

Machine Learning

Neural Networks

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https://www.zubairkhalid.org/ee514_2025.html



Outline

- Neural networks connection with perceptron and logistic regression
- Neural networks notation
- Neural networks 'Forward Pass'
- Activation functions
- Learning neural network parameters
 - Back Propagation.



Connection with Logistic Regression and Perceptron:

- d number of real-valued inputs $x^{(1)}, x^{(2)}, \ldots, x^{(d)} \in \mathbf{R}$.
- Boolean output, $y \in \{0, 1\}$.

Perceptron Model:





Connection with Logistic Regression and Perceptron:

- d number of real-valued inputs $x^{(1)}, x^{(2)}, \ldots, x^{(d)} \in \mathbf{R}$.
- Boolean output, $y \in \{0, 1\}$.

Logistic Regression Model:





Logistic Regression Model, aka Sigmoid Neuron

Connection with Logistic Regression and Perceptron:





Neuron Model:

Compact Representation:



More Compact Representation:



- Neuron model: Characterized by weights, bias and activation function.
 - Weights w, bias b model parameters Activation function g hyperparameter



Neural Networks - Infamous XOR Problem:

• (1969) Minsky and Papert showed that a perceptron cannot classify XOR output.





(1,1)

(1, 0)

 x_1

(0,1)

(0, 0)

- Classes are not linearly separable: linear classifier cannot be used.
- We can either transfrorm features or project the data to higher dimensional space.
- We can however build a network of linear classifiers.



Neural Networks - Infamous XOR Problem:



• This is a neural network; a network of perceptrons, aka multi-layer perceptron (MLP).



Neural Networks

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• A neural network is a set of neurons organized in layers.



• Given the input and parameters of the neurons, we can determine the output by traversing layers from input to output. This is referred to as **Forward Pass**.

Neural Networks:

Example: 3-layer network, 2 hidden layers



- Output is a non-linear function
 - of a linear combination
 - of non-linear functions
 - of linear combinations
 - of non-linear functions
 - of linear combinations of inputs

- We do not count the input layer because there are no parameters assoictaed with it.
- Neural networks with neurons are also referred to as MLPs but we will refer to the network as MLP only when it is constructed using perceptrons.

Feedforward Neural Network: Output from one layer is an input to the next layer.



What kind of functions can be modeled by a neural network?

Intuition: XOR example







What kind of functions can be modeled by a neural network?

Intuition: Example (Sigmoid neuron)







- bias=0.5 indicated.
- weight for x is very large.
- weight for y is zero.

- bias=0.5 indicated.
- weight for y is very large.
- weight for x is zero.



Source: http://neuralnetworksanddeeplearning.com/chap4.html

What kind of functions can be modeled by a neural network?

Intuition: Example (Multi layer)

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What kind of functions can be modeled by a neural network?

Universal Approximation Theorem (Hornik 1991):

"A single hidden layer neural network with a linear output unit can approximate any continuous function arbitrarily well, given enough hidden units."

- The theorem results demonstrates the capability of neural network, but this does not mean there is a learning algorithm that can find the necessary parameter values.
- Since each neuron represents non-linearity, we can keep on increasing the number of neurons in the hidden layer to model the function. But this will also increase the number of parameters defining the model.
- Instead of adding more neurons in the same layer, we prefer to add more hidden layers because non-linear projections of a non-linear projection can model complex functions relatively easy.



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Neural Networks – Notation:

Single Neuron:

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- If we stack n training data in a matrix **X** of size $d \times n$, that is, $\mathbf{X} = [\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_n]$
- Using X and by defining 1 a row vector of ones of length n, we can define 'pre-activatation' operation $\mathbf{w}^T \mathbf{x} + b$ for all inputs compactly, denoted by

z as $\mathbf{z} = \mathbf{w}^T \mathbf{X} + b1$ $(1 \times n) (1 \times d)(d \times n) + (1 \times n)$	Pre-activation (Aggregation)	Linear transformation
Using activation function q , we obtain		

- $\mathbf{a} = g(\mathbf{z})$ Activation Non-linear transformation
- Activation function is operating on each entry of \mathbf{z} .
- **a** a row vector of length n; *i*-th entry represents an output for *i*-th input.

Neural Networks – Notation:

- L number of layers.
- Number of nodes in the $\ell\text{-th}$ layer, $m^{[\ell]}$
- $a_i^{[\ell]}$ denotes the output of *i*-th node in the ℓ -th layer. $\mathbf{a}^{[\ell]}$ vector of outputs of ℓ -th node.
- $\mathbf{a}^{[0]} = \mathbf{x}$ input layer.
- $\mathbf{a}^{[L]} = y$ output layer.

Example: 3-layer network, 2 hidden layers

• *L* = 3

•
$$m^{[1]} = 4, m^{[2]} = 3, m^{[3]} = 1$$





Neural Networks – Notation:

- $\mathbf{w}_i^{[\ell]}$ and $b_i^{[\ell]}$ denote the weight and bias associated with the *i*-th node in the ℓ -th layer respectively.
- $w_{i,j}^{[\ell]}$ denote the weight and bias associated with the j th input of the *i*-th node in the ℓ -th layer respectively.

Example: 3-layer network, 2 hidden layers



Layer 1 output

 $\begin{aligned} a_{1}^{[1]} &= g(z_{1}^{[1]}), \quad z_{1}^{[1]} = \mathbf{w}_{1}^{[1]^{T}} \mathbf{x} + b_{1}^{[1]} \\ a_{2}^{[1]} &= g(z_{2}^{[1]}), \quad z_{2}^{[1]} = \mathbf{w}_{2}^{[1]^{T}} \mathbf{x} + b_{2}^{[1]} \end{aligned}$ $\begin{aligned} a_{3}^{[1]} &= g(z_{3}^{[1]}), \quad z_{3}^{[1]} = \mathbf{w}_{3}^{[1]^{T}} \mathbf{x} + b_{3}^{[1]} \end{aligned}$ $\begin{aligned} a_{4}^{[1]} &= g(z_{4}^{[1]}), \quad z_{4}^{[1]} = \mathbf{w}_{4}^{[1]^{T}} \mathbf{x} + b_{4}^{[1]} \end{aligned}$

Neural Networks – Notation:

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• $\mathbf{W}^{[1]}$ and $\mathbf{b}^{[1]}$ are the parameters of the first layer.

Neural Networks – Forward Pass:

$$\begin{aligned} \mathbf{a}^{[1]} &= g(\mathbf{z}^{[1]}), \quad \mathbf{z}^{[1]} = \mathbf{W}^{[1]}\mathbf{x} + \mathbf{b}^{[1]} \\ \mathbf{z}^{[1]} &= \mathbf{W}^{[1]}\mathbf{a}^{[0]} + \mathbf{b}^{[1]} \end{aligned}$$

- Q. What is the size of W^[1]?
 A. No. of nodes × No. of inputs. 4 × 3
 No. of nodes × No. nodes in the previous layer.
- Q. Can we write output of second layer using the notation we have defined?

$$\mathbf{a}^{[2]} = g(\mathbf{z}^{[2]}), \quad \mathbf{z}^{[2]} = \mathbf{W}^{[2]}\mathbf{a}^{[1]} + \mathbf{b}^{[2]}$$

 $\mathbf{a}^{[3]} = g(\mathbf{z}^{[3]}), \quad \mathbf{z}^{[3]} = \mathbf{W}^{[3]}\mathbf{a}^{[2]} + \mathbf{b}^{[3]}$



- Q. What is the size of $\mathbf{W}^{[2]}$? 3×4
- Q. What is the size of $\mathbf{W}^{[3]}$? 1×3
- $\mathbf{W}^{[\ell]}$ and $\mathbf{b}^{[\ell]}$ are the parameters of the ℓ -th layer.



• Using these equations, we can determine the output given input and parameters of layers (Forward Pass).

<u>Neural Networks – Forward Pass Summary:</u>

$$\begin{aligned} \mathbf{a}^{[1]} &= g(\mathbf{z}^{[1]}), \quad \mathbf{z}^{[1]} = \mathbf{W}^{[1]}\mathbf{x} + \mathbf{b}^{[1]} \\ &\mathbf{z}^{[1]} = \mathbf{W}^{[1]}\mathbf{a}^{[0]} + \mathbf{b}^{[1]} \\ &(4 \times 1) = (4 \times 3)(3 \times 1) + (4 \times 1) \\ \mathbf{a}^{[2]} &= g(\mathbf{z}^{[2]}), \quad \mathbf{z}^{[2]} = \mathbf{W}^{[2]}\mathbf{a}^{[1]} + \mathbf{b}^{[2]} \\ &(3 \times 1) = (3 \times 4)(4 \times 1) + (3 \times 1) \\ \mathbf{a}^{[3]} &= g(\mathbf{z}^{[3]}), \quad \mathbf{z}^{[3]} = \mathbf{W}^{[3]}\mathbf{a}^{[2]} + \mathbf{b}^{[3]} \\ &(1 \times 1) = (1 \times 3)(3 \times 1) + (1 \times 1) \end{aligned}$$

• In general, we have

$$\mathbf{a}^{[\ell]} = g(\mathbf{z}^{[\ell]}), \quad \mathbf{z}^{[\ell]} = \mathbf{W}^{[\ell]} \mathbf{a}^{[\ell-1]} + \mathbf{b}^{[\ell]}$$
for $\ell = 1, 2, \dots, L$, where $\mathbf{a}^{[0]} = \mathbf{x}$.
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- How many parameters do we have by the way?
- This formulation is for one input **x**.
- How can we extend this formulation n inputs?

<u>Neural Networks – Forward Pass – Incorporating all Inputs:</u>



<u>Neural Networks – Forward Pass Summary – All Inputs:</u>

$$\begin{aligned} \mathbf{A}^{[1]} &= g(\mathbf{Z}^{[1]}), \ \mathbf{Z}^{[1]} = \mathbf{W}^{[1]}\mathbf{X} + \mathbf{b}^{[1]} \\ &\mathbf{Z}^{[1]} = \mathbf{W}^{[1]}\mathbf{A}^{[0]} + \mathbf{b}^{[1]} \\ &(4 \times n) = (4 \times 3)(3 \times n) + (4 \times n) \\ \mathbf{A}^{[2]} &= g(\mathbf{Z}^{[2]}), \ \mathbf{Z}^{[2]} = \mathbf{W}^{[2]}\mathbf{A}^{[1]} + \mathbf{b}^{[2]} \\ &(3 \times n) = (3 \times 4)(4 \times n) + (3 \times n) \end{aligned}$$

$$\mathbf{A}^{[3]} = g(\mathbf{Z}^{[3]}), \quad \mathbf{Z}^{[3]} = \mathbf{W}^{[3]}\mathbf{A}^{[2]} + \mathbf{b}^{[3]}$$
$$(1 \times n) = (1 \times 3)(3 \times n) + (1 \times n)$$



• In general, we have

$$\mathbf{A}^{[\ell]} = g(\mathbf{Z}^{[\ell]}), \quad \mathbf{Z}^{[\ell]} = \mathbf{W}^{[\ell]}\mathbf{A}^{[\ell-1]} + \mathbf{b}^{[\ell]} \quad \ell = 1, 2, \dots, L$$



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Activation Function:

- Single neuron is characterized by weights, bias and activation function g.
- We require g to be some non-linear function.
 - Why?
 - If g is a linear function, e.g., identity or $g(z) = \alpha z + \beta$

 $g(\mathbf{w}^T \mathbf{x} + b) = \alpha(\mathbf{w}^T \mathbf{x} + b) + \beta \equiv \tilde{\mathbf{w}}^T \mathbf{x} + \tilde{b}$

- Consequently, different layers of the network can be equivalently represented by a single linear transformation.
- We require active function g to be differentiable if we want to use gradient descent.
- Some standard activation functions:
 - identity (linear), step, rectified linear, leaky rectified linear sigmoid, tanh





Step:

• Step function is defined as

 $g(z) = \begin{cases} 1 & z > 0\\ 0 & z < 0 \end{cases}$

• We have used this activation function before. Perceptron



• Issues: Non-differentiable and only supports binary classification.

Linear:

$g(z) = \alpha z + \beta$

- Constant derivative, $g'(z) = \alpha$; cannot be used for backpropagation.
- Used for simple linear regression model.
- Does not capture non-linearities irrespective of the depth of the network.



Sigmoid:

 $g(z) = \sigma(z) = \frac{1}{1 + e^{-z}}$ (Sigmoid: because of S shaped curve)

- Squishes values in $(-\infty, \infty)$ to (0, 1), bounded, strictly increasing.
- Suitable for output neurons of neural networks used for classification.
- We have used this activation function before. Logistic regression.
- It is differentiable. g'(z) = g(z)(1 g(z))

<u>Issues:</u>

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• Saturation Problem or Vanishing Gradient:

Neuron is saturated considered when it reaches its maximum or minimum value.

g(z) = 0 or g(z) = 1. Consequence: g'(z) = g(z)(1 - g'(z)) = 0 (poor learning for deep networks)

• Sigmoid outputs are not zero-centered:

Due to this, the gradient of all the weights for a neuron is either positive or negative. Consequently, the weights move in one direction. This issue is less severe as gradients are added across the batch and mitigate this.



tanh (Hyperbolic tangent):

$$g(z) = \tanh(z) = 2\sigma(2z) - 1 = \frac{2}{1 + e^{-2z}} - 1 = \frac{e^z - e^{-z}}{e^z + e^{-z}}$$

- Scaled version of sigmoid.
- Squishes values in $(-\infty, \infty)$ to (-1, 1), bounded, strictly increasing.
- Unlike Sigmoid, tanh is a zero-centered function and resolve the issue associated with the sigmoid.
- It is differentiable. $g'(z) = 1 (g(z))^2$

<u>Issues:</u>

• Saturation Problem or Vanishing Gradient:

Neuron is saturated considered when it reaches its maximum or minimum value.

$$g(z) = -1$$
 or $g(z) = 1$. Consequence: $g'(z) = 1 - (g(z))^2 = 0$ (poor learning for deep networks)





Rectifier – Rectified Linear Unit (ReLu):

 $g(z) = \max(0, z) = \begin{cases} z & z \ge 0\\ 0 & z < 0 \end{cases}$ • Super simple.

- It is differentiable. $g'(z) = \begin{cases} 1 & z \ge 0 \\ 0 & z < 0 \end{cases}$
- It is the most used activation function.

Why?

- Unlike Sigmoid and tanh that required the computation of exponents, easier to compute.
- It only activates for which the output is non-negative. It deactives the neurons if the pre-activation output is less than 0. This makes ReLu computationally efficient relative to sigmoid and tanh.

<u>Issues:</u>

- ReLu is not zero centered. As indicated earlier, this is not a major issue and training the network longer can resolve this.
- ReLu does not suffer from saturation problem. Vanishing gradient however occurs for negative values; dead neuron.



Different variants of ReLu have been proposed to overcome these issues.



Leaky Rectified Linear Unit (Leaky ReLu):

$$g(z) = \begin{cases} z & z \ge 0\\ \alpha z & z < 0 \end{cases}$$

- This resolves the issues associated with ReLu to an extent.
 - Due to non-zero output for negative values, it keeps neurons alive.
 - It is not zero centered but close to it.
- If α is any value less than 0.01, randomized ReLu.
- To be precise, $\alpha = 0.01$ for leakly ReLu.

• It is differentiable. $g'(z) = \begin{cases} 1 & z \ge 0 \\ \alpha & z < 0 \end{cases}$



We use rectified linear, leaky rectified linear sigmoid and tanh for hidden layer.



Activation Function for output layer:

- Identity function if the problem is regression.
- Sigmoid function if output needs to be between 0 and 1.
 - e.g., probability value.
 - classification problem.
- Softmax if output needs to be probability distribution.
 - multi-class classification problem.



Choice of the Activation Function:

- For classification tasks;
 - we prefer to use sigmoid, tanh functions and their combinations.
- Due to the saturation problem, sigmoids and tanh functions are sometimes avoided.
- As indicated earlier, ReLU function is mostly used (computationally fast).
 - ReLu variants are used to resolve a dead neuron issue (e.g., Leaky ReLu).
- It must be noted that ReLU function is only used in the hidden layers.
- Start with ReLu or leaky/randomized Relu and if the results are not satisfactory, you may try other activation functions.



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Learning Weights:

• Given the training data, we want to learn the weights (weight matrices+bias vectors) for hidden layers and output layer.

Notation revisit:

- L number of layers.
- Number of nodes in the $\ell\text{-th}$ layer, $m^{[\ell]}$
- $a_i^{[\ell]}$ denotes the output of *i*-th node in the ℓ -th layer.
- $\mathbf{a}^{[\ell]}$ output of ℓ -th layer, $\mathbf{a}^{[0]} = \mathbf{x}$.
- $\mathbf{a}^{[L]} = y$ output layer.
- $\mathbf{w}_i^{[\ell]}$ and $b_i^{[\ell]}$ denote the weight and bias associated with the *i*-th node in the ℓ -th layer respectively.
- $w_{i,j}^{[\ell]}$ denotes the weight associated with the *j*-th input of the *i*-th node in the ℓ -th layer.



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Learning Weights:

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• We assume we have training data D given by

 $D = \{ (\mathbf{x_1}, y_1), (\mathbf{x_2}, y_2), \dots, (\mathbf{x_n}, y_n) \} \subseteq \mathcal{X}^d \times \mathcal{Y}$

- Consider a network with d nodes (features) at the input layer, 1 output node and any number of hidden layers.
- Define the loss function (for regression problem):

$$\mathcal{L} = \frac{1}{2} \sum_{i=1}^{n} \left(\tilde{y}_i - y_i \right)^2$$

We use log loss here if we have a classification problem and output represents probability.

where \tilde{y}_i denotes the output of the neural network for *i*-th input.

- We can use gradient descent to learn the weight matrices and bias vectors.
- Given our prior knowledge, output y is a composite function of input x. Therefore, it is continuous and differentiable and we can use chain rule to compute the gradient.

We use a method called 'Back Propagation' to implement the chain rule for the computation the gradient.

Back Propagation – Key Idea:

• We compute the loss function using forward pass.



- Gradient descent:
- $w_{i,j}^{[\ell]} = w_{i,j}^{[\ell]} \alpha \frac{\partial \mathcal{L}}{\partial w_{i,j}^{[\ell]}}$

Learning problem reduces to the question of calculating gradient (partial derivatives) of loss function.

The weights are the only parameters that can be

modified to make the loss

function as low as possible.

• We compute the derivative by propagating the total loss at the output node back into the neural network to determine the contribution of every node in the loss. (Back Propagation)



Back Propagation – Example:

- 2 layer with 2 neurons in the hidden layer, 2 inputs, 2 outputs network.
- Assuming sigmoid as activation function, that is, $g(z) = \sigma(z)$.



• Given training data

 $x^{(1)}=0.05, \quad x^{(2)}=0.1, \quad y^{(1)}=0.01, \quad y^{(2)}=0.99$

• Initial values of weights and biases:

 $w_{1,1}^{[1]} = 0.15, \ w_{1,2}^{[1]} = 0.2, \ w_{2,1}^{[1]} = 0.25, \ w_{2,2}^{[1]} = 0.3, \ b_1^{[1]} = 0.35, \ b_2^{[1]} = 0.35.$

$$w_{1,1}^{[2]} = 0.4, \ w_{1,2}^{[2]} = 0.45, \ w_{2,1}^{[2]} = 0.5, \ w_{2,2}^{[2]} = 0.55, \ b_1^{[1]} = 0.6, \ b_2^{[1]} = 0.6.$$

Back Propagation – Example:



• Loss function (noting output is a vector): $\mathcal{L} = \frac{1}{2} \| (\tilde{y}^{(1)} - y^{(1)})^2 - (\tilde{y}^{(2)} - y^{(2)})^2 \|^2$ $\mathcal{L} = \frac{1}{2} \| (0.01, 0.99) - (0.7514, 0.7729) \|^2 = 0.2984$

Forward Pass				
$a_1^{[1]} = g(z_1^{[1]}),$	$z_1^{[1]} = \mathbf{w}_1^{[1]^T} \mathbf{x} + b_1^{[1]}$			
$a_2^{[1]} = g(z_2^{[1]}),$	$z_2^{[1]} = \mathbf{w}_2^{[1]^T} \mathbf{x} + b_2^{[1]}$			
$a_1^{[2]} = g(z_1^{[2]}),$	$z_1^{[2]} = \mathbf{w}_1^{[2]^T} \mathbf{x} + b_1^{[2]}$			
$a_2^{[2]} = g(z_2^{[2]}),$	$z_2^{[2]} = \mathbf{w}_2^{[2]^T} \mathbf{x} + b_2^{[2]}$			

$$z_{1}^{[1]} = w_{1,1}^{[1]} x^{(1)} + w_{1,2}^{[1]} x^{(2)} + b_{1}^{[1]} = 0.3775, \quad a_{1}^{[1]} = g(0.3775) = 0.5933$$

$$z_{2}^{[1]} = \mathbf{w}_{2}^{[1]^{T}} \mathbf{x} + b_{2}^{[1]} = 0.3925, \quad a_{2}^{[1]} = g(0.3925) = 0.5969$$

$$z_{1}^{[2]} = \mathbf{w}_{1}^{[2]^{T}} \mathbf{x} + b_{1}^{[2]} = 1.106, \quad a_{1}^{[2]} = g(1.106) = 0.7514 = \tilde{y}^{(1)}$$

$$z_{2}^{[2]} = \mathbf{w}_{2}^{[2]^{T}} \mathbf{x} + b_{2}^{[2]} = 1.225, \quad a_{2}^{[2]} = g(1.225) = 0.7729 = \tilde{y}^{(2)}$$

Nothing fancy so far, we have computed the output and loss by traversing neural network. LUMS Let's compute the contribution of loss by each node; back propagate the loss.

Back Propagation – Example:



• Consider a case when we want to compute $\frac{\partial \mathcal{L}}{\partial w_{1,1}^{[2]}}$

• Traverse the path from the loss function back to the weight $w_{1,1}^{[2]}$:



Back Propagation – Example:



- Consider a case when we want to compute $-\frac{1}{6}$
- Traverse the path from the loss function back to the weight $w_{1,1}^{[1]}$. There are two paths from the output to the weight $w_{1,1}^{[1]}$. In other words, $w_{1,1}^{[1]}$ is contributing to both the outputs.

$$\frac{\partial \mathcal{L}}{\partial w_{1,1}^{[1]}} = \frac{\partial \mathcal{L}}{\partial \tilde{y}^{(1)}} \frac{\partial \tilde{y}^{(1)}}{\partial z_{1}^{[2]}} \frac{\partial z_{1}^{[2]}}{\partial a_{1}^{[1]}} \frac{\partial a_{1}^{[1]}}{\partial z_{1}^{[1]}} \frac{\partial z_{1}^{[1]}}{\partial w_{1,1}^{[1]}} + \frac{\partial \mathcal{L}}{\partial \tilde{y}^{(2)}} \frac{\partial \tilde{y}^{(2)}}{\partial z_{2}^{[2]}} \frac{\partial z_{2}^{[2]}}{\partial a_{1}^{[1]}} \frac{\partial a_{1}^{[1]}}{\partial z_{1}^{[1]}} \frac{\partial z_{1}^{[1]}}{\partial w_{1,1}^{[1]}}$$

• Looking tedious but the concept is very straightforward. I encourage you to write one partial derivative using the same approach to strengthen the concept.





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Back Propagation – Vectorization:

- We compute loss function \mathcal{L} using forward pass.
- We update $\mathbf{W}^{[\ell]}$ and $\mathbf{b}^{[\ell]}$ using gradient descent as:

$$\mathbf{W}^{[\ell]} = \mathbf{W}^{[\ell]} - \alpha \frac{\partial \mathcal{L}}{\partial \mathbf{W}^{[\ell]}} \qquad \mathbf{b}^{[\ell]} = \mathbf{b}^{[\ell]} - \alpha \frac{\partial \mathcal{L}}{\partial \mathbf{b}^{[\ell]}}$$
Partial Derivatives:

$\frac{\partial \mathcal{L}}{\partial \mathbf{W}^{[3]}} = \frac{\partial \mathcal{L}}{\partial \mathbf{a}^{[3]}} \frac{\partial \mathbf{a}^{[3]}}{\partial \mathbf{z}^{[3]}} \frac{\partial \mathbf{z}^{[3]}}{\partial \mathbf{W}^{[3]}}$	$\frac{\partial \mathcal{L}}{\partial \mathbf{b}^{[3]}} =$	$\frac{\partial \mathcal{L}}{\partial \mathbf{a}^{[3]}}$	$\frac{\partial \mathbf{a}^{[3]}}{\partial \mathbf{z}^{[3]}}$	$\frac{\partial \mathbf{z}^{[3]}}{\partial \mathbf{b}^{[3]}}$
$\frac{\partial \mathcal{L}}{\partial \mathbf{W}^{[2]}} = \frac{\partial \mathcal{L}}{\partial \mathbf{a}^{[3]}} \frac{\partial \mathbf{a}^{[3]}}{\partial \mathbf{z}^{[3]}} \frac{\partial \mathbf{z}^{[3]}}{\partial \mathbf{a}^{[2]}} \frac{\partial \mathbf{a}^{[2]}}{\partial \mathbf{z}^{[2]}} \frac{\partial \mathbf{z}^{[2]}}{\partial \mathbf{W}^{[2]}}$				
$\frac{\partial \mathcal{L}}{\partial \mathbf{b}^{[2]}} = \frac{\partial \mathcal{L}}{\partial \mathbf{a}^{[3]}} \frac{\partial \mathbf{a}^{[3]}}{\partial \mathbf{z}^{[3]}} \frac{\partial \mathbf{z}^{[3]}}{\partial \mathbf{a}^{[2]}} \frac{\partial \mathbf{a}^{[2]}}{\partial \mathbf{z}^{[2]}} \frac{\partial \mathbf{z}^{[2]}}{\partial \mathbf{b}^{[2]}}$				
$\frac{\partial \mathcal{L}}{\partial \mathbf{W}^{[1]}} = \frac{\partial \mathcal{L}}{\partial \mathbf{a}^{[3]}} \frac{\partial \mathbf{a}^{[3]}}{\partial \mathbf{z}^{[3]}} \frac{\partial \mathbf{z}^{[3]}}{\partial \mathbf{a}^{[2]}} \frac{\partial \mathbf{a}^{[2]}}{\partial \mathbf{z}^{[2]}} \frac{\partial \mathbf{z}^{[2]}}{\partial \mathbf{a}^{[1]}} \frac{\partial \mathbf{z}^{[2]}}{\partial \mathbf{z}^{[2]}} \frac{\partial \mathbf{z}^{[2]}$	$\mathbf{x}^{[1]} = rac{\partial \mathbf{z}^{[1]}}{\partial \mathbf{W}^{[1]}}$	<u>[]</u>		
$\frac{\partial \mathcal{L}}{\partial \mathbf{b}^{[1]}} = \frac{\partial \mathcal{L}}{\partial \mathbf{a}^{[3]}} \frac{\partial \mathbf{a}^{[3]}}{\partial \mathbf{z}^{[3]}} \frac{\partial \mathbf{z}^{[3]}}{\partial \mathbf{a}^{[2]}} \frac{\partial \mathbf{a}^{[2]}}{\partial \mathbf{z}^{[2]}} \frac{\partial \mathbf{z}^{[2]}}{\partial \mathbf{a}^{[1]}} \frac{\partial \mathbf{a}^{[2]}}{\partial \mathbf{z}^{[2]}} \frac{\partial \mathbf{z}^{[2]}}{\partial \mathbf{z}^{[2]}} \frac{\partial \mathbf{z}^{[2]}$	$rac{\left[1 ight]}{\left[1 ight]}rac{\partial \mathbf{z}^{\left[1 ight]}}{\partial \mathbf{b}^{\left[1 ight]}}$			
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Back Propagation – Vectorization:

Partial Derivatives:

$\frac{\partial \mathcal{L}}{\partial \mathbf{W}^{[3]}} =$	$= \frac{\partial \mathcal{L}}{\partial \mathbf{a}^{[3]}} \frac{\partial \mathbf{a}^{[3]}}{\partial \mathbf{z}^{[3]}} \frac{\partial \mathbf{z}^{[3]}}{\partial \mathbf{W}^{[3]}}$	$rac{\partial \mathcal{L}}{\partial \mathbf{b}^{[3]}} = rac{\partial \mathcal{L}}{\partial \mathbf{a}^{[3]}}$	$\frac{\partial \mathbf{a}^{[3]}}{\partial \mathbf{z}^{[3]}} \frac{\partial \mathbf{z}^{[3]}}{\partial \mathbf{b}^{[3]}}$	$\frac{\partial \mathcal{L}}{\mathbf{W}^{[3]}} =$	$=rac{\partial \mathcal{L}}{\partial \mathbf{z}^{[3]}} rac{\partial \mathbf{z}^{[3]}}{\partial \mathbf{W}^{[3]}}$	$rac{\partial \mathcal{L}}{\mathbf{b}^{[3]}} =$	$rac{\partial \mathcal{L}}{\partial \mathbf{z}^{[3]}} rac{\partial \mathbf{z}^{[3]}}{\partial \mathbf{b}^{[3]}}$
$rac{\partial \mathcal{L}}{\partial \mathbf{W}^{[2]}} =$	$= \frac{\partial \mathcal{L}}{\partial \mathbf{a}^{[3]}} \frac{\partial \mathbf{a}^{[3]}}{\partial \mathbf{z}^{[3]}} \frac{\partial \mathbf{z}^{[3]}}{\partial \mathbf{a}^{[2]}} \frac{\partial \mathbf{a}^{[2]}}{\partial \mathbf{z}^{[2]}} \frac{\partial \mathbf{a}^{[2]}}{\partial \mathbf{z}^{[2]}} \frac{\partial \mathbf{a}^{[2]}}{\partial \mathbf{z}^{[2]}}$	$rac{\partial \mathbf{z}^{[2]}}{\partial \mathbf{W}^{[2]}}$		$rac{\partial \mathcal{L}}{\partial \mathbf{W}^{[2]}}$	$=rac{\partial \mathcal{L}}{\partial \mathbf{z}^{[2]}}rac{\partial \mathbf{z}^{[2]}}{\partial \mathbf{W}^{[2]}}$		
$\frac{\partial \mathcal{L}}{\partial \mathbf{b}^{[2]}} =$	$\frac{\partial \mathcal{L}}{\partial \mathbf{a}^{[3]}} \frac{\partial \mathbf{a}^{[3]}}{\partial \mathbf{z}^{[3]}} \frac{\partial \mathbf{z}^{[3]}}{\partial \mathbf{a}^{[2]}} \frac{\partial \mathbf{a}^{[2]}}{\partial \mathbf{z}^{[2]}} \frac{\partial \mathbf{a}^{$	$rac{\mathbf{z}^{[2]}}{\mathbf{b}^{[2]}}$		$rac{\partial \mathcal{L}}{\partial \mathbf{b}^{[2]}}$ =	$= \frac{\partial \mathcal{L}}{\partial \mathbf{z}^{[2]}} \frac{\partial \mathbf{z}^{[2]}}{\partial \mathbf{b}^{[2]}}$		
$rac{\partial \mathcal{L}}{\partial \mathbf{W}^{[1]}} =$	$\frac{\partial \mathcal{L}}{\partial \mathbf{a}^{[3]}} \frac{\partial \mathbf{a}^{[3]}}{\partial \mathbf{z}^{[3]}} \frac{\partial \mathbf{z}^{[3]}}{\partial \mathbf{a}^{[2]}} \frac{\partial \mathbf{a}^{[2]}}{\partial \mathbf{z}^{[2]}} \frac{\partial \mathbf{a}^{$	$\mathbf{\hat{z}^{[2]}}_{\mathbf{a}^{[1]}} rac{\partial \mathbf{a}^{[1]}}{\partial \mathbf{z}^{[1]}} rac{\partial \mathbf{z}^{[1]}}{\partial \mathbf{W}^{[1]}}$] 1]	$rac{\partial \mathcal{L}}{\partial \mathbf{W}^{[1]}}$ =	$=rac{\partial \mathcal{L}}{\partial \mathbf{z}^{[1]}}rac{\partial \mathbf{z}^{[1]}}{\partial \mathbf{W}^{[1]}}$		
$\frac{\partial \mathcal{L}}{\partial \mathbf{b}^{[1]}} = \frac{1}{2}$	$\frac{\partial \mathcal{L}}{\partial \mathbf{a}^{[3]}} \frac{\partial \mathbf{a}^{[3]}}{\partial \mathbf{z}^{[3]}} \frac{\partial \mathbf{z}^{[3]}}{\partial \mathbf{a}^{[2]}} \frac{\partial \mathbf{z}^{[2]}}{\partial \mathbf{z}^{[2]}} \frac{\partial \mathbf{z}^{$	$\mathbf{z}^{[2]} = \frac{\partial \mathbf{a}^{[1]}}{\partial \mathbf{z}^{[1]}} \frac{\partial \mathbf{z}^{[1]}}{\partial \mathbf{b}^{[1]}}$		$rac{\partial \mathcal{L}}{\partial \mathbf{b}^{[1]}} =$	$\frac{\partial \mathcal{L}}{\partial \mathbf{z}^{[1]}} \frac{\partial \mathbf{z}^{[1]}}{\partial \mathbf{b}^{[1]}}$		

• We need to develop capability to compute $\frac{\partial \mathcal{L}}{\partial \mathbf{z}^{[\ell]}}$, $\frac{\partial \mathbf{z}^{[\ell]}}{\partial \mathbf{W}^{[\ell]}}$ and $\frac{\partial \mathbf{z}^{[\ell]}}{\partial \mathbf{b}^{[\ell]}}$.



Back Propagation – Vectorization:

• We first compute
$$\frac{\partial \mathcal{L}}{\partial \mathbf{z}^{[\ell]}}$$
 for $\ell = L$ (last layer), that is,

$$\frac{\partial \mathcal{L}}{\partial \mathbf{z}^{[L]}} = \frac{\partial \mathcal{L}}{\partial \mathbf{a}^{[L]}} \frac{\partial \mathbf{a}^{[L]}}{\partial \mathbf{z}^{[L]}} \qquad \text{In literature, we often denote } \frac{\partial \mathcal{L}}{\partial \mathbf{z}^{[\ell]}} \text{ with } \delta^{\ell}.$$

 $\frac{\partial \mathcal{L}}{\partial \mathbf{a}^{[L]}} = \mathbf{a}^{[L]} - y$

- Derivative of loss function with respect to activation function output of the last layer:
 - It depends on the definition of the loss function.
 - Regression:

Squared error: $\mathcal{L} = \frac{1}{2} (\mathbf{a}^{[L]} - y)^2 = \frac{1}{2} \|\mathbf{a}^{[L]} - y\|^2$

• Classification:

Log-loss (cross entropy):
$$\mathcal{L} = -y \log \mathbf{a}^{[L]} + (1-y) \log \left(1 - \mathbf{a}^{[L]}\right)$$
 $\frac{\partial \mathcal{L}}{\partial \mathbf{a}^{[L]}} = -\left(\frac{y}{\mathbf{a}^{[L]}} - \frac{1-y}{1-\mathbf{a}^{[L]}}\right)$



Back Propagation – Vectorization:

• Derivative of activation function with respect to pre-activation output:

$$\mathbf{a}^{[\ell]} = g(\mathbf{z}^{[\ell]})$$

$$\frac{\partial \mathbf{a}^{[\ell]}}{\partial \mathbf{z}^{[\ell]}} = g'(\mathbf{z}^{[\ell]}) = \sigma(\mathbf{z}^{[\ell]}) \odot \left(1 - \sigma(\mathbf{z}^{[\ell]})\right)$$

if sigmoid is used as an activation function.

- $\bullet~\odot$ represents the element wise multiplication of matrices or vectors.
- Combining these two, we have

$$\frac{\partial \mathcal{L}}{\partial \mathbf{z}^{[L]}} = \frac{\partial \mathcal{L}}{\partial \mathbf{a}^{[L]}} \odot \frac{\partial \mathbf{a}^{[L]}}{\partial \mathbf{z}^{[L]}} = \frac{\partial \mathcal{L}}{\partial \mathbf{a}^{[L]}} \odot g'(\mathbf{z}^{[L]})$$

• We have computed $\frac{\partial \mathcal{L}}{\partial \mathbf{z}^{[\ell]}}$ for $\ell = L$ (last layer).



Back Propagation – Vectorization:

• Observing this,

 $\frac{\partial \mathcal{L}}{\partial \mathbf{W}^{[1]}} = \frac{\partial \mathcal{L}}{\partial \mathbf{a}^{[3]}} \frac{\partial \mathbf{a}^{[3]}}{\partial \mathbf{z}^{[3]}} \frac{\partial \mathbf{z}^{[3]}}{\partial \mathbf{a}^{[2]}} \frac{\partial \mathbf{a}^{[2]}}{\partial \mathbf{z}^{[2]}} \frac{\partial \mathbf{z}^{[2]}}{\partial \mathbf{a}^{[1]}} \frac{\partial \mathbf{a}^{[1]}}{\partial \mathbf{z}^{[1]}} \frac{\partial \mathbf{z}^{[1]}}{\partial \mathbf{W}^{[1]}}$

we can write

 $\frac{\partial \mathcal{L}}{\partial \mathbf{z}^{[\ell]}} = \frac{\partial \mathcal{L}}{\partial \mathbf{z}^{[\ell+1]}} \frac{\partial \mathbf{z}^{[\ell+1]}}{\partial \mathbf{a}^{[\ell]}} \frac{\partial \mathbf{a}^{[\ell]}}{\partial \mathbf{z}^{[\ell]}}$

• Derivative of pre-activation output of the layer with respect to the input of the current layer or output of the previous layer:

$$\mathbf{z}^{[\ell+1]} = \mathbf{W}^{[\ell+1]} \mathbf{a}^{[\ell]} + \mathbf{b}^{[\ell+1]} \qquad \qquad \frac{\partial \mathbf{z}^{[\ell+1]}}{\partial \mathbf{a}^{[\ell]}} = \mathbf{W}^{[\ell+1]}$$

• Using these results, we can write

$$\frac{\partial \mathcal{L}}{\partial \mathbf{z}^{[\ell]}} = \left(\mathbf{W}^{[\ell+1]^T} \ \frac{\partial \mathcal{L}}{\partial \mathbf{z}^{[\ell+1]}} \right) \ \odot \ g'(\mathbf{z}^{[\ell]})$$

changed order to keep the consistency of the multiplication of matrices.



Back Propagation – Vectorization:

- Derivative of pre-activation output of the layer with respect to weight or bias:
- We know that

$$\mathbf{z}^{[\ell]} = \mathbf{W}^{[\ell]} \mathbf{a}^{[\ell-1]} + \mathbf{b}^{[\ell]} \qquad \qquad \frac{\partial \mathbf{z}^{[\ell]}}{\partial \mathbf{W}^{[\ell]}} = \mathbf{a}^{[\ell-1]} \qquad \qquad \frac{\partial \mathbf{z}^{[\ell]}}{\partial \mathbf{b}^{[\ell]}} = 1$$

• Finally, we obtain

$$rac{\partial \mathcal{L}}{\partial \mathbf{W}^{[\ell]}} = rac{\partial \mathcal{L}}{\partial \mathbf{z}^{[\ell]}} rac{\partial \mathbf{z}^{[\ell]}}{\partial \mathbf{W}^{[1]}} = rac{\partial \mathcal{L}}{\partial \mathbf{z}^{[\ell]}} \ \mathbf{a}^{[\ell-1]^T}$$

$\partial \mathcal{L}$	$\partial \mathcal{L}$	$\partial \mathbf{z}^{[\ell]}$		$\partial \mathcal{L}$
$\overline{\mathbf{b}^{[\ell]}} =$	$\overline{\partial \mathbf{z}^{[\ell]}}$	$\overline{\partial \mathbf{b}^{[1]}}$	=	$\overline{\partial \mathbf{z}^{[\ell]}}$



Back Propagation – Vectorization:

Key Equations:

• Gradients with respect to weight and bias:

$$\frac{\partial \mathcal{L}}{\partial \mathbf{W}^{[\ell]}} = \frac{\partial \mathcal{L}}{\partial \mathbf{z}^{[\ell]}} \ \mathbf{a}^{[\ell-1]^T} \qquad \qquad \frac{\partial \mathcal{L}}{\partial \mathbf{b}^{[\ell]}} = \frac{\partial \mathcal{L}}{\partial \mathbf{z}^{[\ell]}}$$

• We compute $\frac{\partial \mathcal{L}}{\partial \mathbf{z}^{[\ell]}}$ as

$$\frac{\partial \mathcal{L}}{\partial \mathbf{z}^{[\ell]}} = \left(\mathbf{W}^{[\ell+1]^T} \ \frac{\partial \mathcal{L}}{\partial \mathbf{z}^{[\ell+1]}} \right) \ \odot \ g'(\mathbf{z}^{[\ell]})$$

• Base case:

$$\frac{\partial \mathcal{L}}{\partial \mathbf{z}^{[L]}} = \frac{\partial \mathcal{L}}{\partial \mathbf{a}^{[L]}} \odot g'(\mathbf{z}^{[L]})$$

• For sigmoid activation function:

$$g'(\mathbf{z}^{[\ell]}) = \sigma(\mathbf{z}^{[\ell]}) \odot \left(1 - \sigma(\mathbf{z}^{[\ell]})\right)$$



Back Propagation – Vectorization:

Interpretation of Key Equations:



Back Propagation – Vectorization:

• Assuming squared error and sigmoid activation, let's see if it all makes sense. We want to compute:



$$\frac{\partial \mathcal{L}}{\mathbf{W}^{[1]}} = \frac{\partial \mathcal{L}}{\partial \mathbf{z}^{[1]}} \mathbf{a}^{[0]^T}$$
$$\times 3 \qquad 4 \times 1 \qquad 1 \times 3$$

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References:

- TM Chapter 4
- CB Chapter 5 (See Section 5.3 for back propagation)
- 'Neural Networks: A Comprehensive Foundation' and 'Neural Networks and Learning Machines' by Simon Haykin
- <u>http://neuralnetworksanddeeplearning.com/</u>

