)}} = \frac{\partial E}{\partial a_j^{(1)}} x_i = \delta_j^{(1)} x_i, \qquad \delta_j^{(1)} = \left( \sum_k \delta_k^{(2)} W_{j,k}^{(2)} \right) g'(a_j^{(1)}) \tag{5}$$



# The recursive relationship

For unit $j$ of layer $\ell$, $\delta_j^{(\ell)} = \dfrac{\partial E}{\partial a_j^{(\ell)}}$.

$$\delta_j^{(\ell)} = \begin{cases} \dfrac{\partial E}{\partial z_j^{(\ell)}} \times g'(a_j^{(\ell)}), & \text{base case, } j \text{ is an output unit} \\ \left( \sum_k \delta_k^{(\ell+1)} W_{j,k}^{(\ell+1)} \right) \times g'(a_j^{(\ell)}), & \text{recursive case, } j \text{ is a hidden unit} \end{cases} \tag{6}$$



# A concrete example of forward and backward pass

Calculate $W^{(2)}_{j,k}$ and $W^{(1)}_{i,j}$ given the information below.

- The error function is the sum of squares error.

$$E = \sum_k (\hat{y}_k - y_k)^2$$

- The activation function is the sigmoid function.

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

# The derivative of $g(x)$

Sigmoid Function Derivative:

$$\frac{\partial g(x)}{\partial x} = \frac{1}{1+e^{-x}} \frac{e^{-x}}{1+e^{-x}} = g(x)(1-g(x))$$

It means that during forward propagation, we can save the intermediate values of $g(x)$ to directly compute $\frac{\partial g(x)}{\partial x}$.

# The recursive relationship

For the $i$-th layer output $x^{(i)}$:

$$\frac{\partial g(x^{(i)})}{\partial x^{(i)}} =$$

$$\begin{pmatrix} g(x_1^{(i)})(1 - g(x_1^{(i)})) & 0 & \cdots & 0 \\ 0 & g(x_2^{(i)})(1 - g(x_2^{(i)})) & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & g(x_d^{(i)})(1 - g(x_d^{(i)})) \end{pmatrix}$$

where $j$ indexes the $j$-th element in the $i$-th vector $g(x_j^{(i)})$.

# The recursive relationship

At i-th layer, assuming there are $d$ neurons:

Through backward propagation, the derivative w.r.t to $g(x_i)$ is denoted as $\delta_i = \frac{\partial E}{\partial g(x^{(i)})} \in \mathbb{R}^d$.

$$\delta_{i-1} = \frac{\partial E}{\partial g(x^{i-1})} = \frac{\partial E}{\partial g(x^{(i)})} \cdot \frac{\partial g(x^{(i)})}{\partial x^{(i)}} \cdot \frac{\partial x^{(i)}}{\partial g(x^{(i-1)})}$$

According to definition: $\frac{\partial x^{(i)}}{\partial g(x^{(i-1)})} = W_i \in \mathbb{R}^{d \times d'}$, where $d'$ is the number of neurons in $i-1$-th layer.

Therefore, we can conclude:

$$\delta_{i-1} = \delta_i \cdot \frac{\partial g(x^{(i)})}{\partial x^{(i)}} \cdot W_i$$

where $\delta_{i-1} \in \mathbb{R}^{d'}$

# The recursive relationship

Backward Propagation Algorithm:

- Initialize $W_i$ for all the layers.
- Feedforward $x$ into neural network and save intermediate values $g(x^{(1)}), g(x^{(2)}), \cdots$.
- Compute $\delta_n = \frac{\partial E}{\partial z}$.
- For i = n $\rightarrow$ 1; do
  - $\delta_{i-1} = \delta_i \cdot \frac{\partial g(x^{(i)})}{\partial x^{(i)}} \cdot W_i$
  - Compute $\frac{\partial E}{\partial W_i} = \delta_i \cdot \frac{\partial g(x^{(i)})}{\partial x^{(i)}} \cdot g(x^{(i-1)})$
- Obtain all $\frac{\partial E}{\partial W_i}$ for gradient descent.

# When should we use Neural Network?

- High dimensional or real-valued inputs, noisy (sensor) data.
- Form of target function is unknown (no model).
- Not important for humans to explain the learned function.

# When should we NOT use Neural Network?

- Difficult to determine the network structure (number of layers, number of neurons).
- Difficult to interpret weights, especially in multi-layered networks.
- Tendency to overfit in practice (poor predictions outside of the range of values it was trained on).

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- Time available for training and classification. → DT: fast. NN: slow to train and test.

# Revisiting Learning Goals

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