Intro to Neural Networks

Foundations of Deep Learning

BOSTON UNIVERSITY
MACHINE INTELLIGENCE
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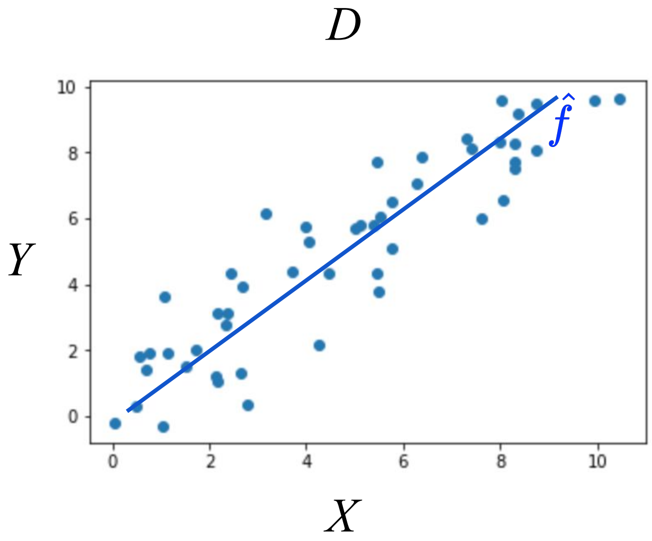
Building up to Neural Networks

Regression

What is learning?

The approximation of some unknown function f based on some data D.



$$f : X \rightarrow Y$$

$$\hat{f} = \theta_0 + \theta_1 x$$

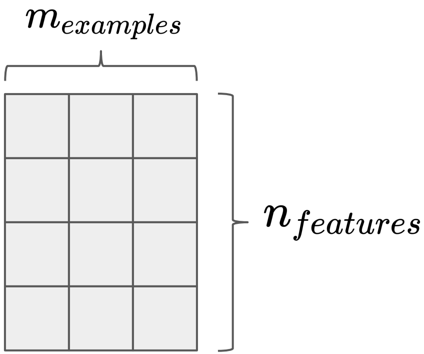
How do we set the parameters?
How do we know what assumptions to make?

Dataset

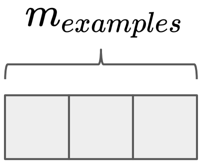
$$X_i = \begin{bmatrix} feature_1 \\ feature_2 \\ \vdots \\ feature_n \end{bmatrix}$$

$$Y_i = label_1$$

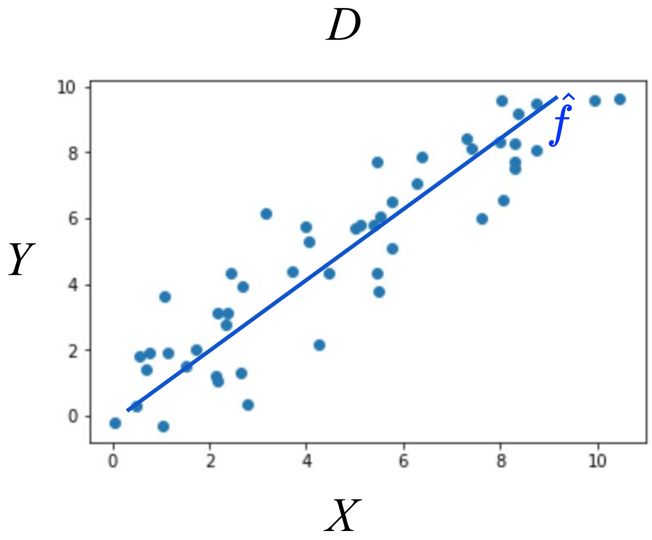
$$X =$$



$$Y =$$



Linear Regression



One dimensional input

$$y = mx + b$$

Multi dimensional input

$$y = w_1 x_1 + \cdots + w_n x_n + b$$

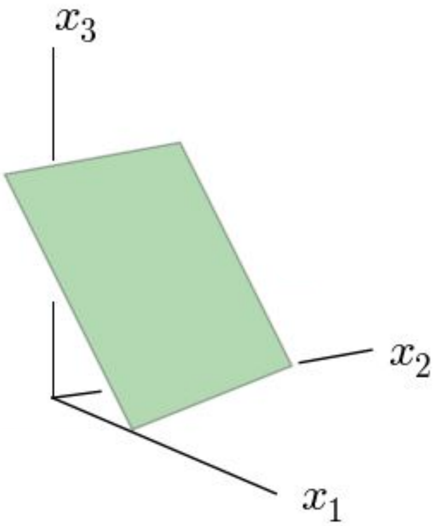
Linear Regression example

Say you want to predict house prices given some features about the house

$$x_1 = 5(bedrooms), x_2 = 3(bathrooms), x_3 = 3000(squarefeet)$$

Then the house price could be:

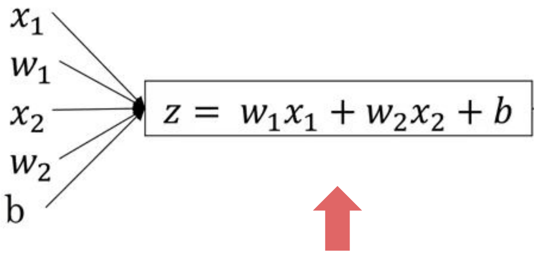
$$z = 5w_1 + 3w_2 + 3000w_3 + b$$



Logistic Regression (1)

1. **Has a linear combination / made up of weights and a bias**

$$z = w_1x_1 + w_2x_2 + \ldots + w_nx_n + b$$



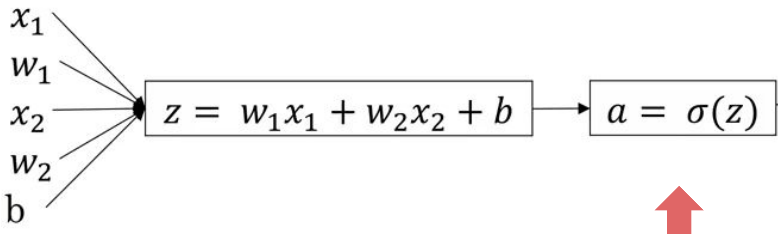
Logistic Regression (2)

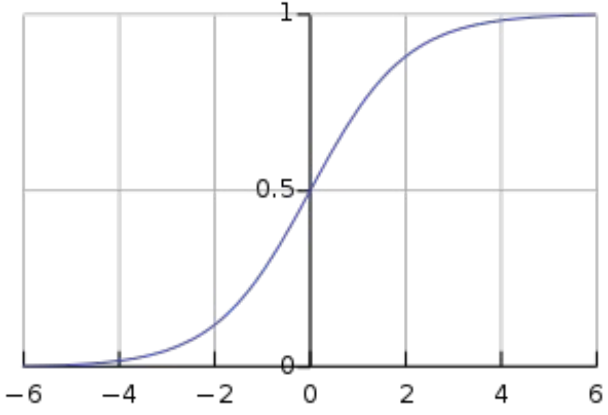
1. Has a linear combination / made up of weights and a bias

$$z = w_1x_1 + w_2x_2 + \ldots + w_nx_n + b$$

2. Is fed through an activation function (such as a sigmoid function)

$$a = \hat{y} = \sigma(z)$$





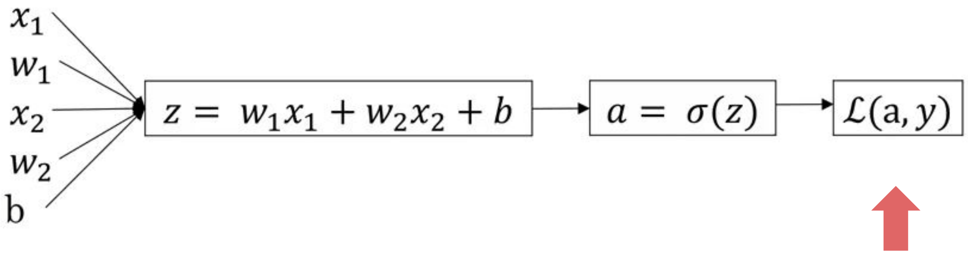
Logistic Regression (3)

$$z = w_1x_1 + w_2x_2 + \ldots + w_nx_n + b$$

$$a = \hat{y} = \sigma(z)$$

3. The output is used to measure the difference from the actual data.

$$L(a, y) = y - a$$



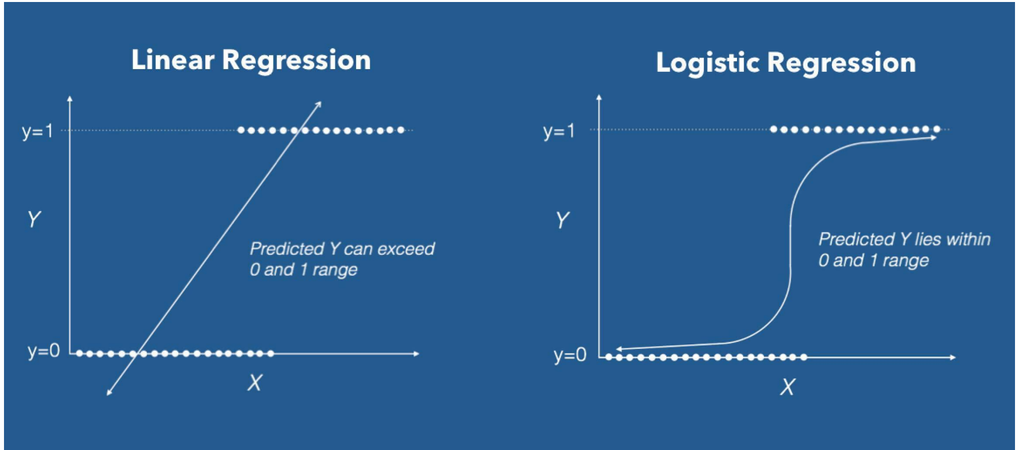
Logistic Regression (example)

Now say we want to determine if we can afford the house or not.

In this case we would use a sigmoid function to output values between 0 or 1.

This can be a metric of how affordable the house is.

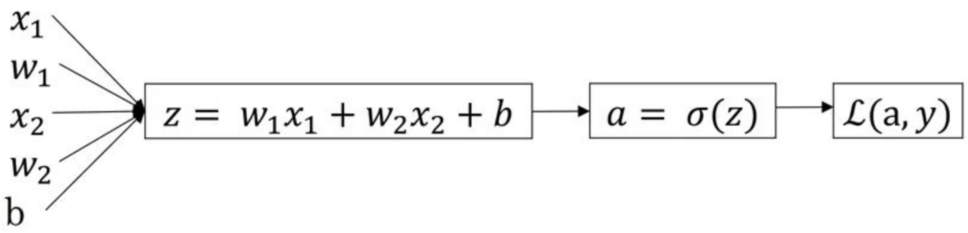
$$a = y = \sigma(z)$$



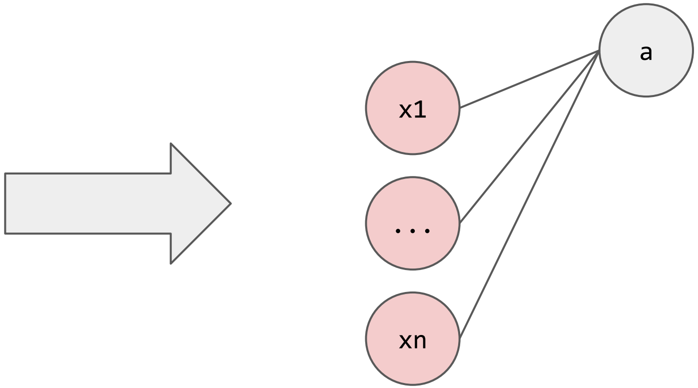
Logistic Regression to Neural Networks (1)

Single logistic regression

$$a = \sigma(w_1 x_2 + \cdots + w_n x_n + b)$$



Expanded representation



Compact representation

Logistic Regression to Neural Networks (2)

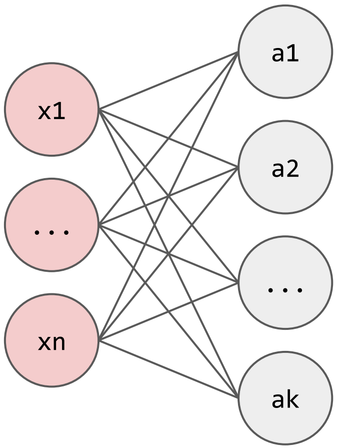
Multiple logistic regressions

$$a_1 = \sigma(w_1^{(1)} x_1 + \cdots + w_n^{(1)} x_n + b^{(1)})$$

$$a_2 = \sigma(w_1^{(2)} x_1 + \cdots + w_n^{(2)} x_n + b^{(2)})$$

$$\vdots$$

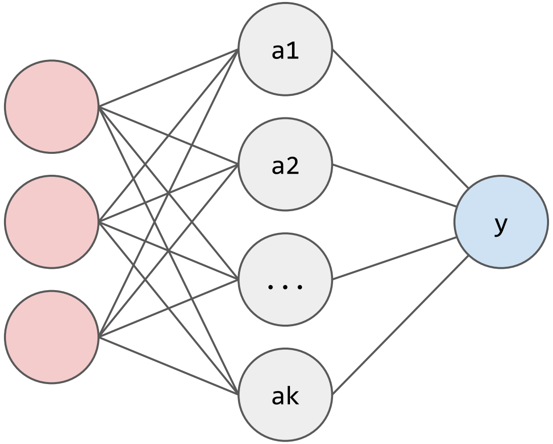
$$a_k = \sigma(w_1^{(k)} x_1 + \cdots + w_n^{(k)} x_n + b^{(k)})$$



Logistic Regression to Neural Networks (2)

Logistic regression on the outputs of other logistic regressions

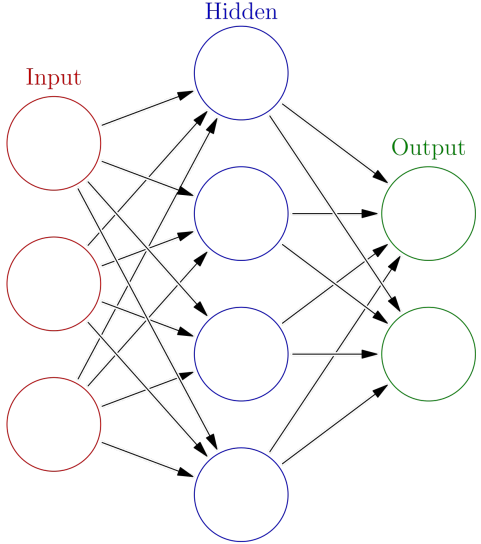
$$\hat{y} = \sigma(w_1^{(y)} a_1 + \cdots + w_k^{(y)} a_k + b^{(y)})$$



Shallow Neural Networks

The foundation of new AI

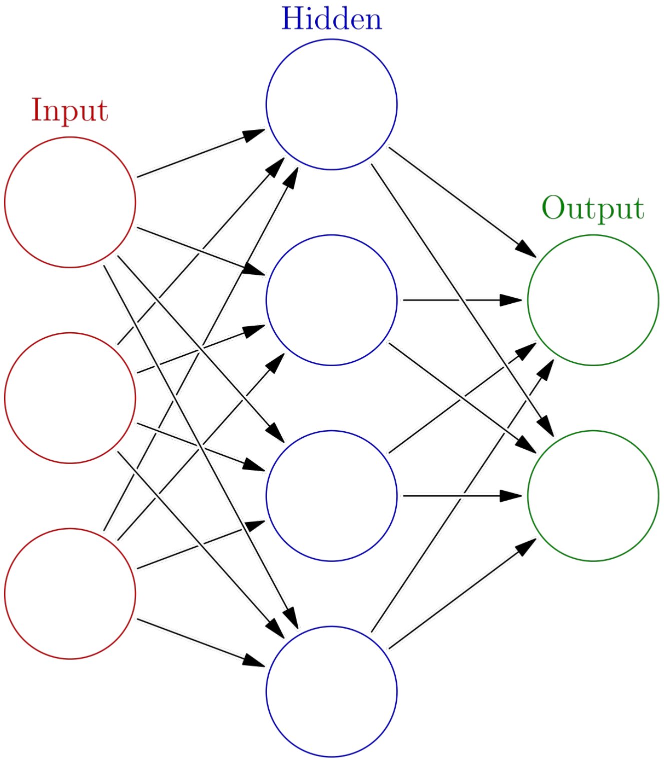
Neural Network



1. A neural network is a bunch of activations in layers
    a. The middle layers are called a hidden layer
2. Each activation takes in inputs from the previous layer
    a. The hidden layer is built from the input layer
    b. The output layer is built from the hidden layer
3. Adding more layers means we can learn more complicated functions

Activations (Neuron)

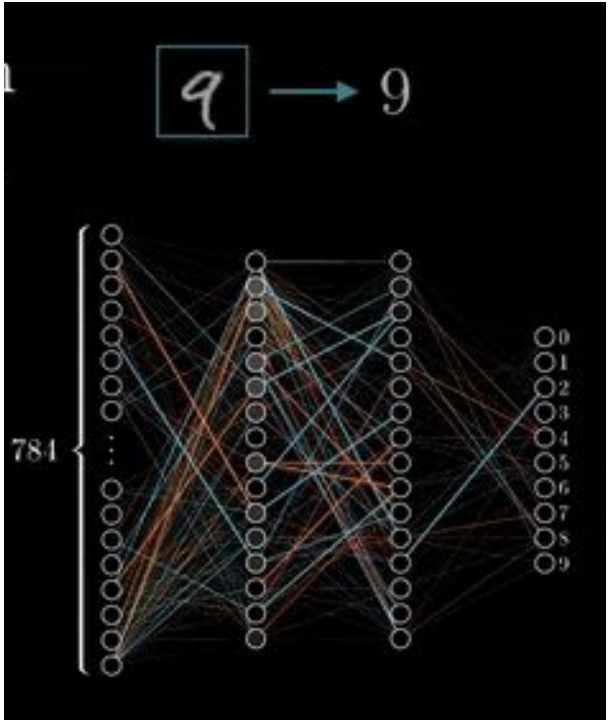
1. **Affine function**
   a. $z = w_1 a_1^{[l-1]} + \cdots + w_n a_n^{[l-1]} + b$
   b. **Gathers and weights features**
2. **Activation**
   a. $a = g(z)$
      i. $g(x)$ **is an activation function**
   b. **Acts as a significance threshold**



Where are the weights in this diagram?

Three steps to training a neural network

1. Forward propagation
   a. Push example through the network to get a predicted output
2. Compute the cost
   a. Calculate difference between predicted output and actual data
3. Backward propagation
   a. Push back the derivative of the error and apply to each weight, such that next time it will result in a lower error



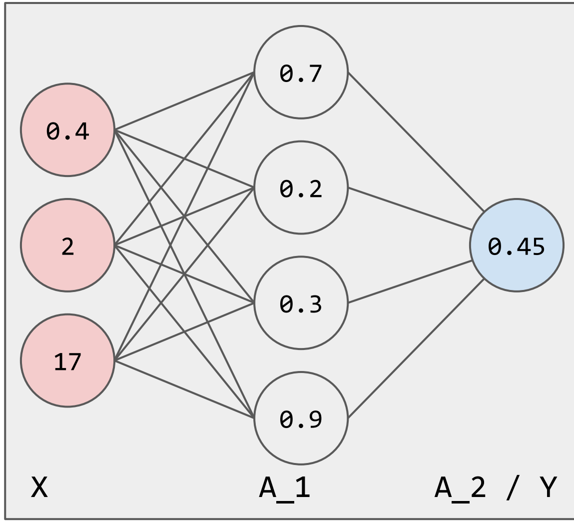
Shallow Neural Networks (example)

Say you want to predict if it is worth going to class or not

$$X = \begin{bmatrix} \text{difficulty of material} \\ \text{number of assignments due} \\ \text{days until midterm} \end{bmatrix} \qquad Y = \begin{bmatrix} \text{probability of going to class} \end{bmatrix}$$

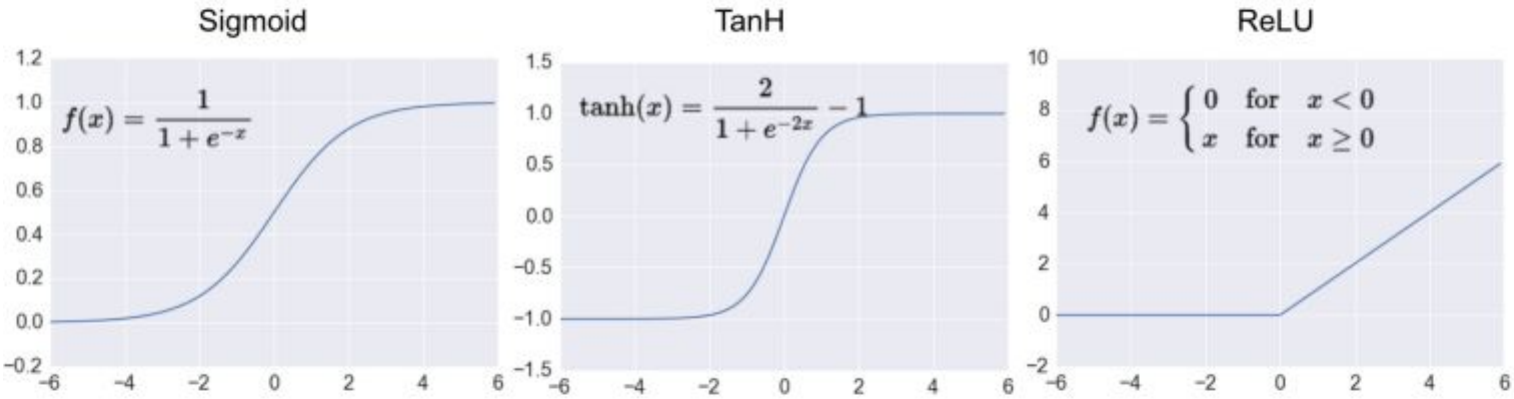
$$a_i^{[1]} = g(z) = g(w_1 x_1 + w_2 x_2 + w_3 x_3 + b)$$

$$a^{[2]} = g(w_1 a_1^{[1]} + w_2 a_2^{[1]} + w_3 a_3^{[1]} + w_4 a_4^{[1]} + b)$$



Activation Functions

1. **Sigmoid: output is between 0,1**
2. **Tanh: output is between -1,1**
3. **ReLu: output is positive real numbers**

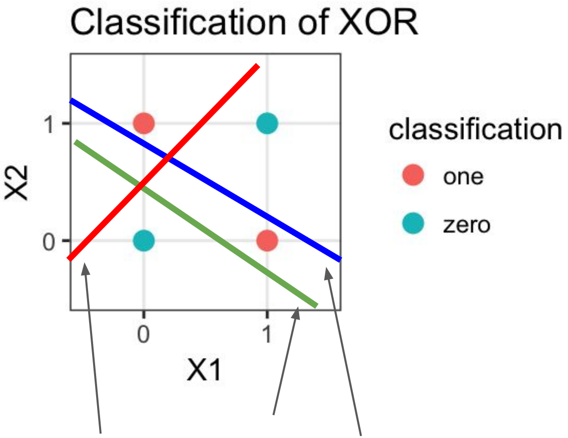


Why do you need nonlinear activation functions?

XOR Problem

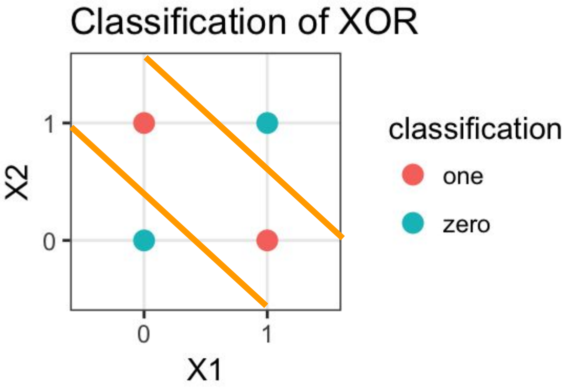
There is no way to correctly classify all inputs with a linear decision boundary

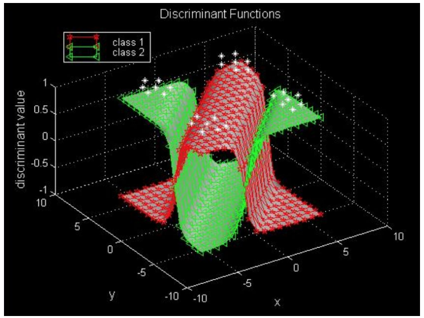
Linear Classifier



Possible linear decision boundaries

Two Layer Neural Network w/ Sigmoid Activation





Linear Activation Functions

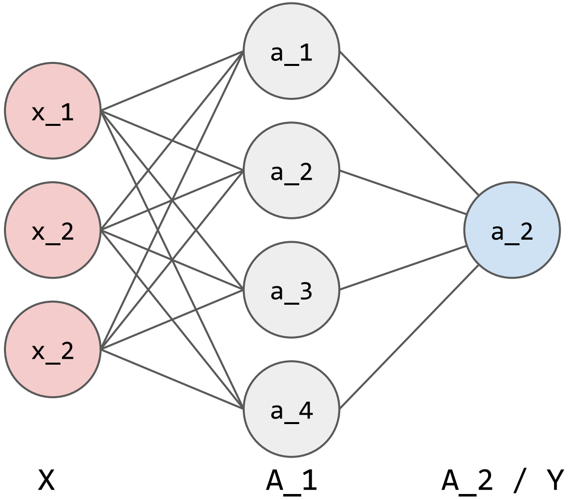
If we removed the activation function from our model that can be called a linear activation function.

$$a_1 = w_1 x + b_1 \qquad a_2 = w_2 a_1 + b_2$$

$$\begin{aligned} a_2 &= w_2(w_1 x + b_1) + b_2 \\ &= w_2 w_1 x + \underbrace{w_2 b_1 + b_2} \\ &= wx + b \end{aligned}$$

Forward Propagation

1. **We've seen neural nets with one pass through, however usually, we have multiple samples.**
2. **One way is to do this iteratively**




```
for each sample i:
    for each layer l:
        for each activation j:
```

$$a_j^{[l]} = g^{[l]}(\sum_k w_{jk}^{[l]} a_k^{[l-1]} + b_j^{[l]}) = g^{[l]}(z_j^{[l]})$$

```
finally, use the final activations to compute
the cost
```

Computing the cost

In order to train our neural network, we need some way to tell us how far off its estimate was from the actual value.

We define the cost function, $J(\hat{y}, y)$ **as the sum of losses,** $\sum_{i=0}^{m} L(\hat{y}, y)$

a. Loss = Error for a single training example

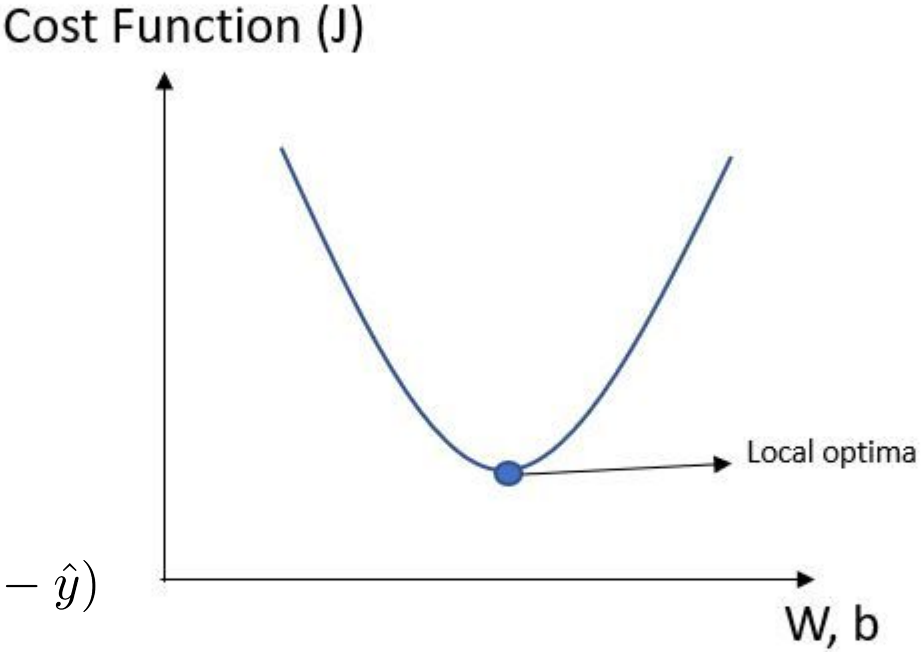
b. Cost = Sum of all Losses

Example cost functions

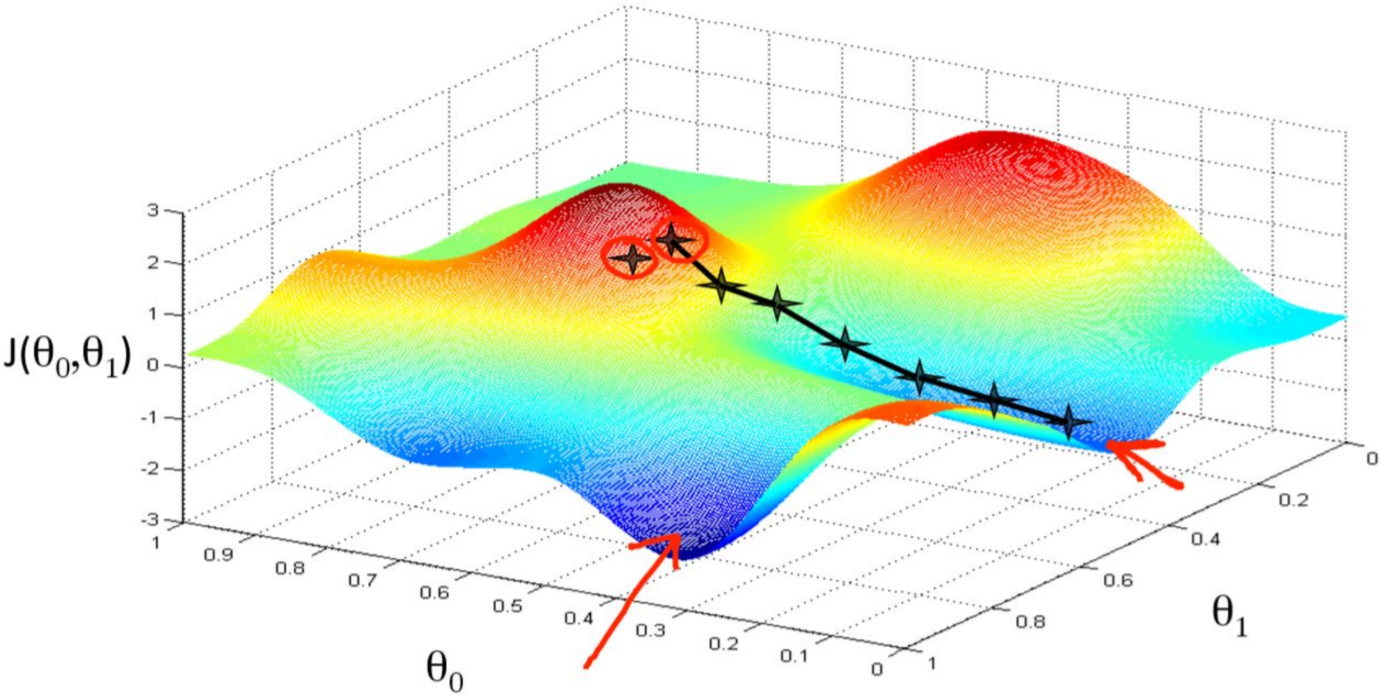
$$\text{MSE} = \frac{1}{n} \sum_{i=1}^{n} (y_i - \tilde{y}_i)^2$$

$$L_{\text{cross-entropy}}(\hat{\mathbf{y}}, \mathbf{y}) = -\sum_i y_i \log(\hat{y}_i)$$

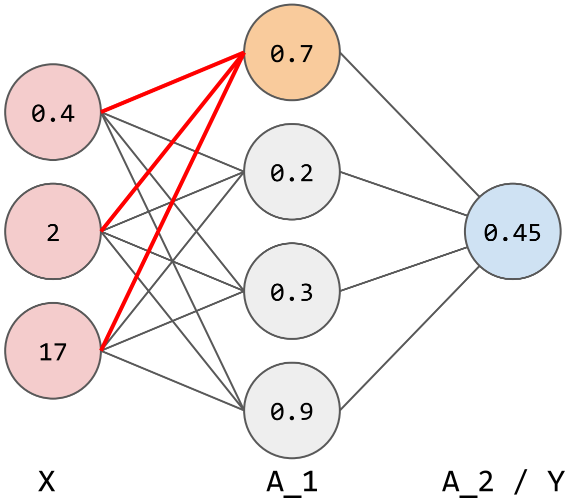
$$L(\hat{y}, y) = -y \log \hat{y} - (1 - y) \log(1 - \hat{y})$$



Cost function for gradient descent

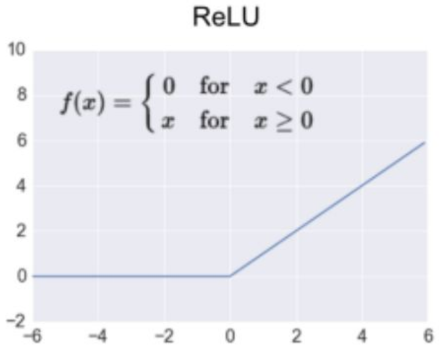


Forward Propagation (example)

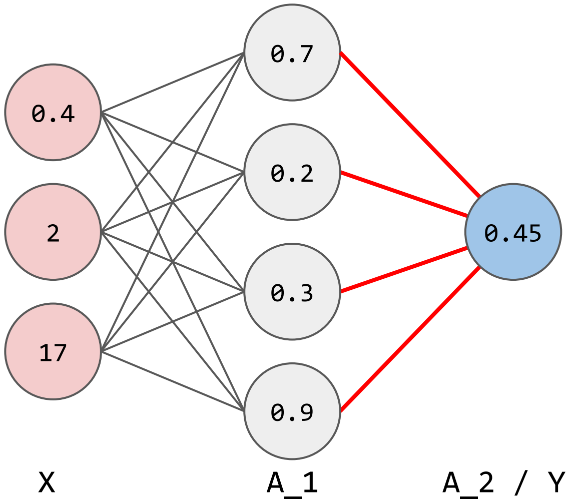


$$z_1^{[1]} = w_1^{[1]}x_1 + w_1^{[1]}x_2 + w_3^{[1]}x_3 + b$$
$$= 0.5 * 0.4 + 0.1 \times 2 + 0.0058 \times 17 + 0.2 = 0.7$$

$$a_1^{[1]} = g(0.7) = \mathrm{ReLU}(0.7) = 0.7$$



Forward Propagation (example)

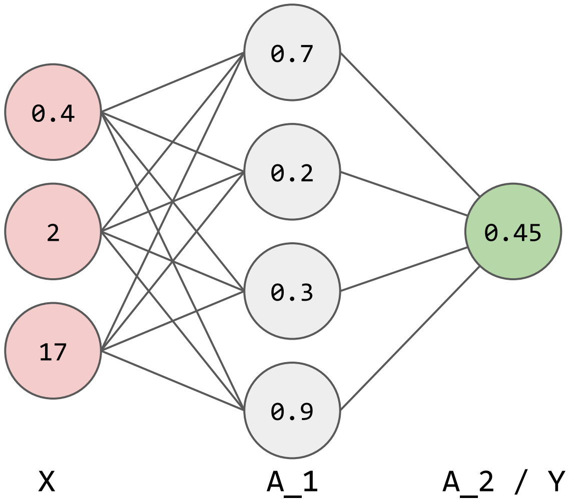


$$z_1^{[1]} = w_1^{[1]}x_1 + w_1^{[1]}x_2 + w_3^{[1]}x_3 + b$$
$$= 0.5 * 0.4 + 0.1 \times 2 + 0.0058 \times 17 + 0.2 = 0.7$$

$$a_1^{[1]} = g(0.7) = \mathrm{ReLU}(0.7) = 0.7$$

$$z_1^{[2]} = w_1^{[2]}a_1^{[1]} + w_2^{[2]}a_2^{[1]} + w_3^{[2]}a_3^{[1]} + w_4^{[2]}a_4^{[1]} + b$$

Forward Propagation (example)



$$z_1^{[1]} = w_1^{[1]} x_1 + w_1^{[1]} x_2 + w_3^{[1]} x_3 + b$$
$$= 0.5 * 0.4 + 0.1 \times 2 + 0.0058 \times 17 + 0.2 = 0.7$$

$$a_1^{[1]} = g(0.7) = \mathrm{ReLU}(0.7) = 0.7$$

$$z_1^{[2]} = w_1^{[2]} a_1^{[1]} + w_2^{[2]} a_2^{[1]} + w_3^{[2]} a_3^{[1]} + w_4^{[2]} a_4^{[1]} + b$$

$$\hat{y} = a_1^{[2]} = g(z_1^{[2]}) = 0.45$$

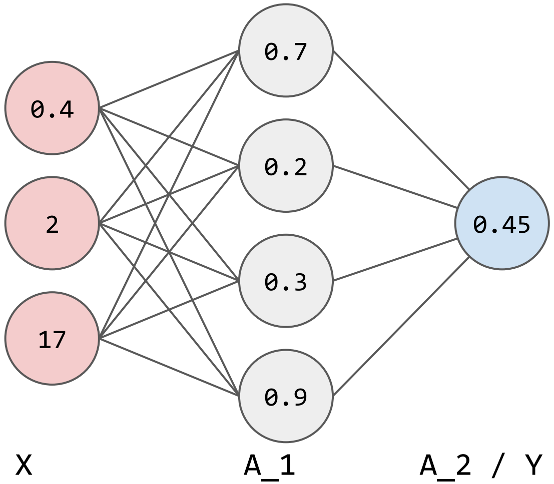
$$y = 1$$

$$L(\hat{y}, y) = -y \log \hat{y} - (1 - y) \log(1 - \hat{y})$$

$$-(1) \log(0.45) - (1 - (1)) \log(1 - (0.45)) = 0.798508$$

Back to the example

Say you want to predict if it is worth going to class or not



$$\hat{y} = a_1^{[2]} = g(z_1^{[2]}) = 0.45$$

```
if y > 0.5:
    goto_class()
else:
    skip()
```

But it turns out midterm material was covered...

$$y = 1$$

Here is his mistake in numerical form

$$L(\hat{y}, y) = \ 0.798508$$

Training a network with Calculus

Gradient descent

Terminology for later - Parameters vs Hyperparameters

Parameters are values that are <u>learned</u> through training or backpropagation. (E.g. W, b)

Hyperparameters are values that are <u>set manually</u> without a learning method. (E.g. the learning rate, α)

Cost Function: revisited

The cost function is the sum of losses for all training examples

- combined error for all training examples.

$$J(\hat{y}, y) = \sum_{i=1}^{m} L(\hat{y}^{(i)}, y^{(i)})$$

This is the general form of writing the cost function

$$J(\theta) = \text{Cost Function}$$

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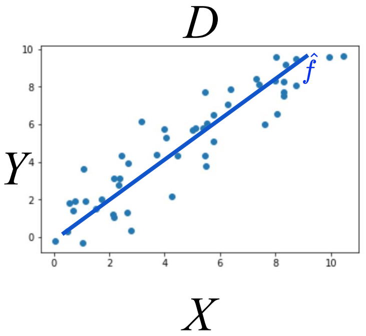
Learning the weights

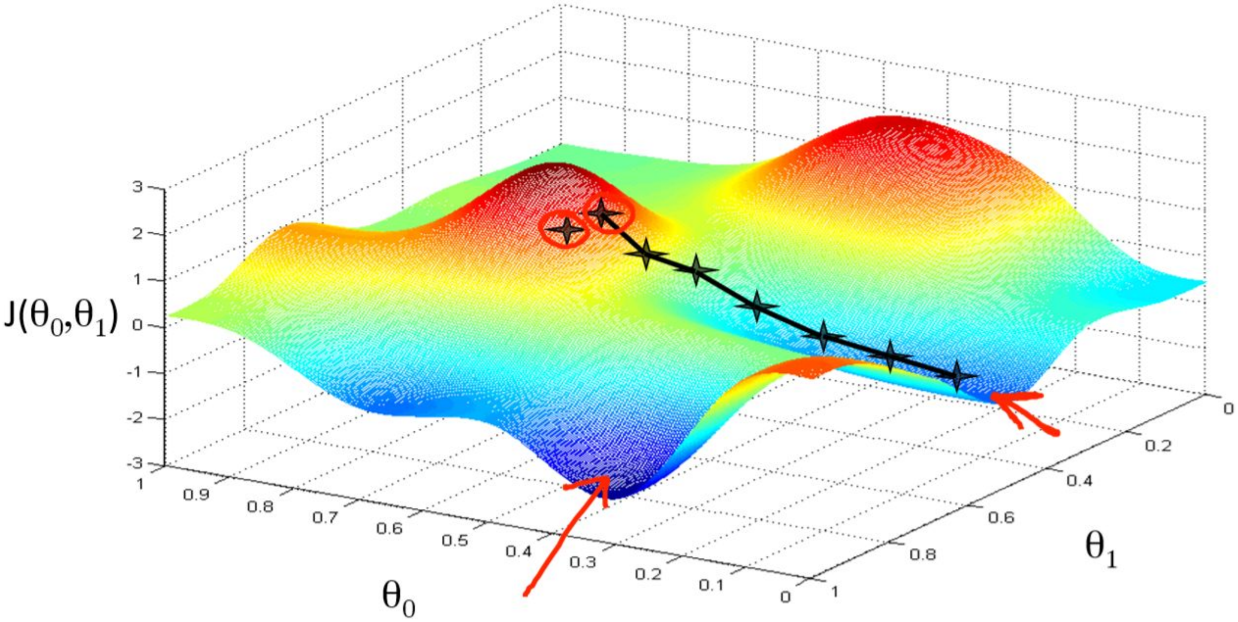
1. Goal: we want to change all of the weights so that our predictions fit the data better



2. Method: the error between our predicted values and actual values tells us how much we need to change each individual weight (increase or decrease)
   a. By calculating the derivative from the cost function we get the numerical value of change.
   b. The derivative is equivalent to the slope that that point, and tells us where the error is minimized

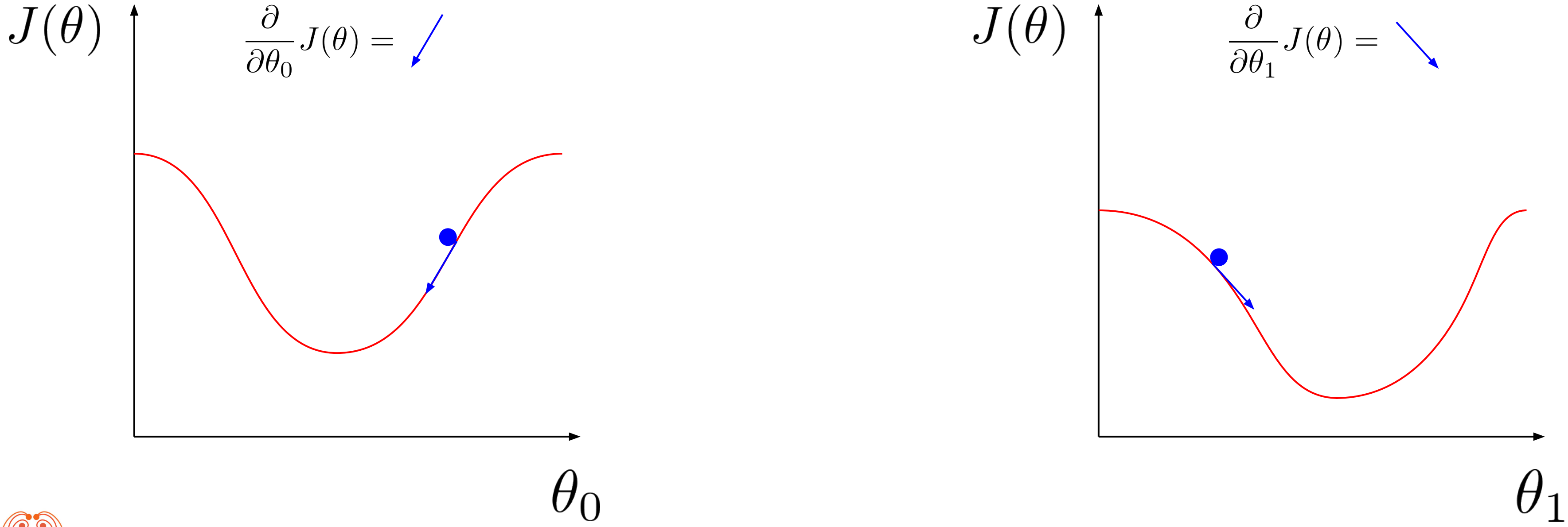
Gradient descent

We find the direction of steepest slope, then take one step in that direction.



Gradient descent

Finding the slope for each individual parameter



Gradient descent

To find the slope, we compute the derivative of the cost (gradient) with respect to a single parameter.

Scalar learning rate

$$\theta_j := \theta_j - \alpha \overbrace{\frac{\partial}{\partial \theta_j} J(\theta)}^{\text{Also written } \nabla J(\theta)}$$

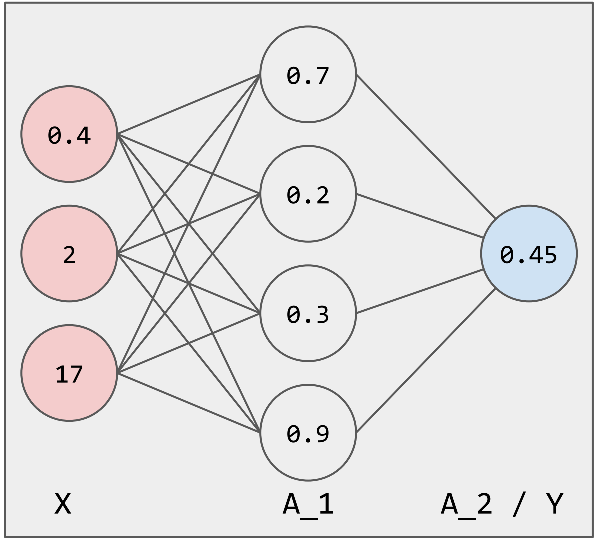
Individual weights

Vector of weights

Cost/objective/loss function

Gradient descent for Neural Networks

Goal: update the **weights** and **biases** such that the **cost function** will output a smaller value (i.e. the difference actual and predicted values will be minimized)



Repeat for many iterations (training steps):

Compute forward pass and the cost function, **J**

$$W^{[1]} := W^{[1]} - \alpha \frac{\partial J}{\partial W^{[1]}}$$

$$b^{[1]} := b^{[1]} - \alpha \frac{\partial J}{\partial b^{[1]}}$$

$$W^{[2]} := W^{[2]} - \alpha \frac{\partial J}{\partial W^{[2]}}$$

$$b^{[2]} := b^{[2]} - \alpha \frac{\partial J}{\partial b^{[2]}}$$

Chain Rule

1. To get the direction that a parameter must change in order reduce prediction error, we use the **chain rule** from calculus.

$$\frac{d}{dx}f(g(x)) = f'(g(x))g'(x)$$

$$\frac{\partial J}{\partial W^{[2]}} = \frac{\partial J}{\partial a^{[2]}}\frac{\partial a^{[2]}}{\partial z^{[2]}}\frac{\partial z^{[2]}}{\partial W^{[2]}}$$

$$\frac{\partial J}{\partial W^{[1]}} = \frac{\partial J}{\partial a^{[2]}}\frac{\partial a^{[2]}}{\partial z^{[2]}}\frac{\partial z^{[2]}}{\partial a^{[1]}}\frac{\partial a^{[1]}}{\partial z^{[1]}}\frac{\partial z^{[1]}}{\partial W^{[1]}}$$

$$J(\hat{y}, y) = \sum_{i=1}^{m} L(\hat{y}^{(i)}, y^{(i)})$$

$$L(\hat{y}, y) = -y \log \hat{y} - (1 - y) \log(1 - \hat{y})$$

$$a^{[2]} = g^{[2]}(z^{[2]})$$

$$z^{[2]} = W^{[2]} a^{[1]} + b^{[2]}$$

$$a^{[1]} = g^{[1]}(z^{[1]})$$

$$z^{[1]} = W^{[1]} x + b^{[1]}$$