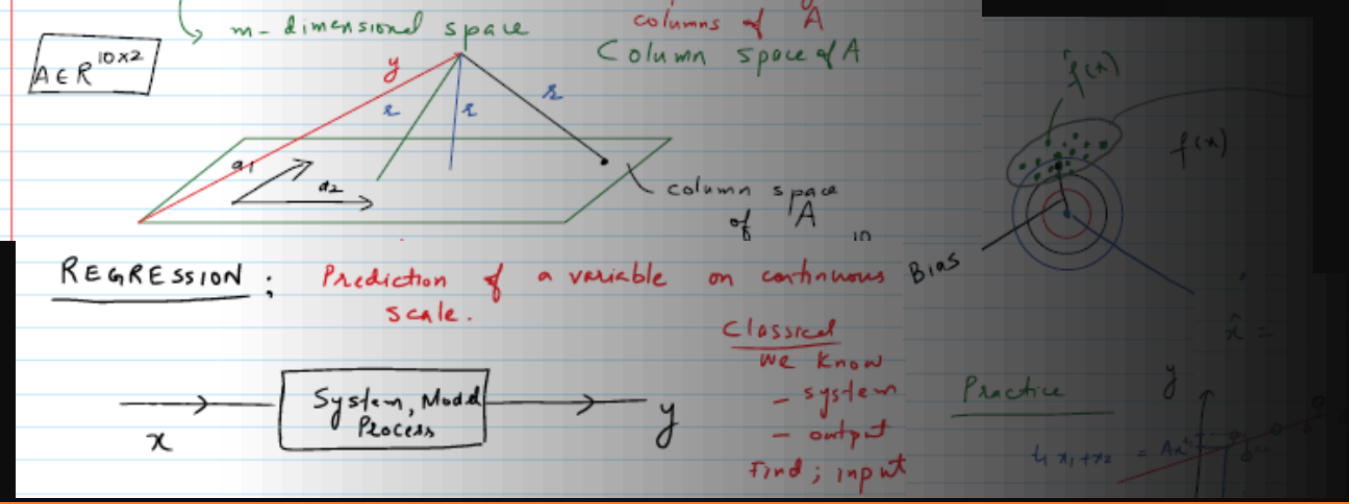

Machine Learning
EE514 – CS535

Neural Networks

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https://www.zubairkhalid.org/ee514_2023.html

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Outline

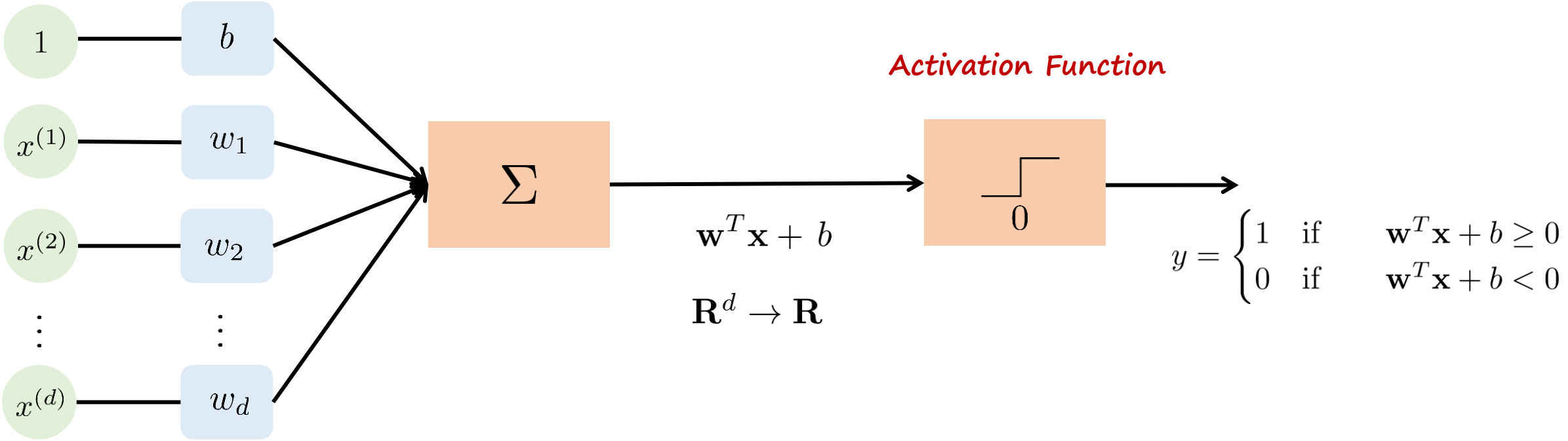
- Neural networks connection with perceptron and logistic regression
- Neural networks notation
- Neural networks 'Forward Pass'
- Activation functions
- Learning neural network parameters
  - Back Propagation.

Neural Networks

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:

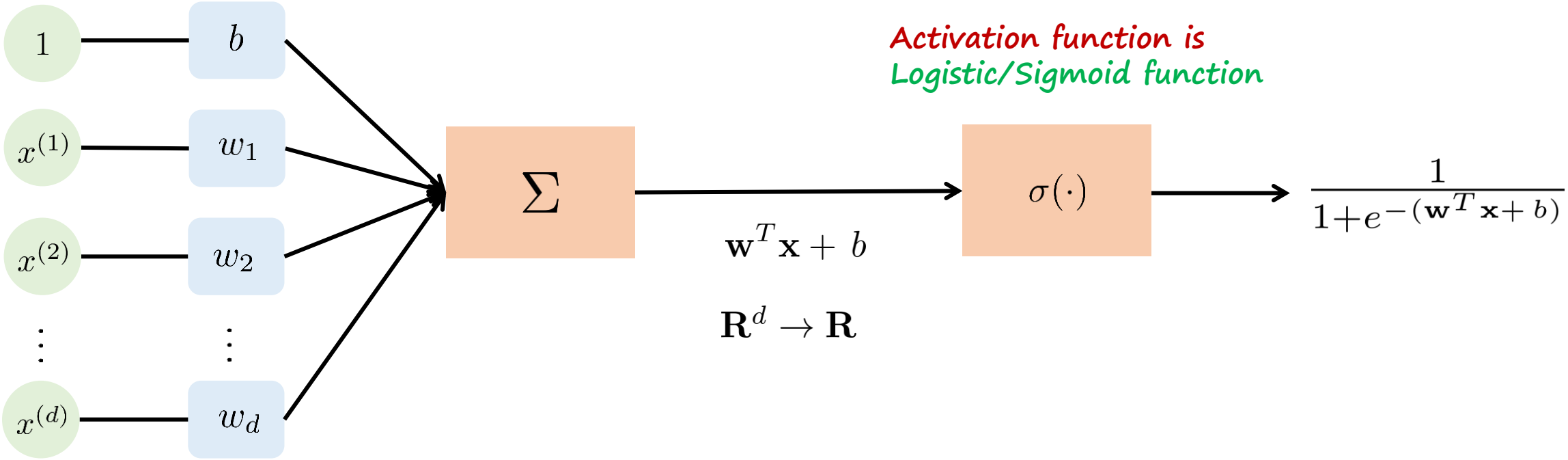


Neural Networks

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:



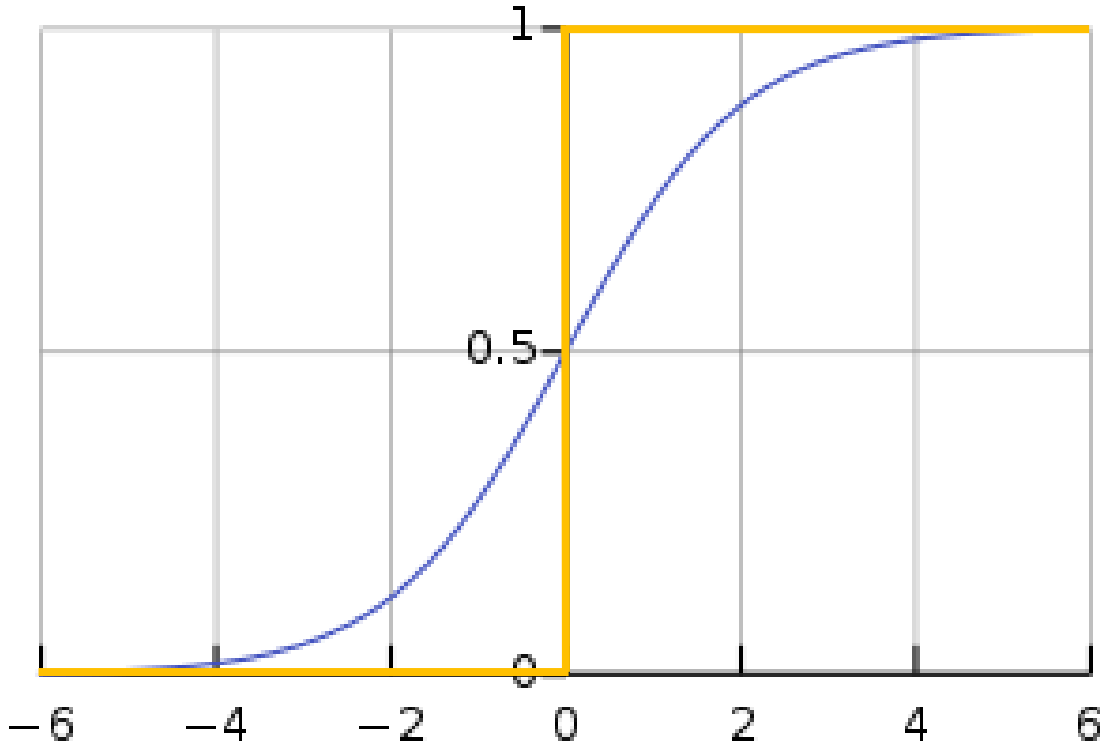
Logistic Regression Model, aka Sigmoid Neuron

Neural Networks

Connection with Logistic Regression and Perceptron:

Activation Function

Perceptron vs Sigmoid Neuron



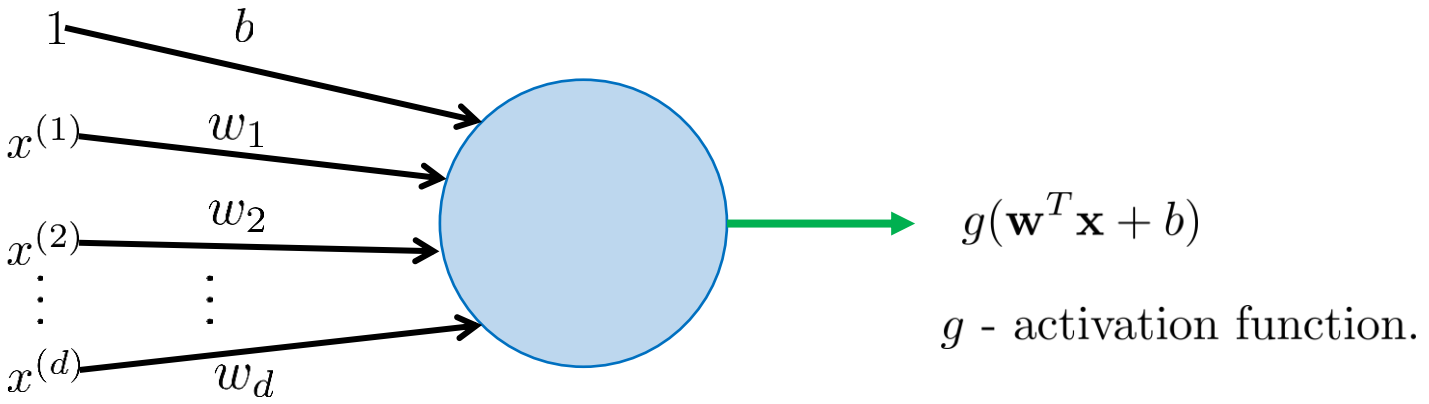
Weighted sum of inputs + bias

$$\mathbf{w}^T\mathbf{x} + b$$

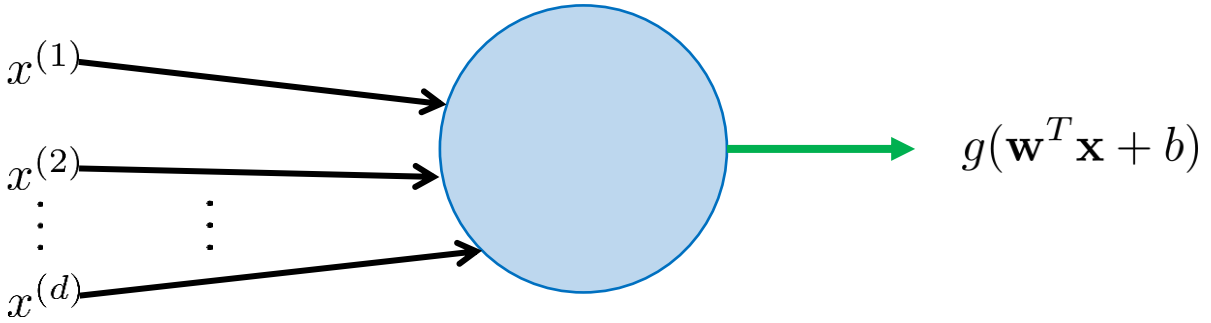
Neural Networks

Neuron Model:

Compact Representation:



More Compact Representation:



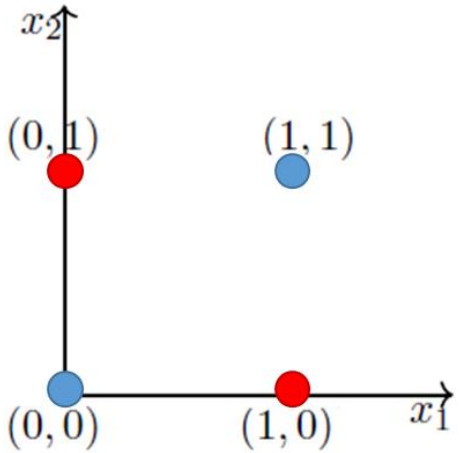
- Neuron model: Characterized by weights, bias and activation function.
  - Weights $\mathbf{w}$, bias b - model parameters
  - Activation function g - hyperparameter

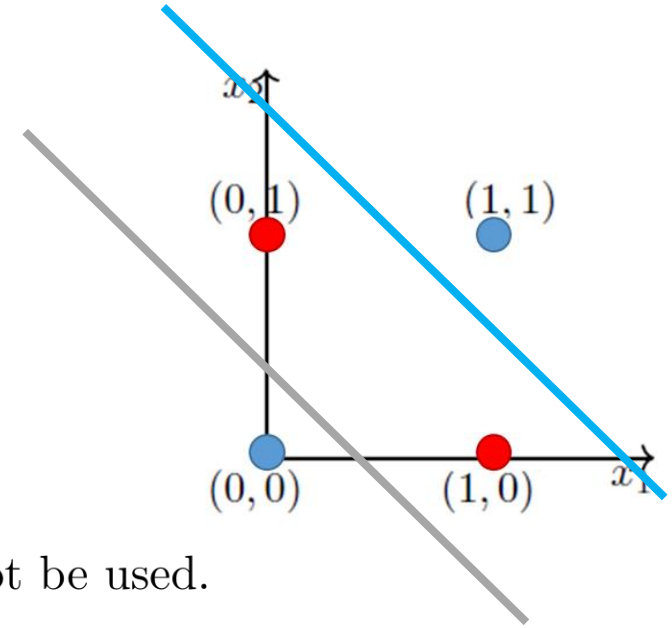
Neural Networks

Neural Networks - Infamous XOR Problem:

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

x_1	x_2	XOR
0	0	0
1	0	1
0	1	1
1	1	0



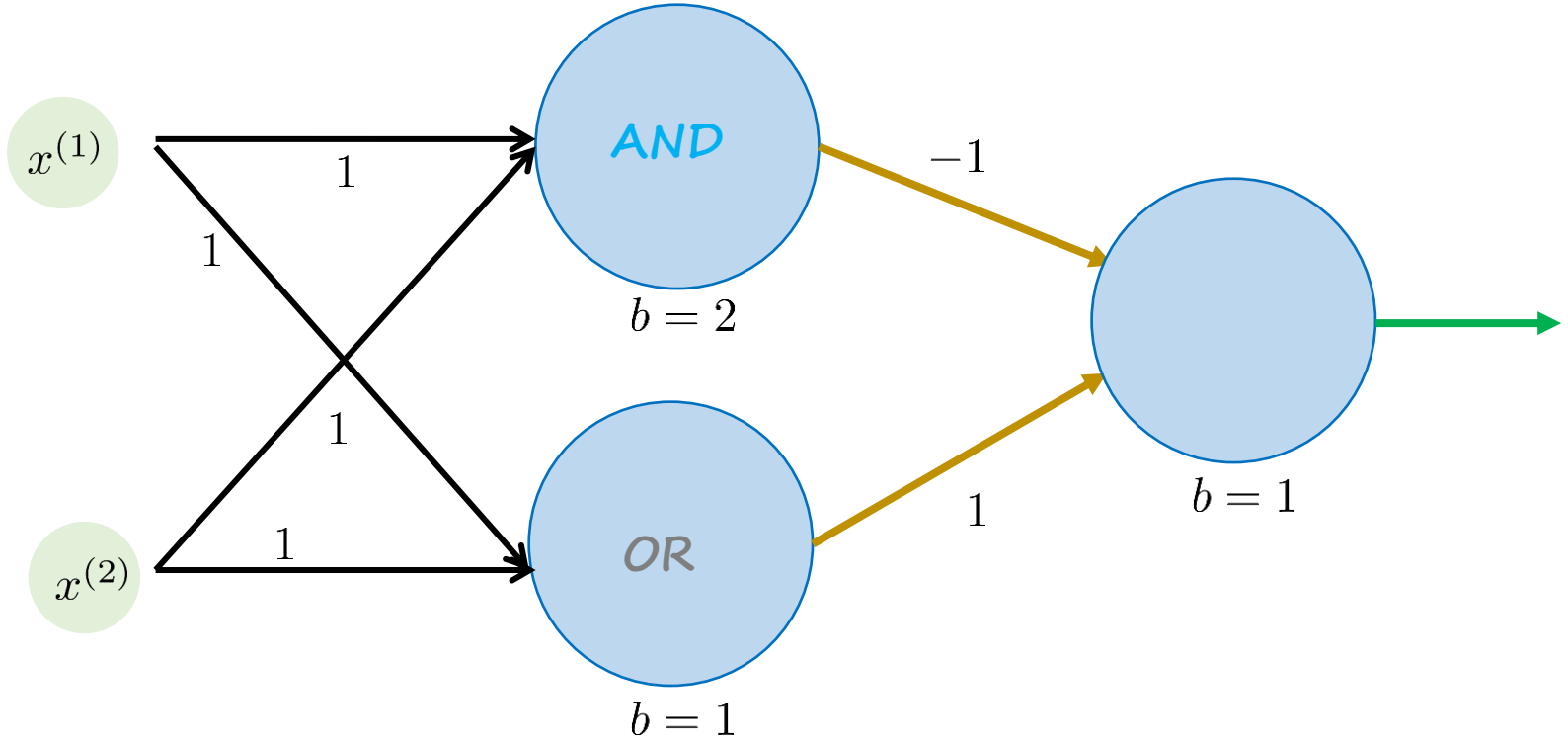


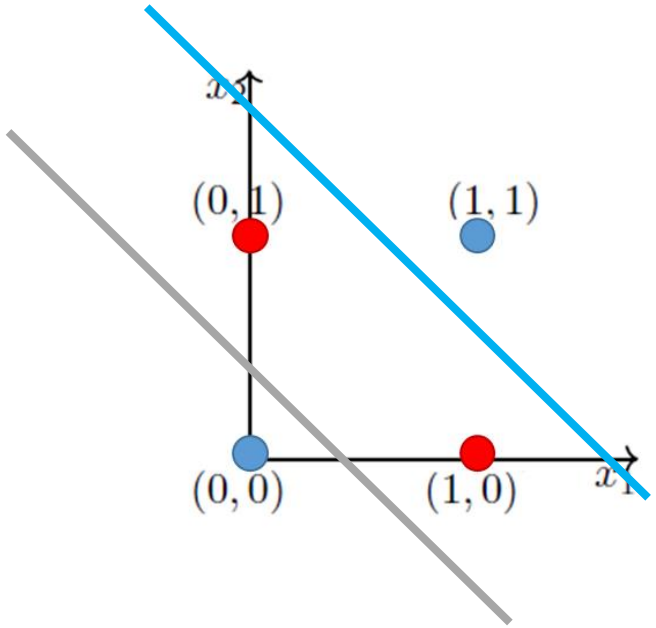
Idea:
Learn AND and OR boundaries.

- 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

Neural Networks - Infamous XOR Problem:



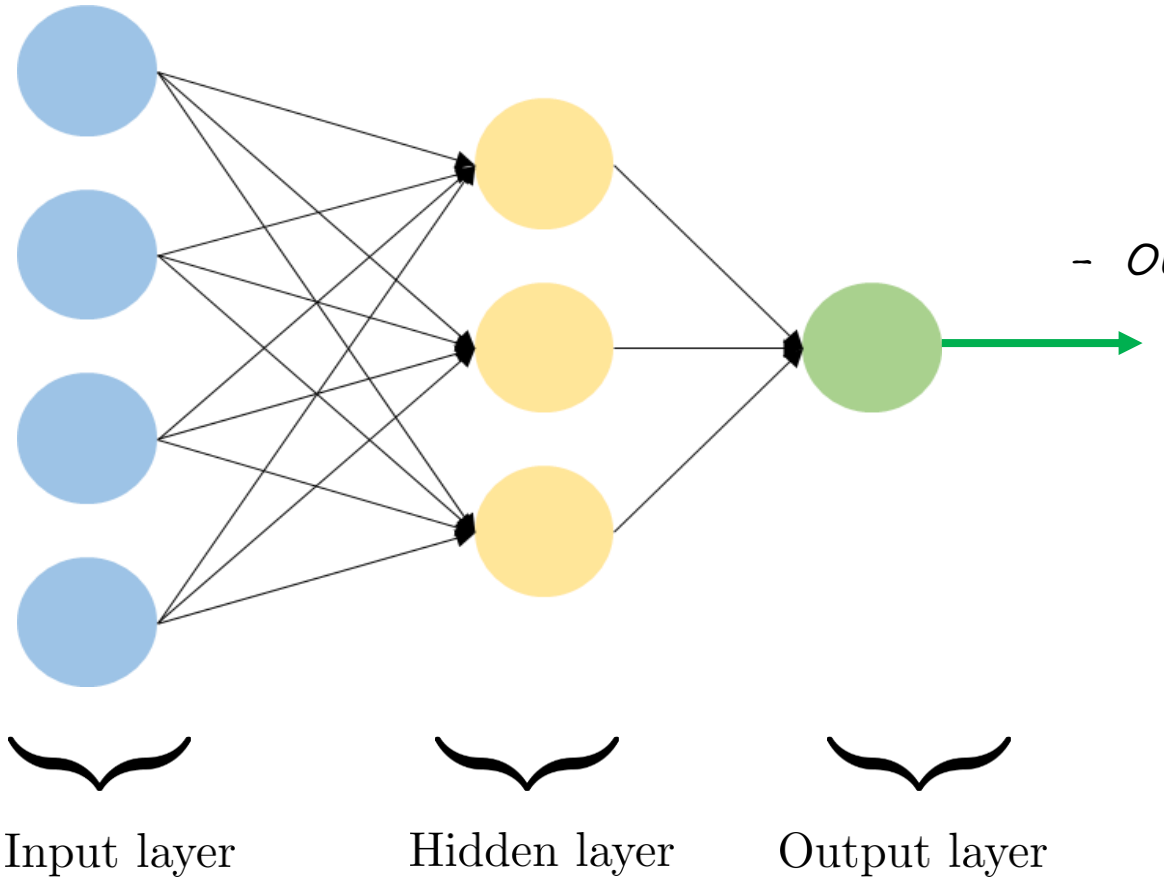


- This is a neural network; a network of perceptrons, aka multi-layer perceptron (MLP).

Neural Networks

Neural Networks

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



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

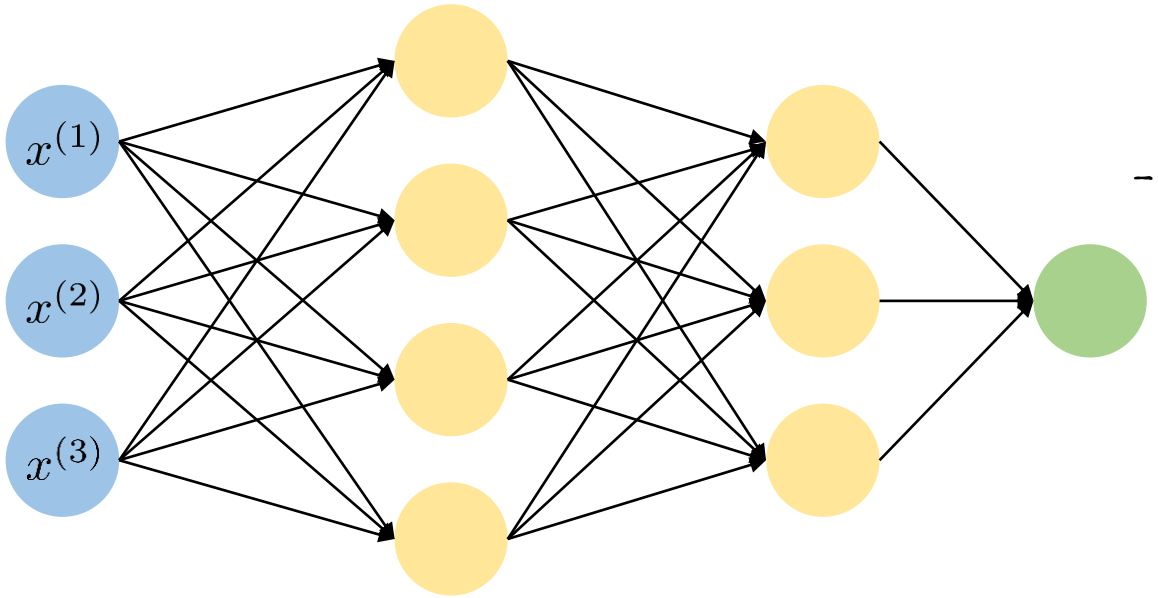
Each unit in the network is called a neuron and the network of neurons is called Neural Network.

- 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

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

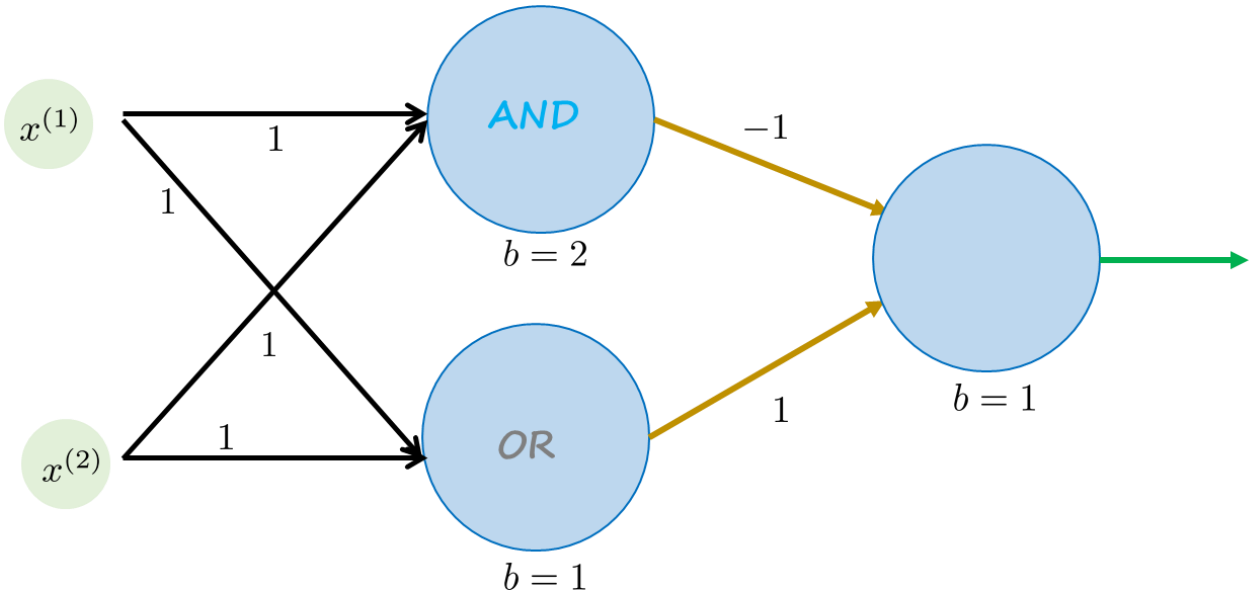
- We do not count the input layer because there are no parameters associated with it.
- Neural networks with neurons are also referred to as MLPs but we will refer to the network as MLP only when it is constructed using perceptrons.

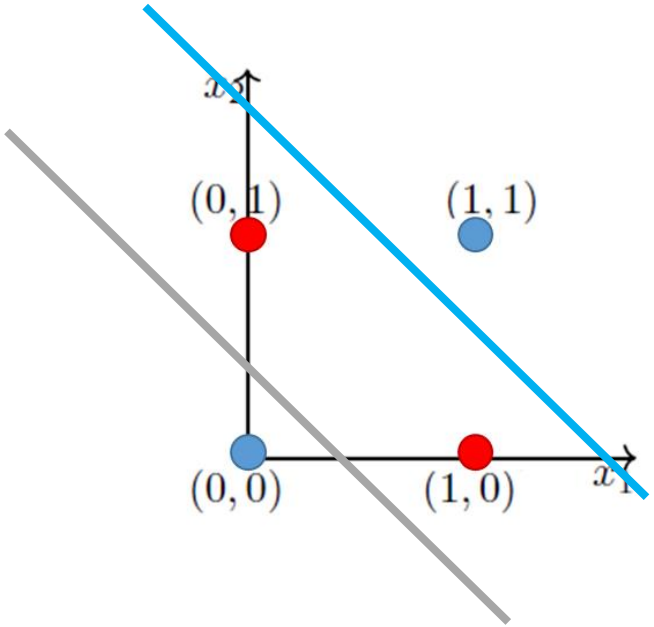
Feedforward Neural Network: **Output from one layer is an input to the next layer.**

Neural Networks

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

Intuition: *XOR example*

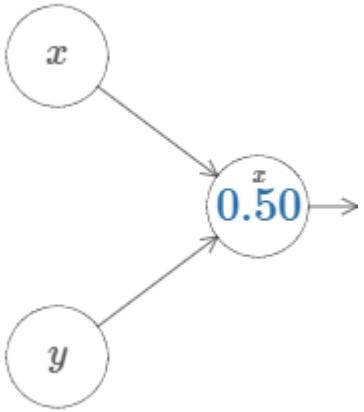


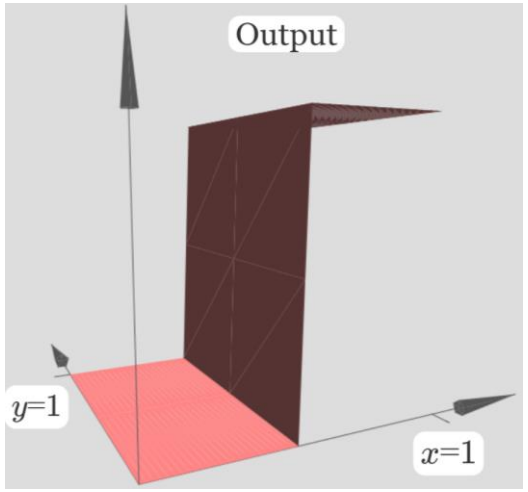


Neural Networks

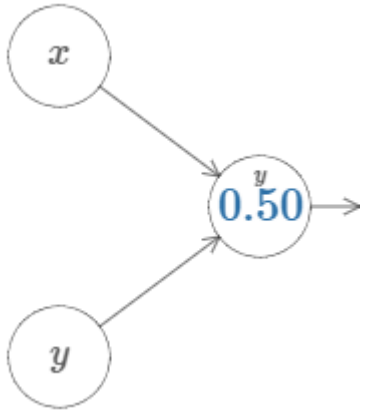
What kind of functions can be modeled by a neural network?

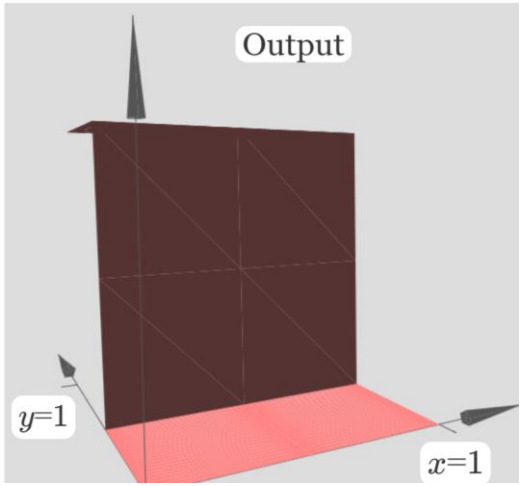
Intuition: *Example (Sigmoid neuron)*





- 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.

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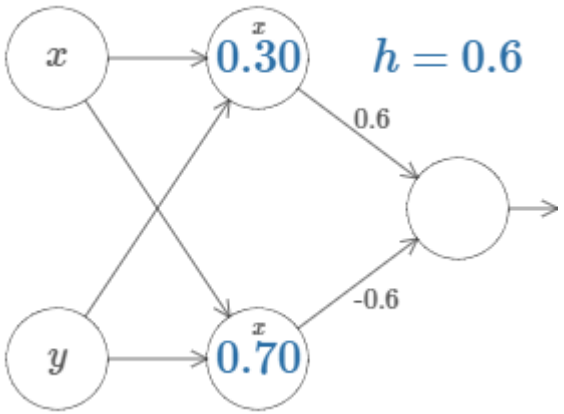
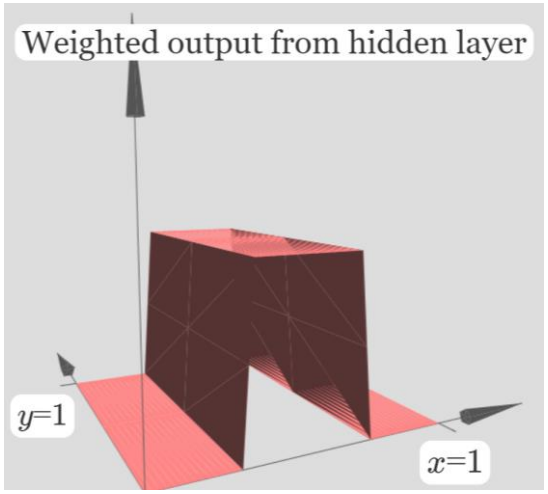
Source: http://neuralnetworksanddeeplearning.com/chap4.html

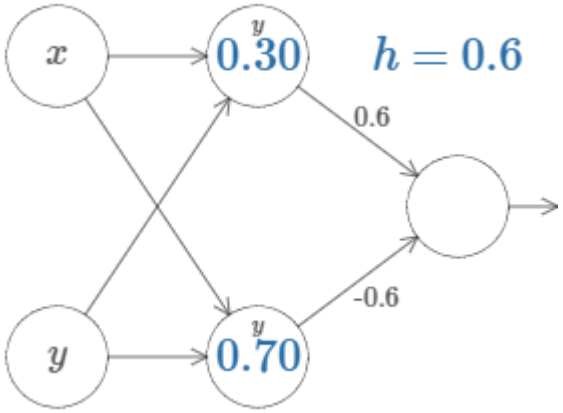
Neural Networks

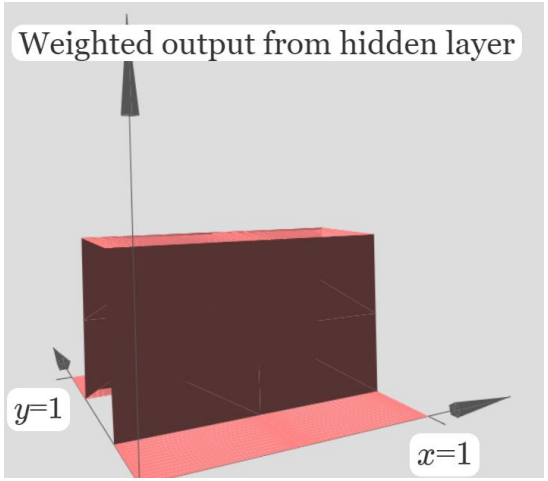
What kind of functions can be modeled by a neural network?

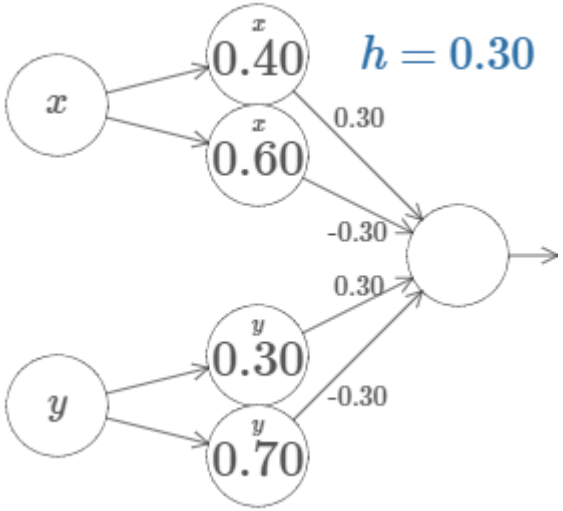
Intuition: *Example (Multi layer)*

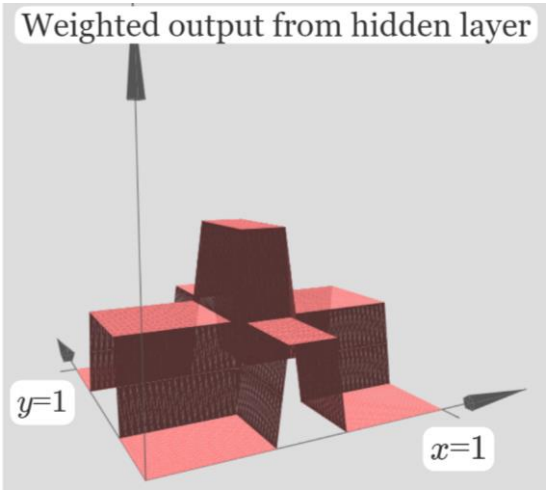












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Source: http://neuralnetworksanddeeplearning.com/chap4.html

Neural Networks

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.

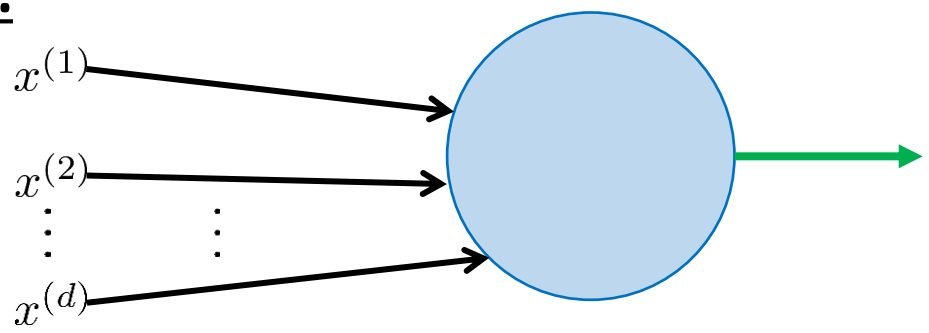
Outline

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

Neural Networks

Neural Networks – Notation:

Single Neuron:



$g(\mathbf{w}^T\mathbf{x} + b)$

$z = \mathbf{w}^T\mathbf{x} + b$ **Pre-activation**

$g(z)$ **Activation**

- If we stack n training data in a matrix $\mathbf{X}$ of size $d \times n$, that is, $\mathbf{X} = [\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_n]$
- Using $\mathbf{X}$ and by defining $\mathbf{1}$ 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 $\mathbf{z}$ as

$$\underset{(1\times n)}{\mathbf{z}} = \underset{(1\times d)(d\times n)}{\mathbf{w}^T\mathbf{X}} + \underset{(1\times n)}{b\mathbf{1}}$$

Pre-activation (Aggregation) **Linear transformation**

- Using activation function g, we obtain

$$\mathbf{a} = g(\mathbf{z})$$

Activation **Non-linear transformation**

  - Activation function is operating on each entry of $\mathbf{z}$.
  - $\mathbf{a}$ - a row vector of length n; i-th entry represents an output for i-th input.

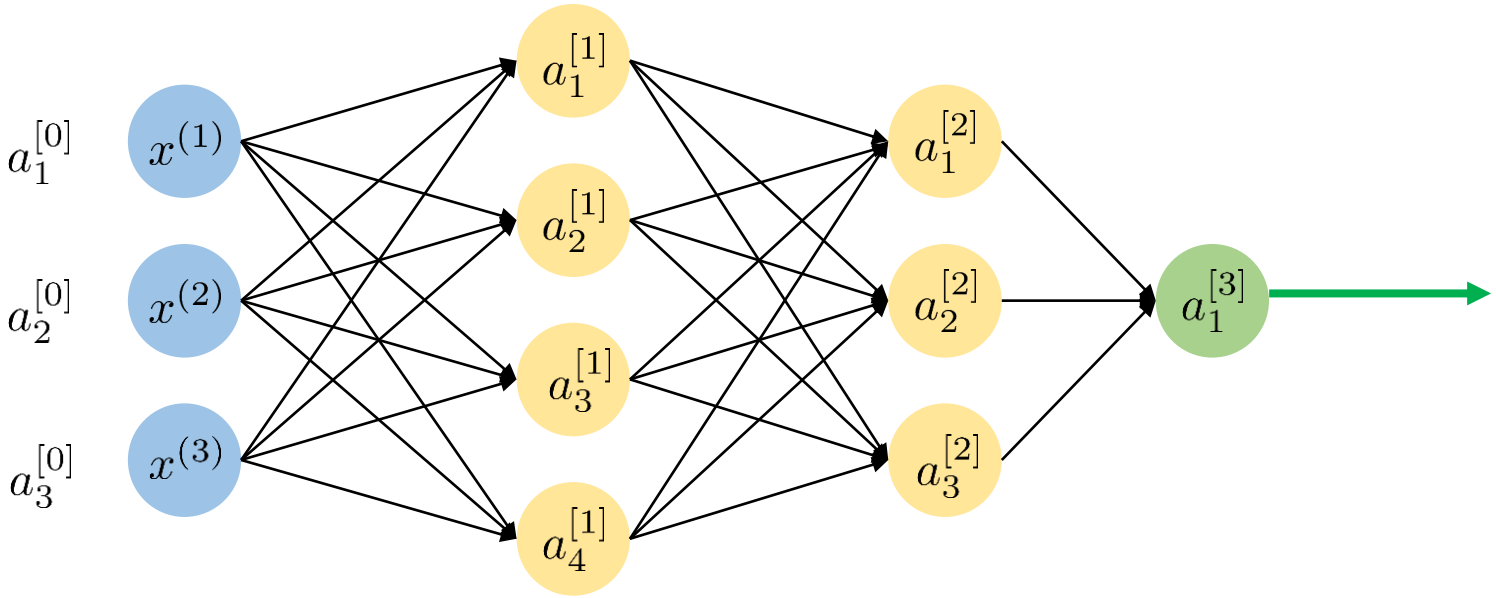
Neural Networks

Neural Networks – Notation:

- L - number of layers.
- Number of nodes in the ℓ-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

- $L = 3$
- $m^{[1]} = 4,\ m^{[2]} = 3,\ m^{[3]} = 1$

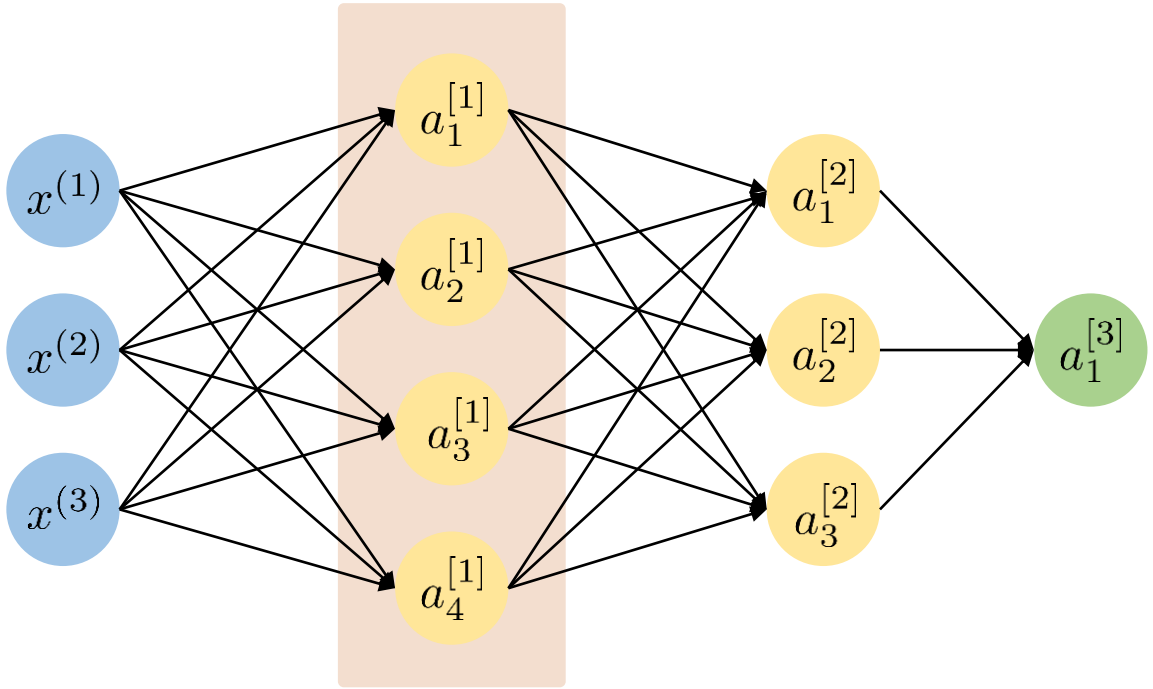


Neural Networks

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

$$a_1^{[1]} = g(z_1^{[1]}), \quad z_1^{[1]} = \mathbf{w}_1^{[1]T}\mathbf{x} + b_1^{[1]}$$

$$a_2^{[1]} = g(z_2^{[1]}), \quad z_2^{[1]} = \mathbf{w}_2^{[1]T}\mathbf{x} + b_2^{[1]}$$

$$a_3^{[1]} = g(z_3^{[1]}), \quad z_3^{[1]} = \mathbf{w}_3^{[1]T}\mathbf{x} + b_3^{[1]}$$

$$a_4^{[1]} = g(z_4^{[1]}), \quad z_4^{[1]} = \mathbf{w}_4^{[1]T}\mathbf{x} + b_4^{[1]}$$

Neural Networks

Neural Networks – Notation:

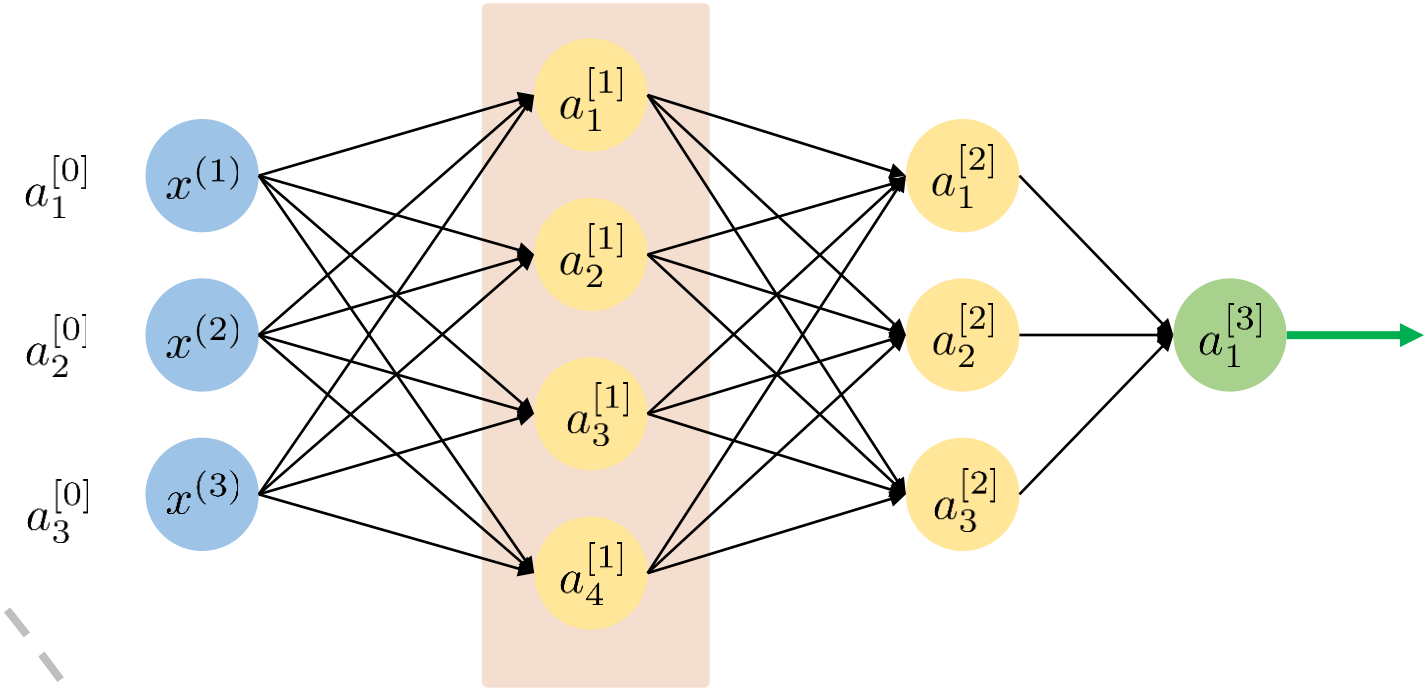
Layer 1 output

$$a_1^{[1]} = g(z_1^{[1]}), \quad z_1^{[1]} = \mathbf{w}_1^{[1]T}\mathbf{x} + b_1^{[1]}$$

$$a_2^{[1]} = g(z_2^{[1]}), \quad z_2^{[1]} = \mathbf{w}_2^{[1]T}\mathbf{x} + b_2^{[1]}$$

$$a_3^{[1]} = g(z_3^{[1]}), \quad z_3^{[1]} = \mathbf{w}_3^{[1]T}\mathbf{x} + b_3^{[1]}$$

$$a_4^{[1]} = g(z_4^{[1]}), \quad z_4^{[1]} = \mathbf{w}_4^{[1]T}\mathbf{x} + b_4^{[1]}$$



$$\mathbf{W}^{[1]} = \begin{bmatrix} \mathbf{w}_1^{[1]T} \\ \mathbf{w}_2^{[1]T} \\ \mathbf{w}_3^{[1]T} \\ \mathbf{w}_4^{[1]T} \end{bmatrix} \quad \mathbf{b}^{[1]} = \begin{bmatrix} b_1^{[1]T} \\ b_2^{[1]T} \\ b_3^{[1]T} \\ b_4^{[1]T} \end{bmatrix} \quad \mathbf{z}^{[1]} = \begin{bmatrix} z_1^{[1]T} \\ z_2^{[1]T} \\ z_3^{[1]T} \\ z_4^{[1]T} \end{bmatrix}$$

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

$$\mathbf{z}^{[1]} = \mathbf{W}^{[1]}\mathbf{a}^{[0]} + \mathbf{b}^{[1]}$$

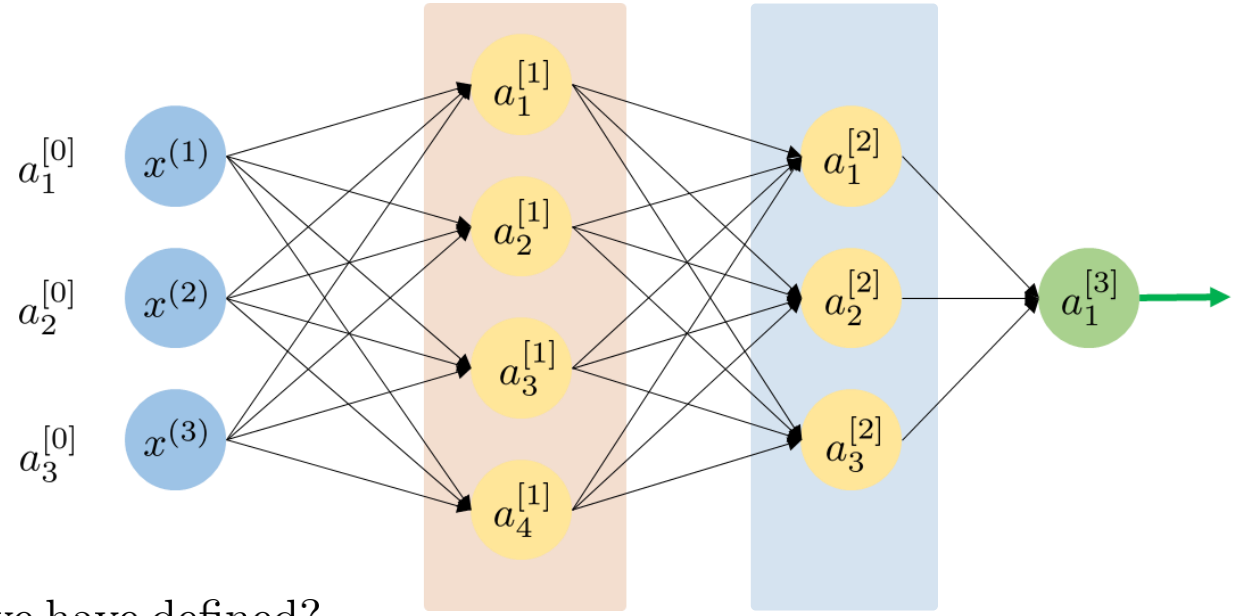
- $\mathbf{W}^{[1]}$ and $\mathbf{b}^{[1]}$ are the parameters of the first layer.

Neural Networks

Neural Networks – Forward Pass:

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

$$\mathbf{z}^{[1]} = \mathbf{W}^{[1]}\mathbf{a}^{[0]} + \mathbf{b}^{[1]}$$



- Q. What is the size of $\mathbf{W}^{[1]}$?

A. No. of nodes $\times$ No. of inputs. 4×3

No. of nodes $\times$ 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)**.

Neural Networks

Neural Networks – Forward Pass Summary:

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

$$\mathbf{z}^{[1]} = \mathbf{W}^{[1]}\mathbf{a}^{[0]} + \mathbf{b}^{[1]}$$

$$(4 \times 1) = (4 \times 3)(3 \times 1) + (4 \times 1)$$

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

$$(3 \times 1) = (3 \times 4)(4 \times 1) + (3 \times 1)$$

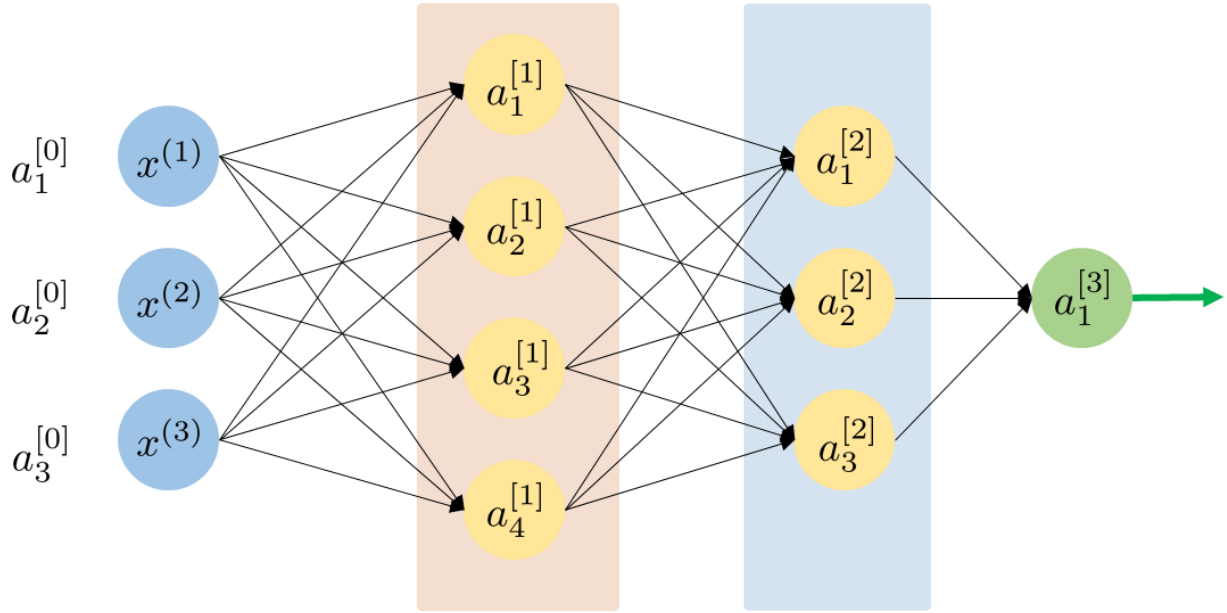
$$\mathbf{a}^{[3]} = g(\mathbf{z}^{[3]}), \quad \mathbf{z}^{[3]} = \mathbf{W}^{[3]}\mathbf{a}^{[2]} + \mathbf{b}^{[3]}$$

$$(1 \times 1) = (1 \times 3)(3 \times 1) + (1 \times 1)$$

- 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 $\ell = 1, 2, \ldots, L$, where $\mathbf{a}^{[0]} = \mathbf{x}$.



- How many parameters do we have by the way?
- This formulation is for one input $\mathbf{x}$.
- How can we extend this formulation n inputs?

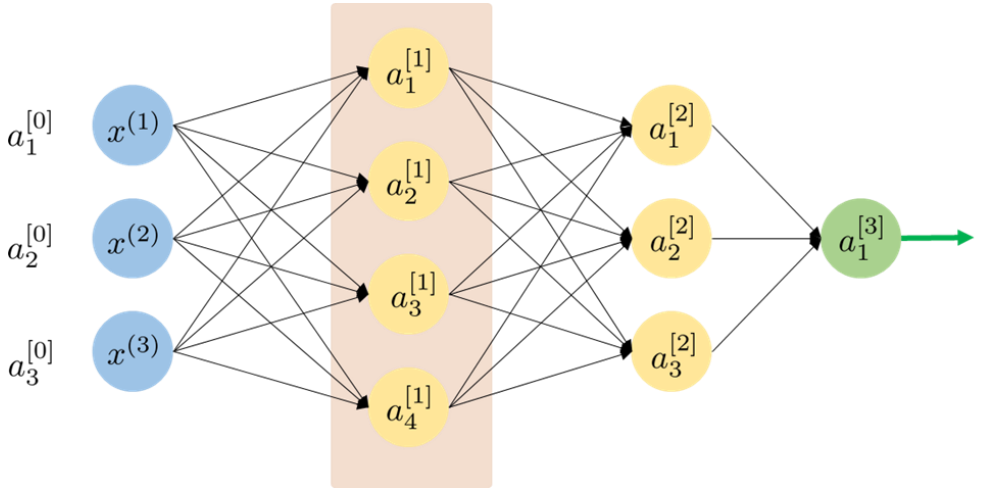
Neural Networks

Neural Networks – Forward Pass – Incorporating all Inputs:

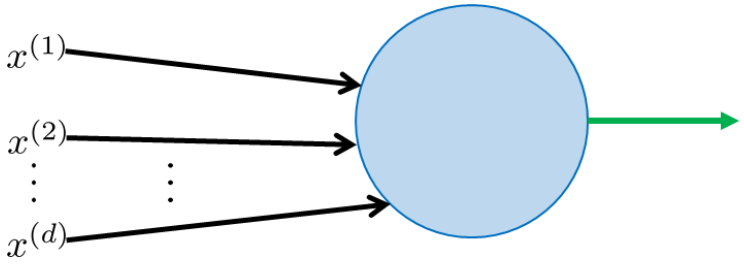
$$\mathbf{a}^{[1]} = g(\mathbf{z}^{[1]}), \quad \mathbf{z}^{[1]} = \mathbf{W}^{[1]}\mathbf{x} + \mathbf{b}^{[1]}$$

$$\mathbf{z}^{[1]} = \mathbf{W}^{[1]}\mathbf{a}^{[0]} + \mathbf{b}^{[1]}$$

$$(4 \times 1) = (4 \times 3)(3 \times 1) + (4 \times 1)$$



Recall:



$g(\mathbf{w}^T\mathbf{x} + b)$

$z = \mathbf{w}^T\mathbf{x} + b$

$g(z)$

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

$$\mathbf{Z}^{[1]} = \mathbf{W}^{[1]}\mathbf{A}^{[0]} + \mathbf{b}^{[1]}$$

$$(4 \times n) = (4 \times 3)(3 \times n) + (4 \times n)$$

- For single neuron, we developed the following formulation incorporating all inputs simultaneously.

$$\mathbf{z} = \mathbf{w}^T\mathbf{X} + b\mathbf{1}$$

$$\mathbf{a} = g(\mathbf{z})$$

- $\mathbf{a}$ - a row vector of length n;
  i-th entry represents an output for i-th input.

Neural Networks

Neural Networks – Forward Pass Summary – All Inputs:

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

$$\mathbf{Z}^{[1]} = \mathbf{W}^{[1]}\mathbf{A}^{[0]} + \mathbf{b}^{[1]}$$

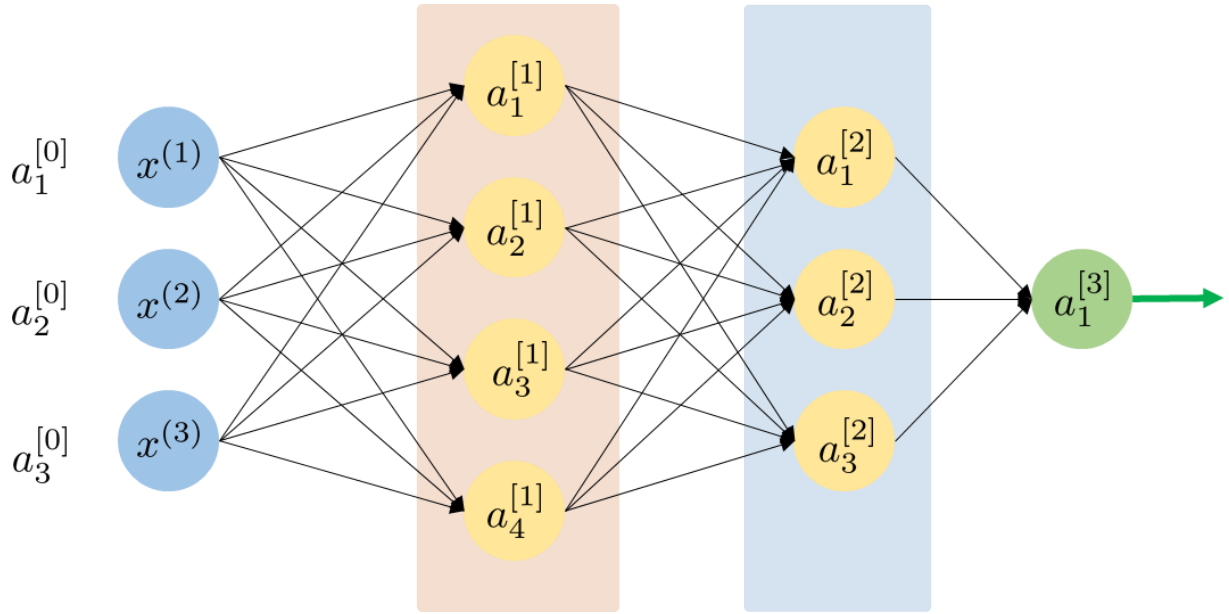
$$(4 \times n) = (4 \times 3)(3 \times n) + (4 \times n)$$

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

$$(3 \times n) = (3 \times 4)(4 \times n) + (3 \times n)$$

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

$$(1 \times n) = (1 \times 3)(3 \times n) + (1 \times n)$$



- In general, we have

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

Outline

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

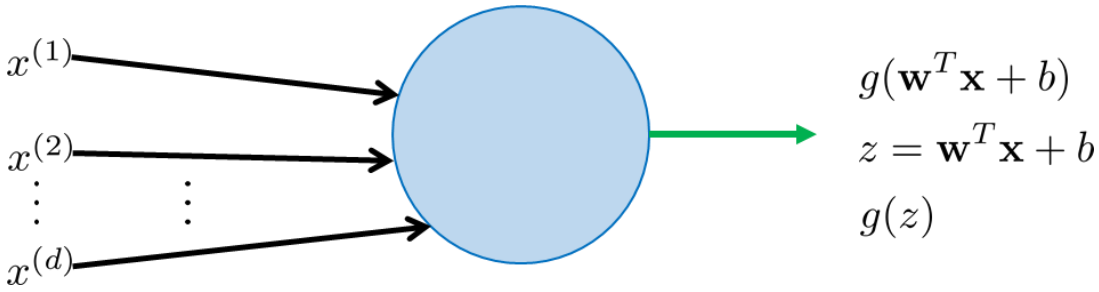
Neural Networks

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 functon, e.g., identity or $\mathrm{g(z)} = \alpha\, z + \beta$

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

  - Consequently, different layers of the network can be equivalently represented by a single linear transformation.



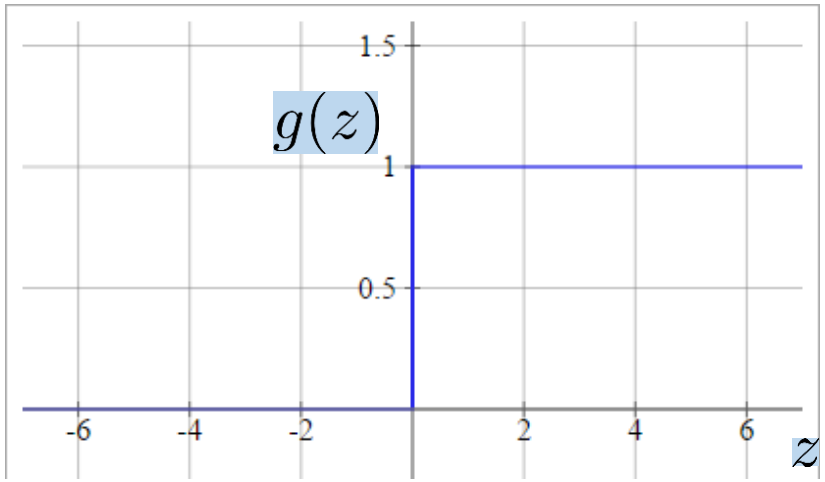
- We require active function g to be differentiable if we want to use gradient descent.
- Some standard activation functions:
  - identity (linear), step, rectified linear, leaky rectified linear sigmoid, tanh

Neural Networks

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:

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

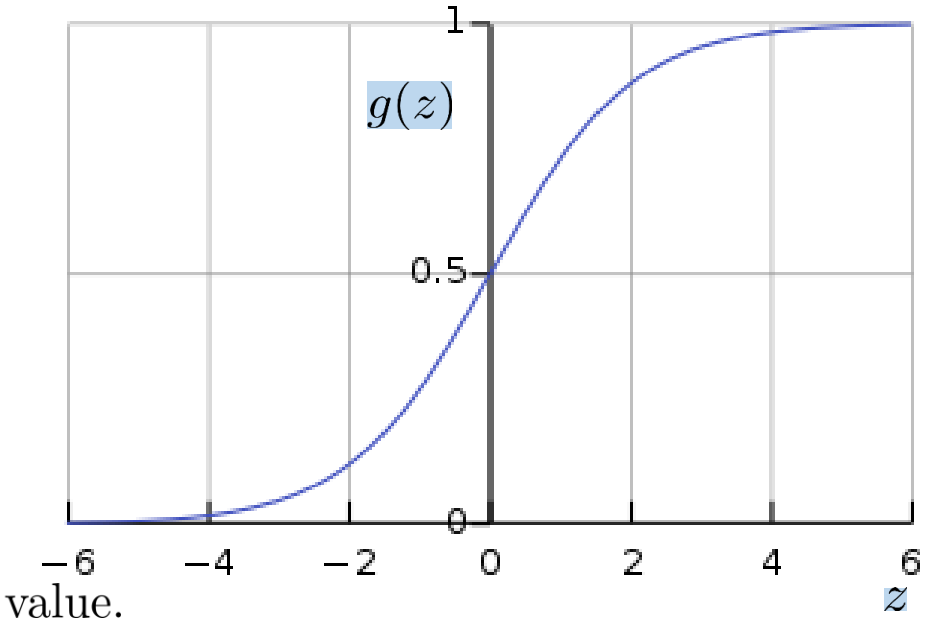
- Constant derivative, $g'(z) = \alpha$; cannot be used for backpropagation.
- Used for simple linear regression model.
- Does not capture non-linearities irrespective of the depth of the network.

Neural Networks

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. $g'(z) = g(z)\big(1 - g(z)\big)$



Issues:

- Saturation Problem or Vanishing Gradient:

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

  $g(z) = 0$ or $g(z) = 1$. Conseqeunce: $g'(z) = g(z)\big(1 - g'(z)\big) = 0$ (poor learning for deep networks)

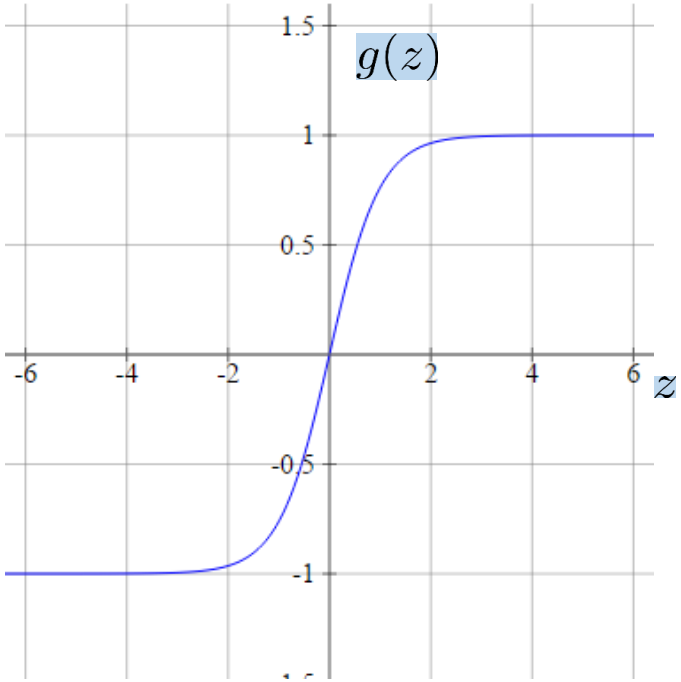
- Sigmoid outputs are not zero-centered:

  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.

Neural Networks

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. $g'(z) = 1 - \big(g(z)\big)^2$

Issues:

- Saturation Problem or Vanishing Gradient:

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

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

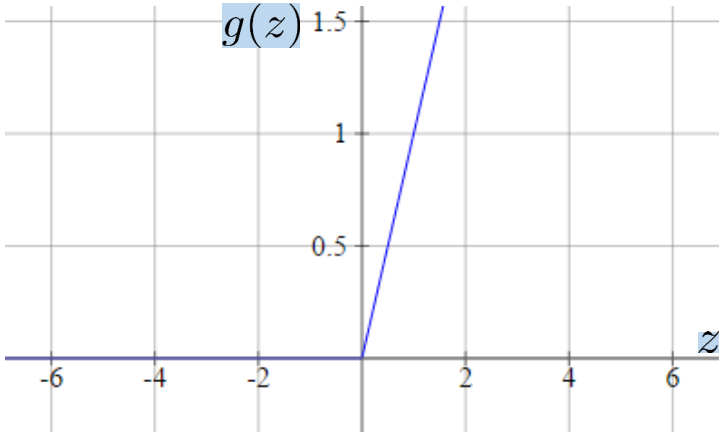
Neural Networks

Rectifier – Rectified Linear Unit (ReLu):

$$g(z) = \max(0, z) = \begin{cases} z & z \geq 0 \\ 0 & z < 0 \end{cases}$$

- Super simple.

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



- 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.

Issues:

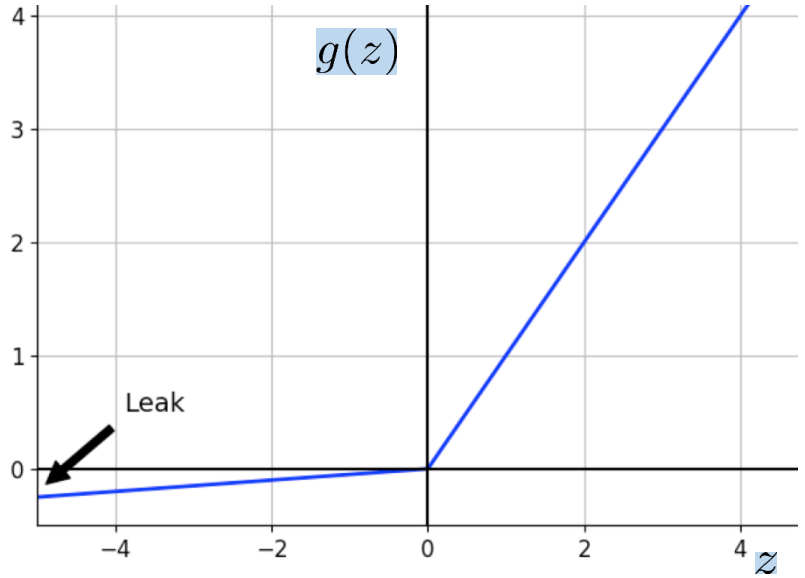
- ReLu is not zero centered.
  As indicated earlier, this is not a major issue and training the network longer can resolve this.
- ReLu does not suffer from saturation problem. Vanishing gradient however occurs for negative values; dead neuron.

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

Neural Networks

Leaky Rectified Linear Unit (Leaky ReLu):

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



- 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. $g'(z) = \begin{cases} 1 & z \geq 0 \\ \alpha & z < 0 \end{cases}$

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

Neural Networks

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.

Neural Networks

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.

Outline

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

Neural Networks

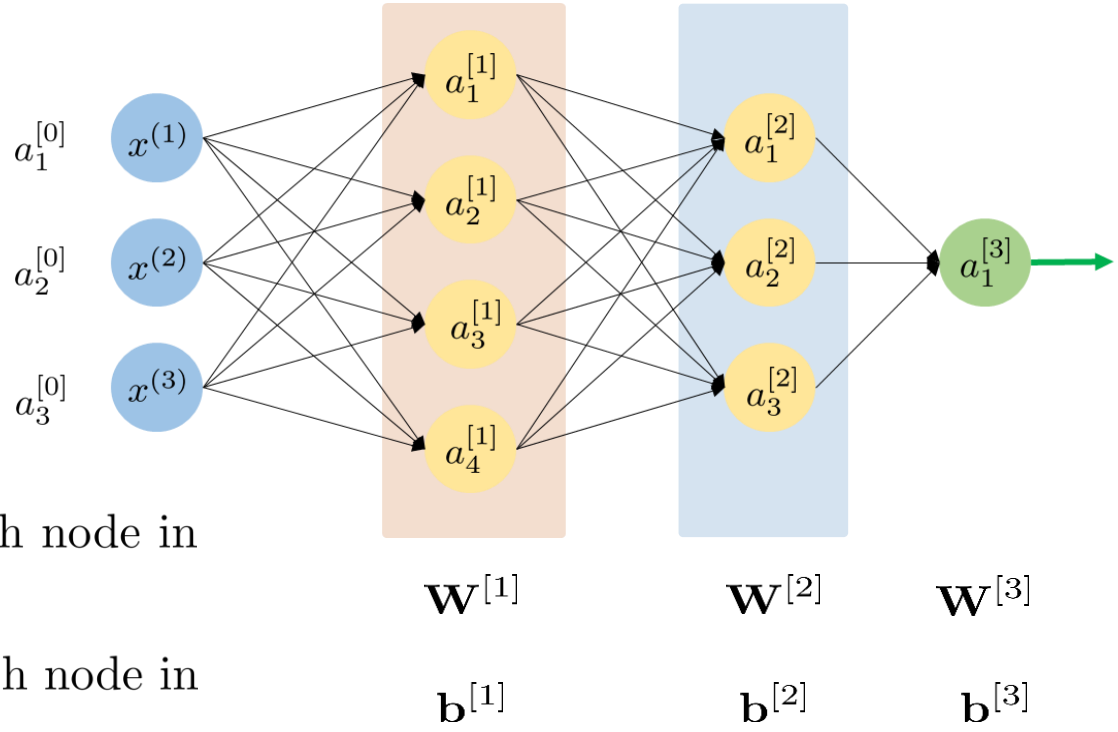
Learning Weights:

- 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 ℓ-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.

Example:



Parameters we need to learn!

Neural Networks

Learning Weights:

- We assume we have training data D given by

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

- 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):

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

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

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

- We can use gradient descent to learn the weight matrices and bias vectors.

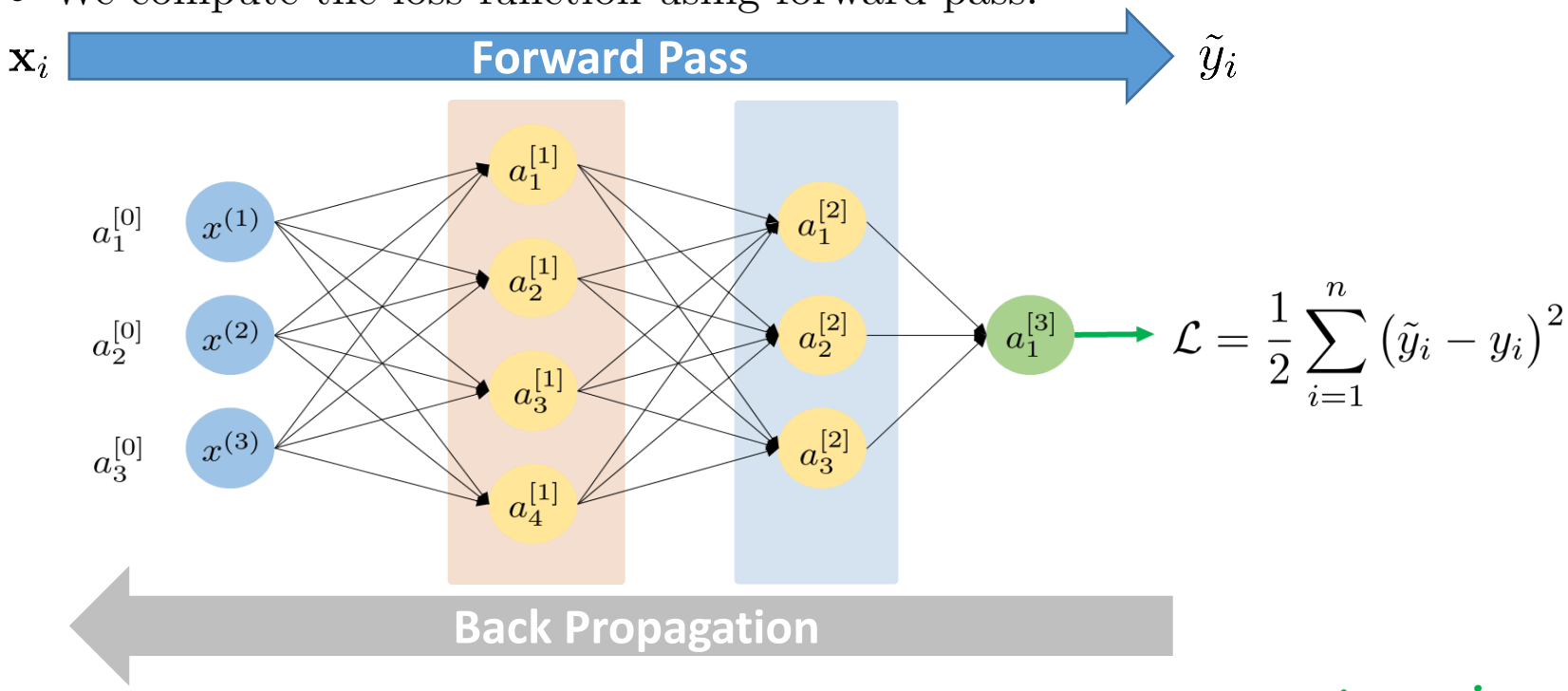
- Given our prior knowledge, output y is a composite function of input $\mathbf{x}$. Therefore, it is continuous and differentiable and we can use chain rule to compute the gradient.

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

Neural Networks

Back Propagation – Key Idea:

- We compute the loss function using forward pass.



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

The weights are the only parameters that can be modified to make the loss function as low as possible.

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

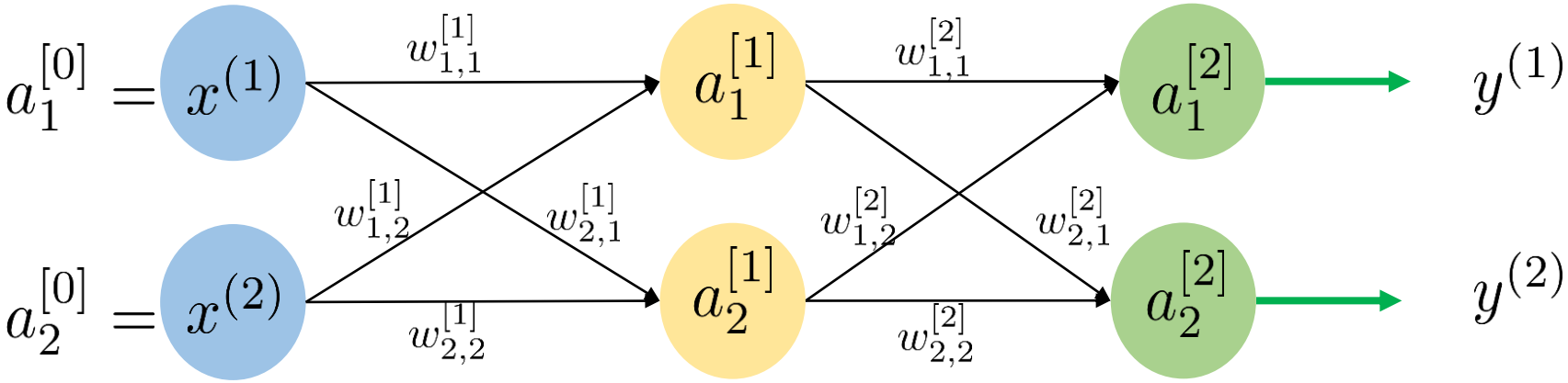
Learning problem reduces to the question of calculating gradient (partial derivatives) of loss function.

- 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**)

Neural Networks

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

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

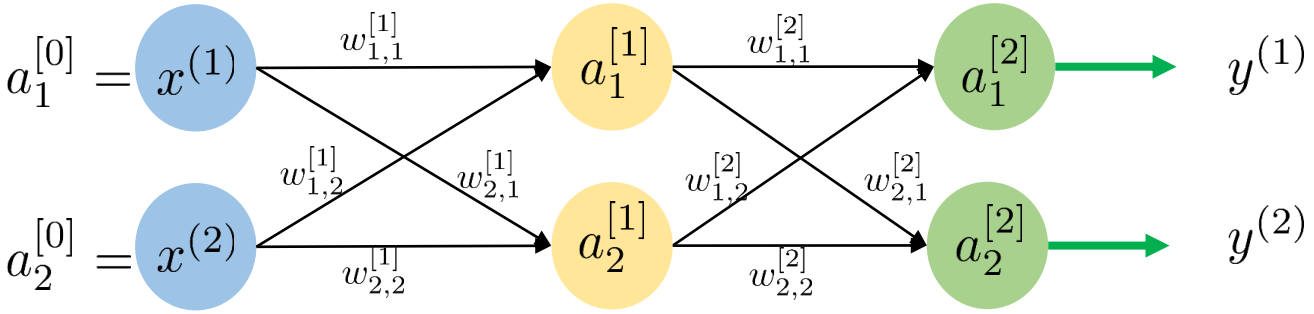
- Initial values of weights and biases:

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

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

Neural Networks

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

$$a_1^{[1]} = g(z_1^{[1]}), \quad z_1^{[1]} = \mathbf{w}_1^{[1]T}\mathbf{x} + b_1^{[1]}$$

$$a_2^{[1]} = g(z_2^{[1]}), \quad z_2^{[1]} = \mathbf{w}_2^{[1]T}\mathbf{x} + b_2^{[1]}$$

$$a_1^{[2]} = g(z_1^{[2]}), \quad z_1^{[2]} = \mathbf{w}_1^{[2]T}\mathbf{x} + b_1^{[2]}$$

$$a_2^{[2]} = g(z_2^{[2]}), \quad z_2^{[2]} = \mathbf{w}_2^{[2]T}\mathbf{x} + b_2^{[2]}$$

$$z_1^{[1]} = w_{1,1}^{[1]}x^{(1)} + w_{1,2}^{[1]}x^{(2)} + b_1^{[1]} = 0.3775, \quad a_1^{[1]} = g(0.3775) = 0.5933$$

$$z_2^{[1]} = \mathbf{w}_2^{[1]T}\mathbf{x} + b_2^{[1]} = 0.3925, \quad a_2^{[1]} = g(0.3925) = 0.5969$$

$$z_1^{[2]} = \mathbf{w}_1^{[2]T}\mathbf{x} + b_1^{[2]} = 1.106, \quad a_1^{[2]} = g(1.106) = 0.7514 = \tilde{y}^{(1)}$$

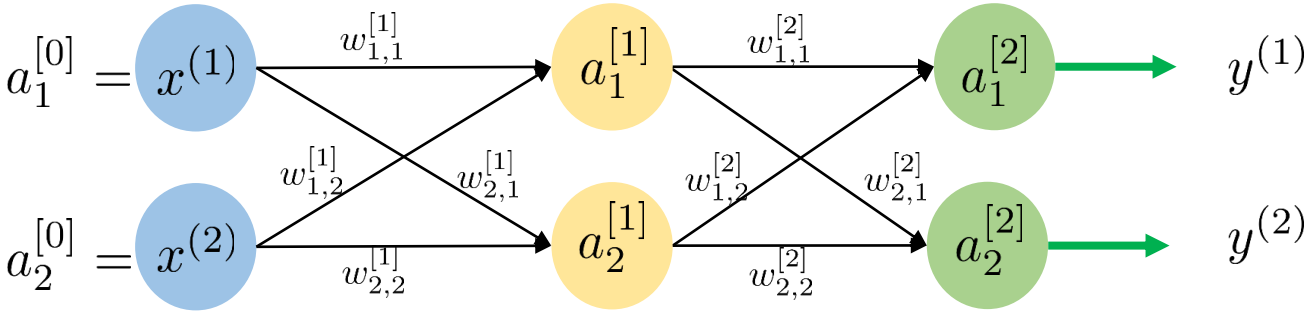
$$z_2^{[2]} = \mathbf{w}_2^{[2]T}\mathbf{x} + b_2^{[2]} = 1.225, \quad a_2^{[2]} = g(1.225) = 0.7729 = \tilde{y}^{(2)}$$

Nothing fancy so far, we have computed the output and loss by traversing neural network.

Let's compute the contribution of loss by each node; back propagate the loss.

Neural Networks

Back Propagation – Example:



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

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

$$\mathcal{L} = \frac{1}{2}\|(\tilde{y}^{(1)} - y^{(1)})^2 - (\tilde{y}^{(2)} - y^{(2)})^2\|^2$$

$$\tilde{y}^{(1)} = \sigma(z_1^{[2]})$$

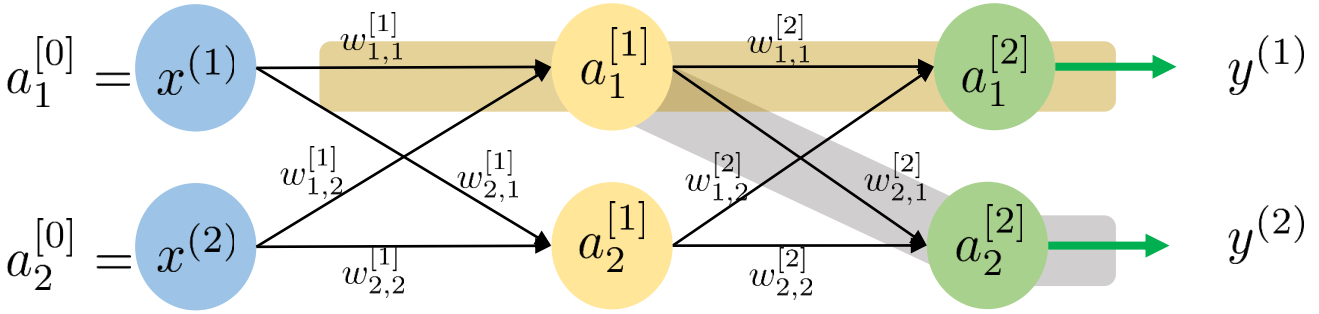
$$z_1^{[2]} = w_{1,1}^{[2]} a_1^{[1]} + w_{1,2}^{[2]} a_2^{[1]} + b_1^{[2]}$$

$$\left.\begin{aligned} \frac{\partial \mathcal{L}}{\partial w_{1,1}^{[2]}} &= \frac{\partial \mathcal{L}}{\partial \tilde{y}^{(1)}} \frac{\partial \tilde{y}^{(1)}}{\partial z_1^{[2]}} \frac{\partial z_1^{[2]}}{\partial w_{1,1}^{[2]}} \\ &= 0.0821 \end{aligned}\right\}$$

$$\left\{\begin{aligned} \frac{\partial \mathcal{L}}{\partial \tilde{y}^{(1)}} &= \tilde{y}^{(1)} - y^{(1)} = 0.7414 \\ \frac{\partial \tilde{y}^{(1)}}{\partial z_1^{[2]}} &= \sigma(\partial z_1^{[2]})\left(1 - \sigma(\partial z_1^{[2]})\right) = 0.1868 \\ \frac{\partial z_1^{[2]}}{\partial w_{1,1}^{[2]}} &= a_1^{[a]} = 0.5933 \end{aligned}\right.$$

Neural Networks

Back Propagation – Example:



$$\mathcal{L} = \frac{1}{2}\|(\tilde{y}^{(1)} - y^{(1)})^2 - (\tilde{y}^{(2)} - y^{(2)})^2\|^2$$

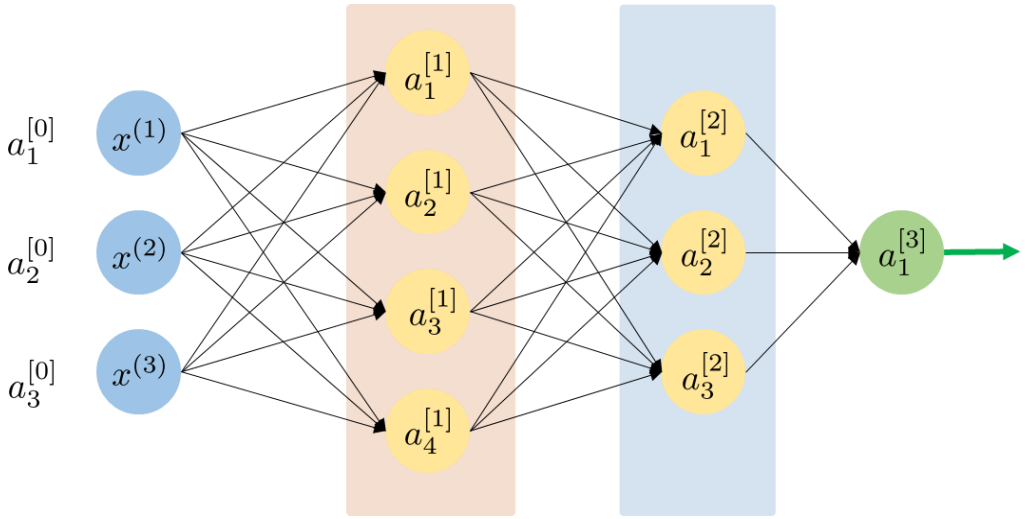
- Consider a case when we want to compute $\dfrac{\partial \mathcal{L}}{\partial w_{1,1}^{[1]}}$
- Traverse the path from the loss function back to the weight $w_{1,1}^{[1]}$. There are two paths from the output to the weight $w_{1,1}^{[1]}$. In other words, $w_{1,1}^{[1]}$ is contributing to both the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

Neural Networks

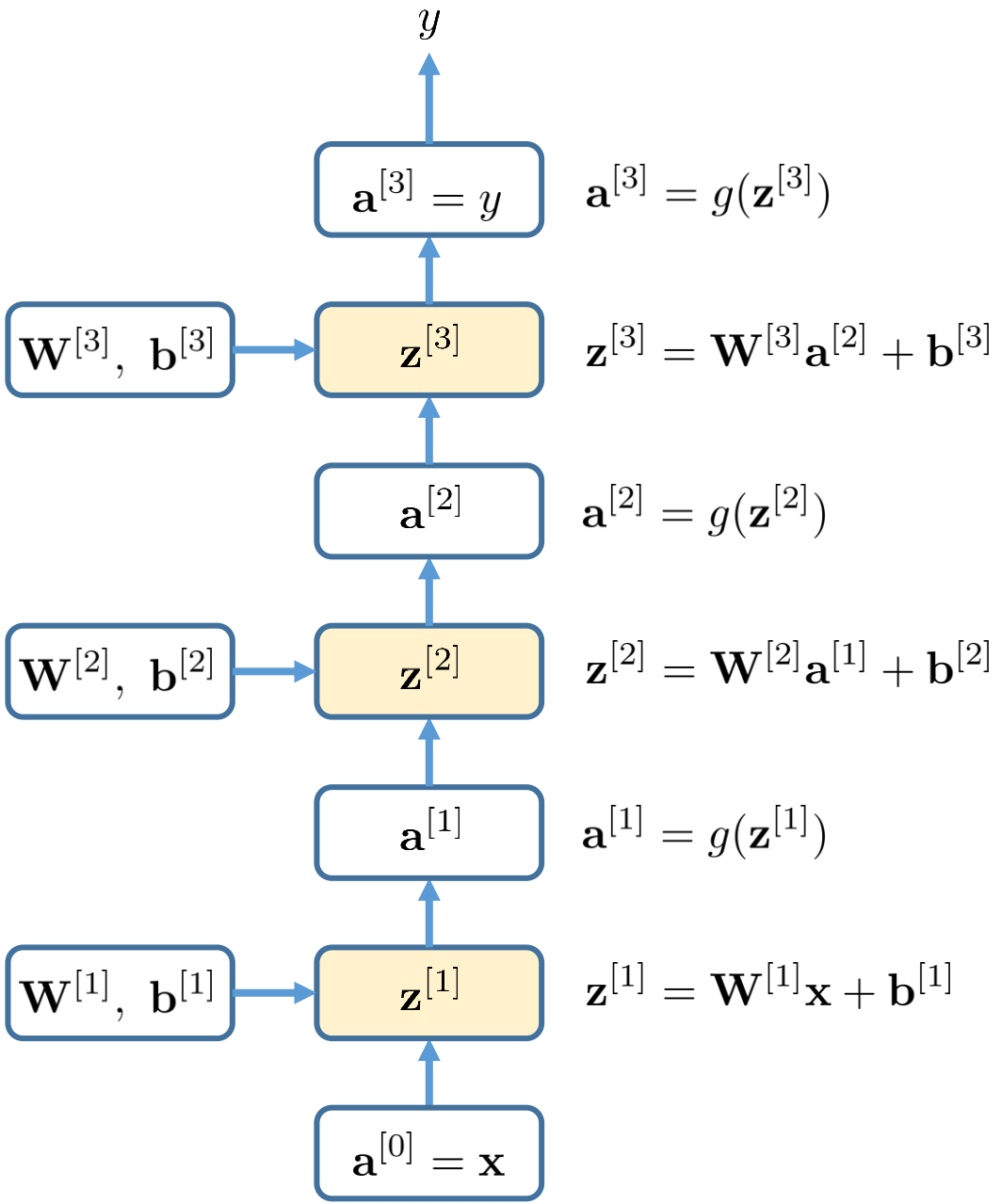
Back Propagation – Vectorization:



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

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

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



Neural Networks

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:

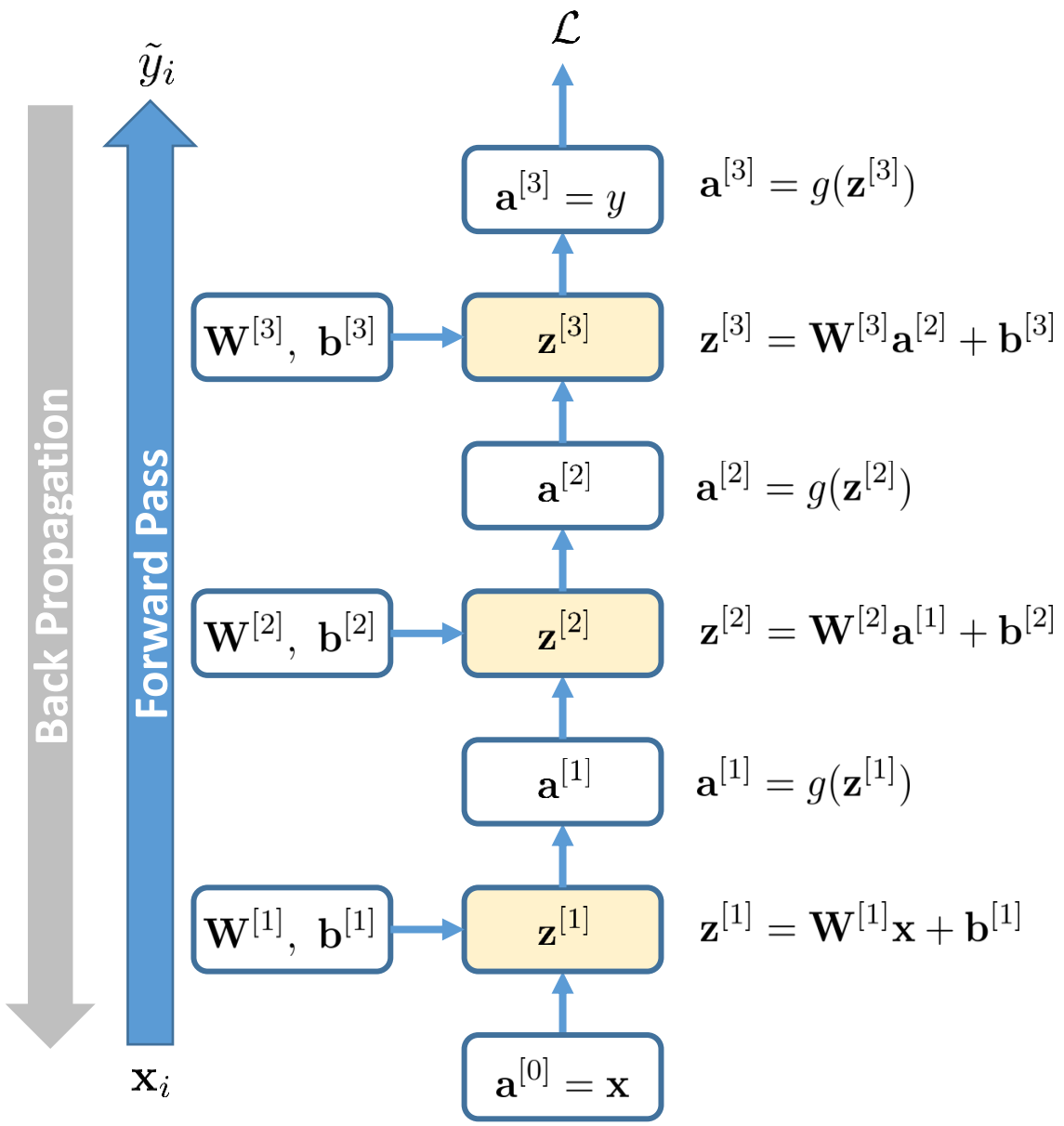
$$\frac{\partial \mathcal{L}}{\partial \mathbf{W}^{[3]}} = \frac{\partial \mathcal{L}}{\partial \mathbf{a}^{[3]}} \frac{\partial \mathbf{a}^{[3]}}{\partial \mathbf{z}^{[3]}} \frac{\partial \mathbf{z}^{[3]}}{\partial \mathbf{W}^{[3]}} \qquad \frac{\partial \mathcal{L}}{\partial \mathbf{b}^{[3]}} = \frac{\partial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

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

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

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

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



Neural Networks

Back Propagation – Vectorization:

Partial Derivatives:

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

$$\frac{\partial \mathcal{L}}{\mathbf{W}^{[3]}} = \frac{\partial \mathcal{L}}{\partial \mathbf{z}^{[3]}} \frac{\partial \mathbf{z}^{[3]}}{\partial \mathbf{W}^{[3]}} \qquad \frac{\partial \mathcal{L}}{\mathbf{b}^{[3]}} = \frac{\partial \mathcal{L}}{\partial \mathbf{z}^{[3]}} \frac{\partial \mathbf{z}^{[3]}}{\partial \mathbf{b}^{[3]}}$$

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

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

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

$$\frac{\partial \mathcal{L}}{\partial \mathbf{b}^{[2]}} = \frac{\partial \mathcal{L}}{\partial \mathbf{z}^{[2]}} \frac{\partial \mathbf{z}^{[2]}}{\partial \mathbf{b}^{[2]}}$$

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

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

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

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

- 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 $\frac{\partial \mathbf{z}^{[\ell]}}{\partial \mathbf{b}^{[\ell]}}$.

Neural Networks

Back Propagation – Vectorization:

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

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

In literature, we often denote $\frac{\partial \mathcal{L}}{\partial \mathbf{z}^{[\ell]}}$ with δ^{ℓ}.

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

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

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

  - Classification:

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

$$\frac{\partial \mathcal{L}}{\partial \mathbf{a}^{[L]}} = -\left(\frac{y}{\mathbf{a}^{[L]}} - \frac{1-y}{1-\mathbf{a}^{[L]}}\right)$$

Neural Networks

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.

- $\odot$ 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).

Neural Networks

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:

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

- 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.

Neural Networks

Back Propagation – Vectorization:

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

- We know that

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

- Finally, we obtain

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

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

Neural Networks

Back Propagation – Vectorization:

Key Equations:

- Gradients with respect to weight and bias:

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

- 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:

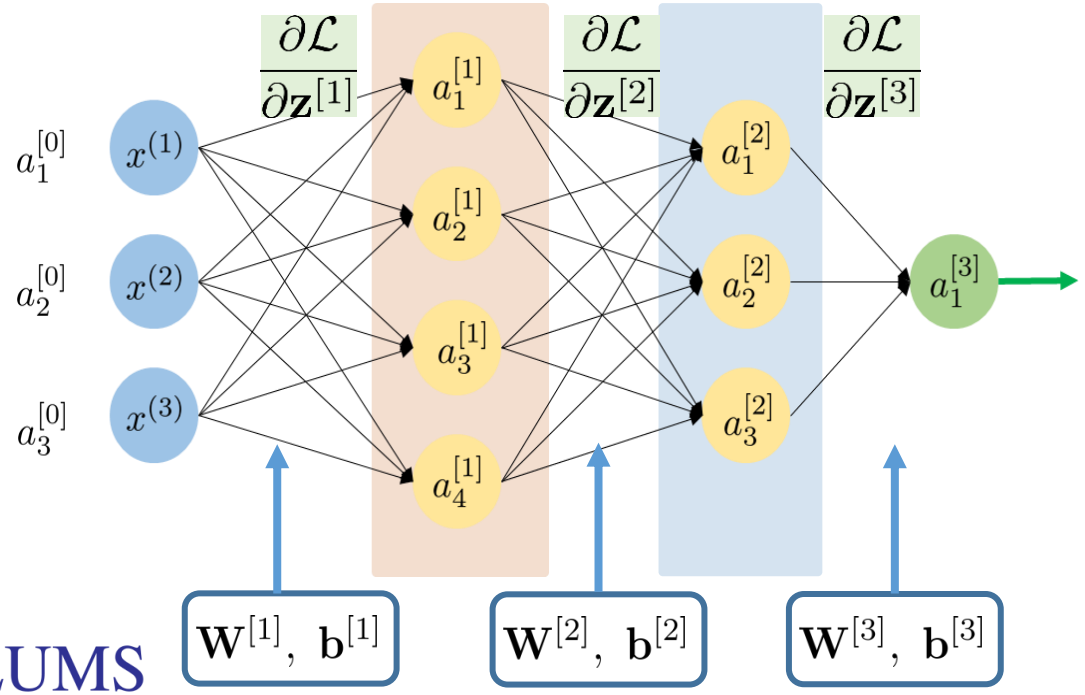
$$g'(\mathbf{z}^{[\ell]}) = \sigma(\mathbf{z}^{[\ell]}) \odot \left(1 - \sigma(\mathbf{z}^{[\ell]})\right)$$

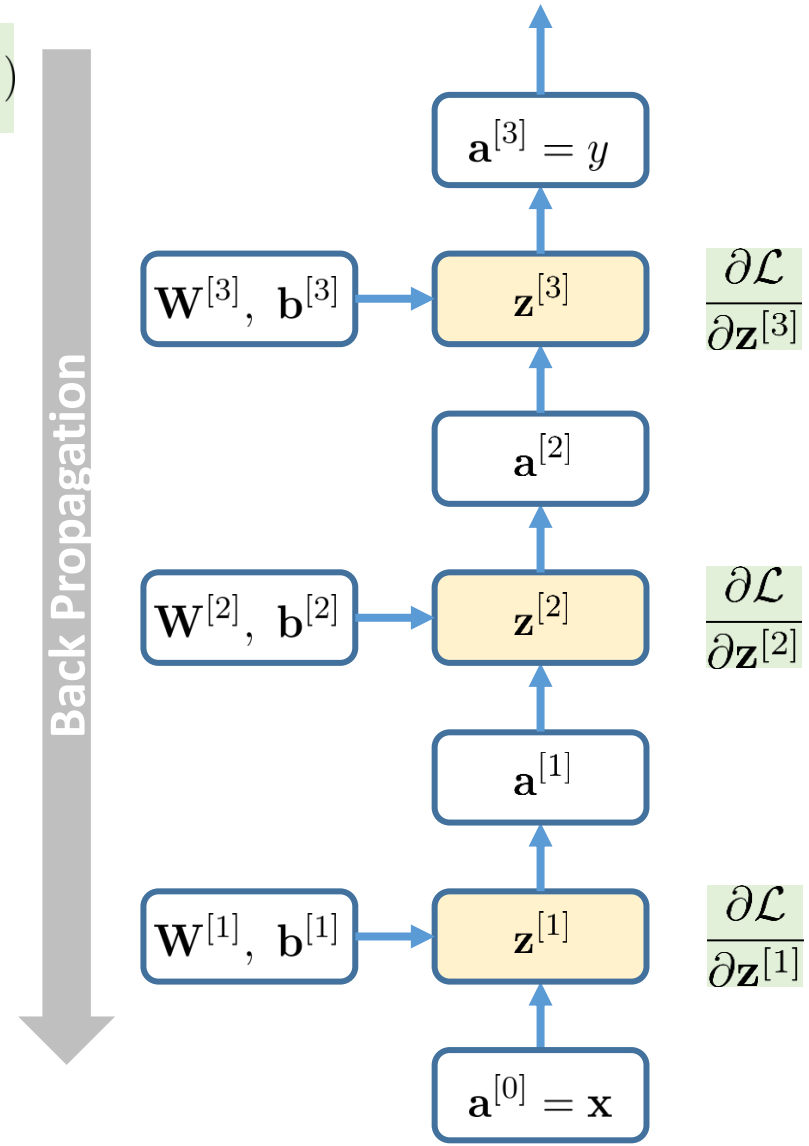
Neural Networks

Back Propagation – Vectorization:

Interpretation of Key Equations:

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





Neural Networks

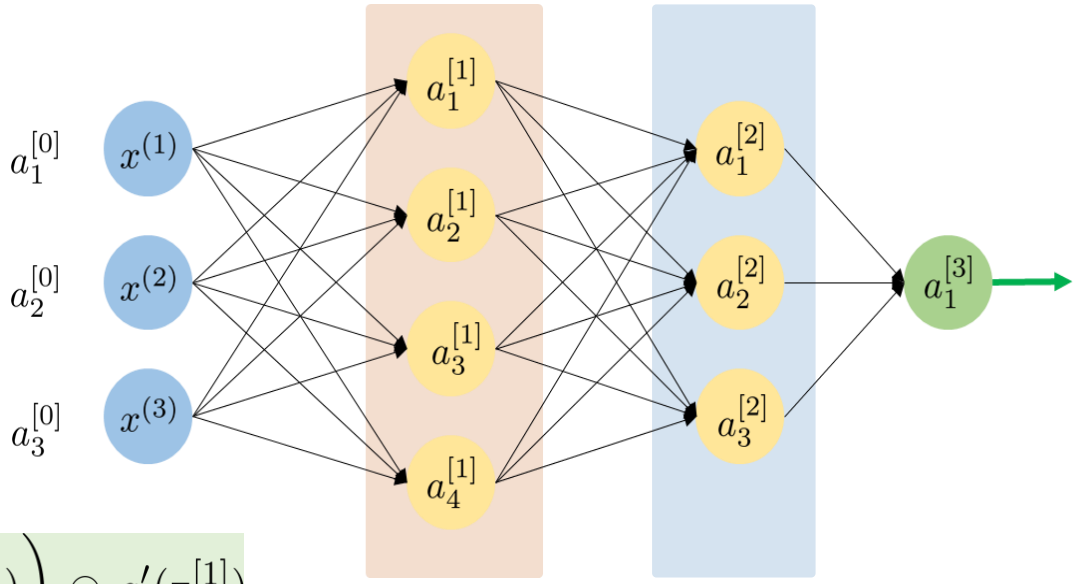
Back Propagation – Vectorization:

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

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

- Base case:

$$\frac{\partial \mathcal{L}}{\partial \mathbf{z}^{[3]}} = \frac{\partial \mathcal{L}}{\partial \mathbf{a}^{[3]}} \odot g'(\mathbf{z}^{[3]}) = (\mathbf{a}^{[L]} - y) \odot g'(\mathbf{z}^{[3]}) \qquad 1 \times 1$$



$$\frac{\partial \mathcal{L}}{\partial \mathbf{z}^{[1]}} = \left(\mathbf{W}^{[2]^T} \frac{\partial \mathcal{L}}{\partial \mathbf{z}^{[2]}}\right) \odot g'(\mathbf{z}^{[1]}) = \left(\mathbf{W}^{[2]^T} \left((\mathbf{W}^{[3]^T} \frac{\partial \mathcal{L}}{\partial \mathbf{z}^{[3]}}) \odot g'(\mathbf{z}^{[2]})\right) \odot g'(\mathbf{z}^{[1]})\right)$$

$4 \times 3 \qquad 3 \times 1 \qquad 3 \times 1 \qquad 4 \times 1$

- Finally:

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

$4 \times 3 \qquad 4 \times 1 \qquad 1 \times 3$

Neural Networks

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
- http://neuralnetworksanddeeplearning.com/