Scientific Computing

April 14, 2025

Announcements

- Homework 5 due Fri, 11:59pm
- No class Fri Apr 18, Mon Apr 21 (Easter Break)
- Homework 6 is going to be an assignment to watch and learn from some online videos. More info on Wednesday.

Today

- Intro to Neural Networks
- Coding NN and Batching

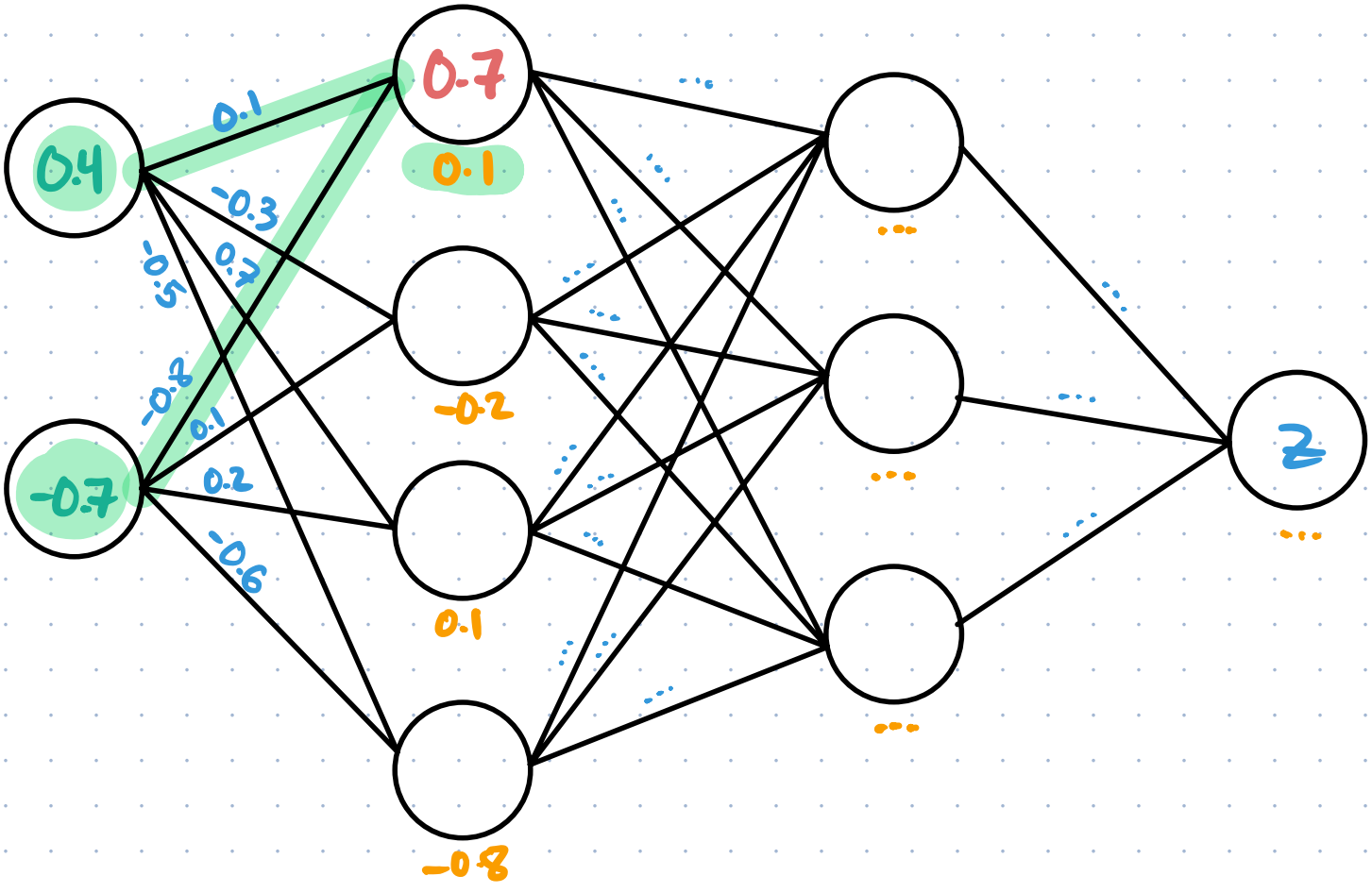
Office Hours:

Mon + Fri

9:30am - 10:30am

Cudahy 307

Example: A NN that takes 2 inputs and has 1 output
$f(u,v) = z$



To calculate the value for a neuron, we multiply the value of each connected neuron from the last layer by the weight of the connection, add these all up, and add the bias

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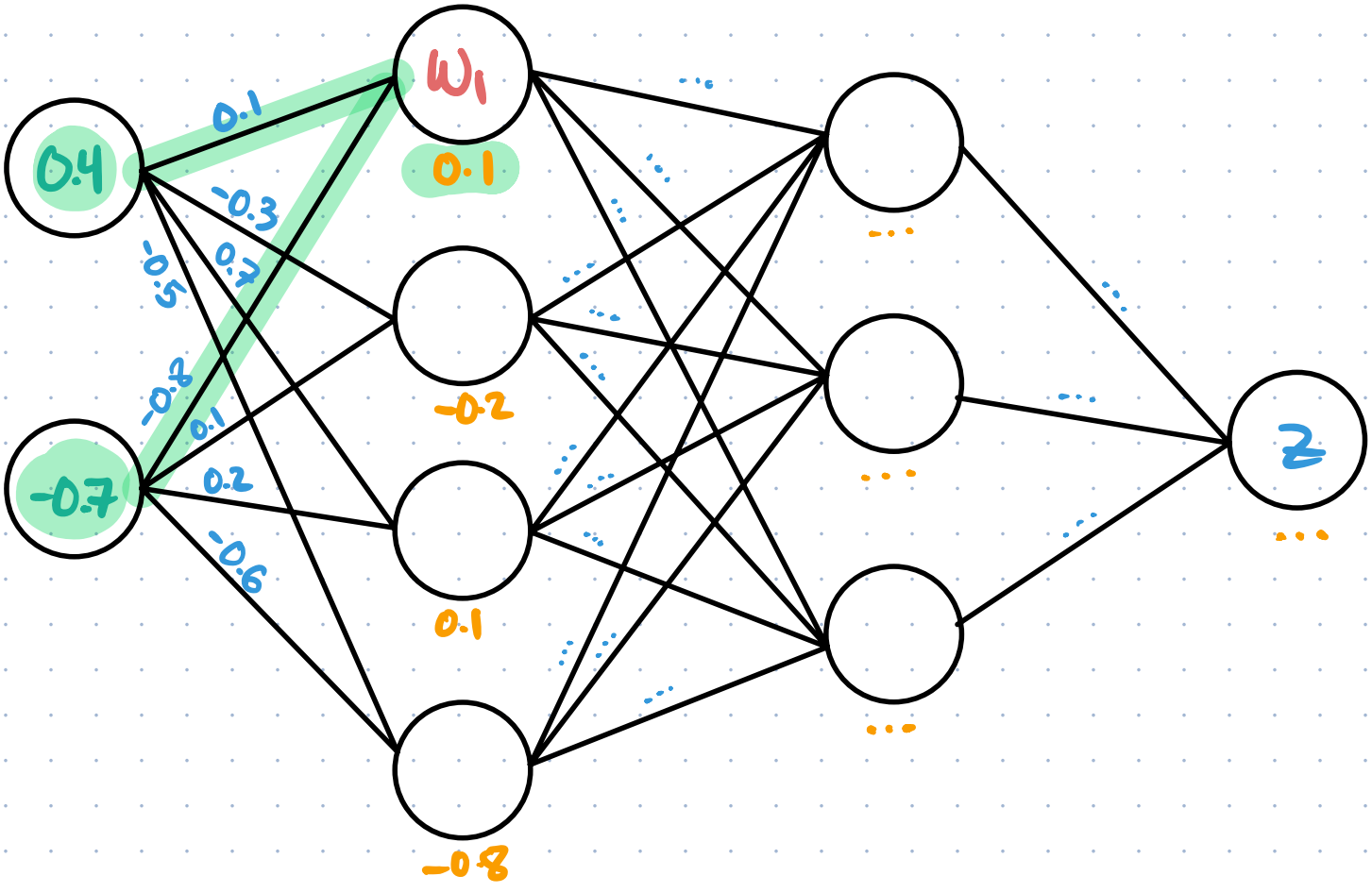
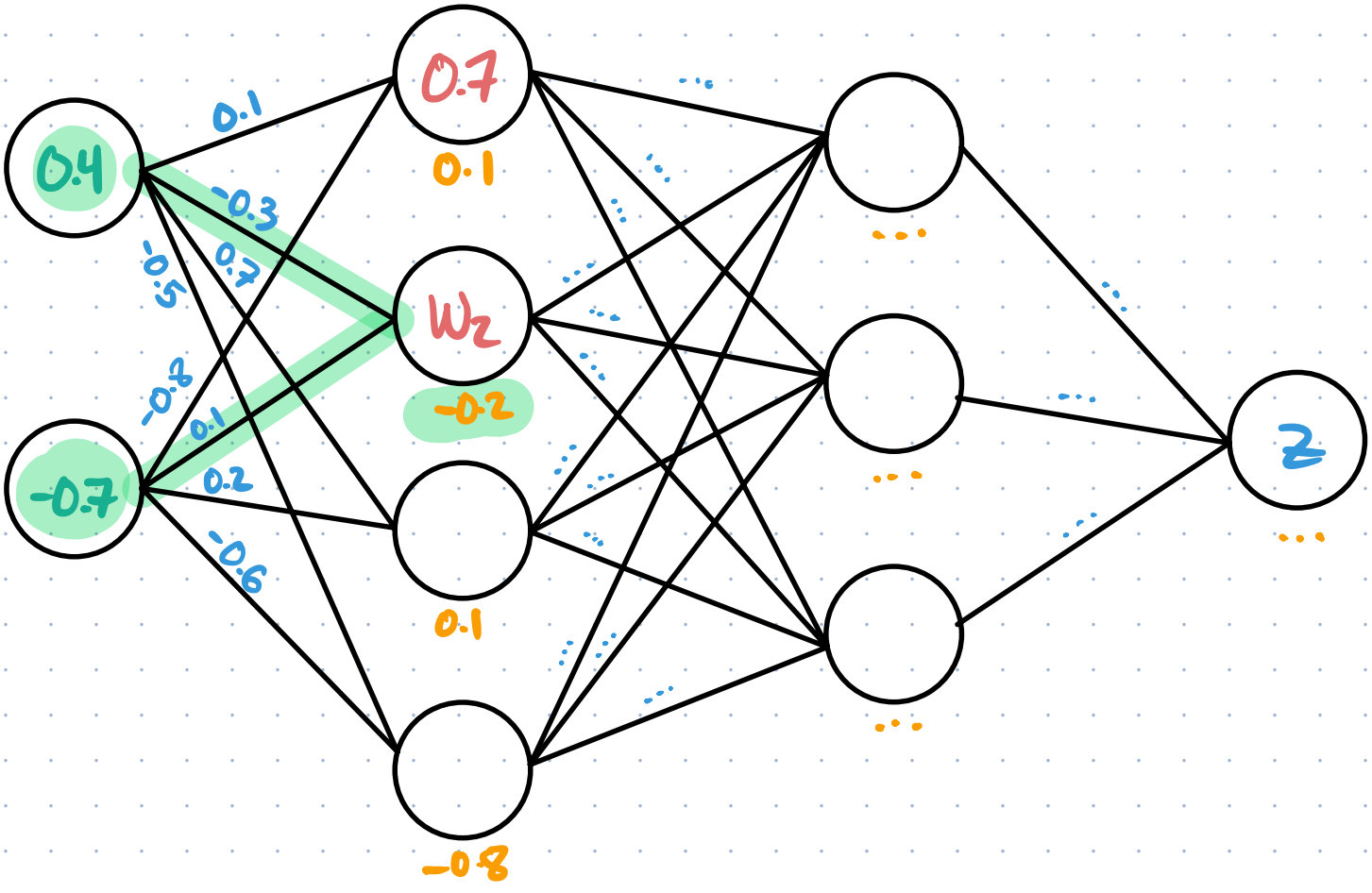


$W_1 = (0.4)(0.1) + (-0.7)(-0.8) + 0.1$

$= 0.7$

Example: A NN that takes 2 inputs and has 1 output

$f(u,v) = z$

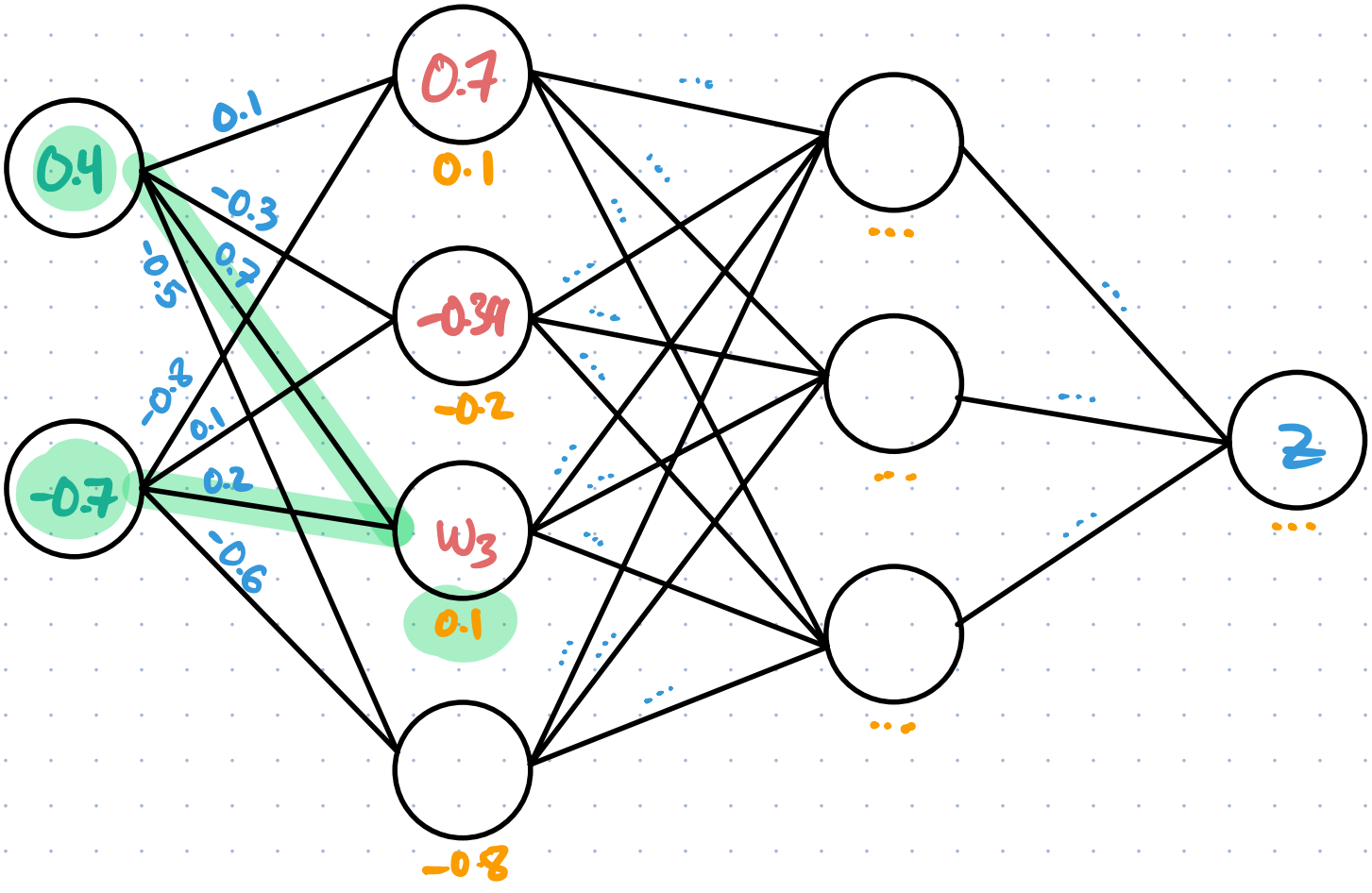


$W_2 = (0.4)(-0.3) + (-0.7)(0.1) + -0.2$

$= -0.39$

Example: A NN that takes 2 inputs and has 1 output

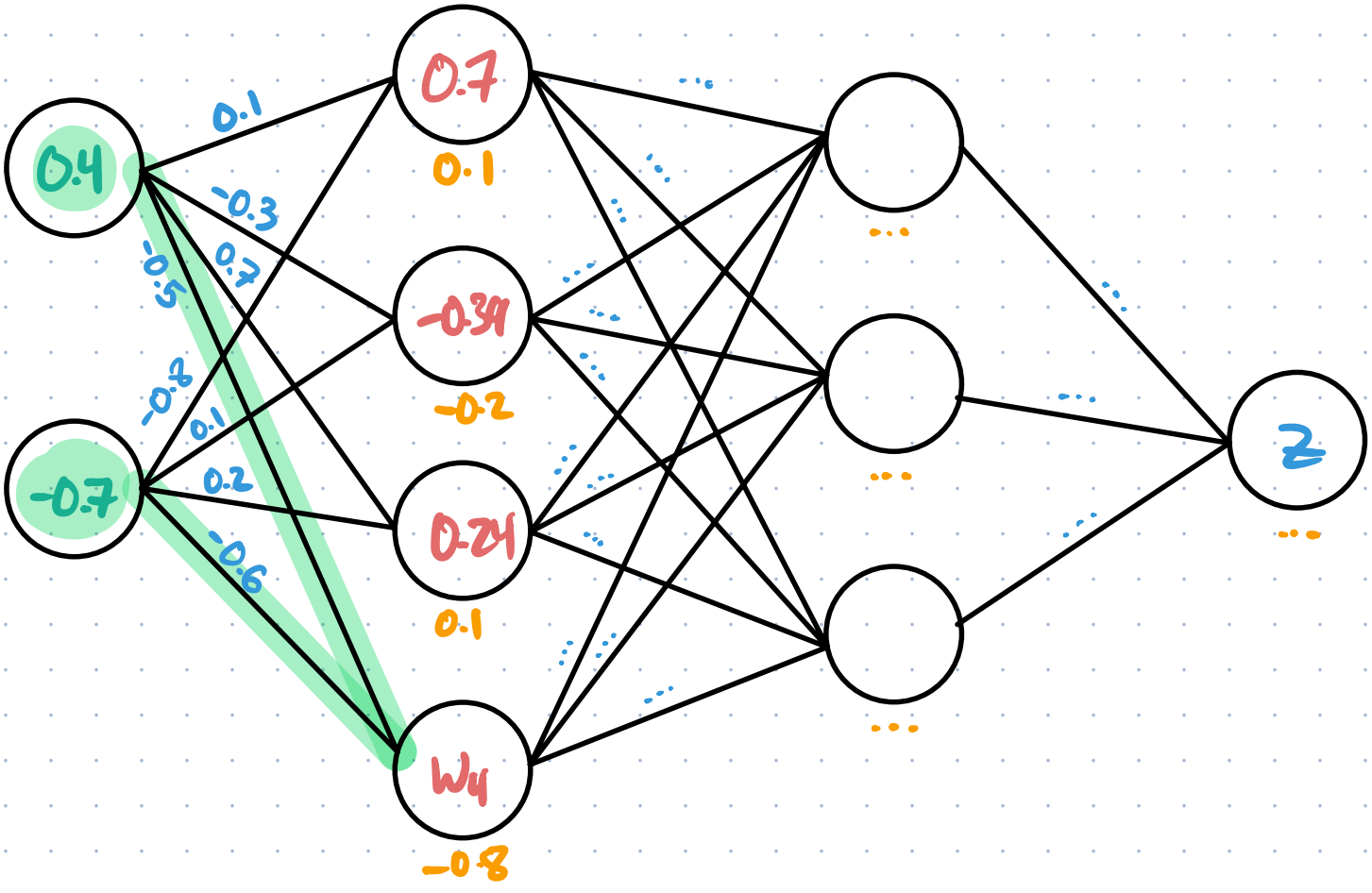
$f(u,v) = z$



$$w_3 = (0.4)(0.7) + (-0.7)(0.2) + 0.1$$
$$= 0.24$$

Example: A NN that takes 2 inputs and has 1 output

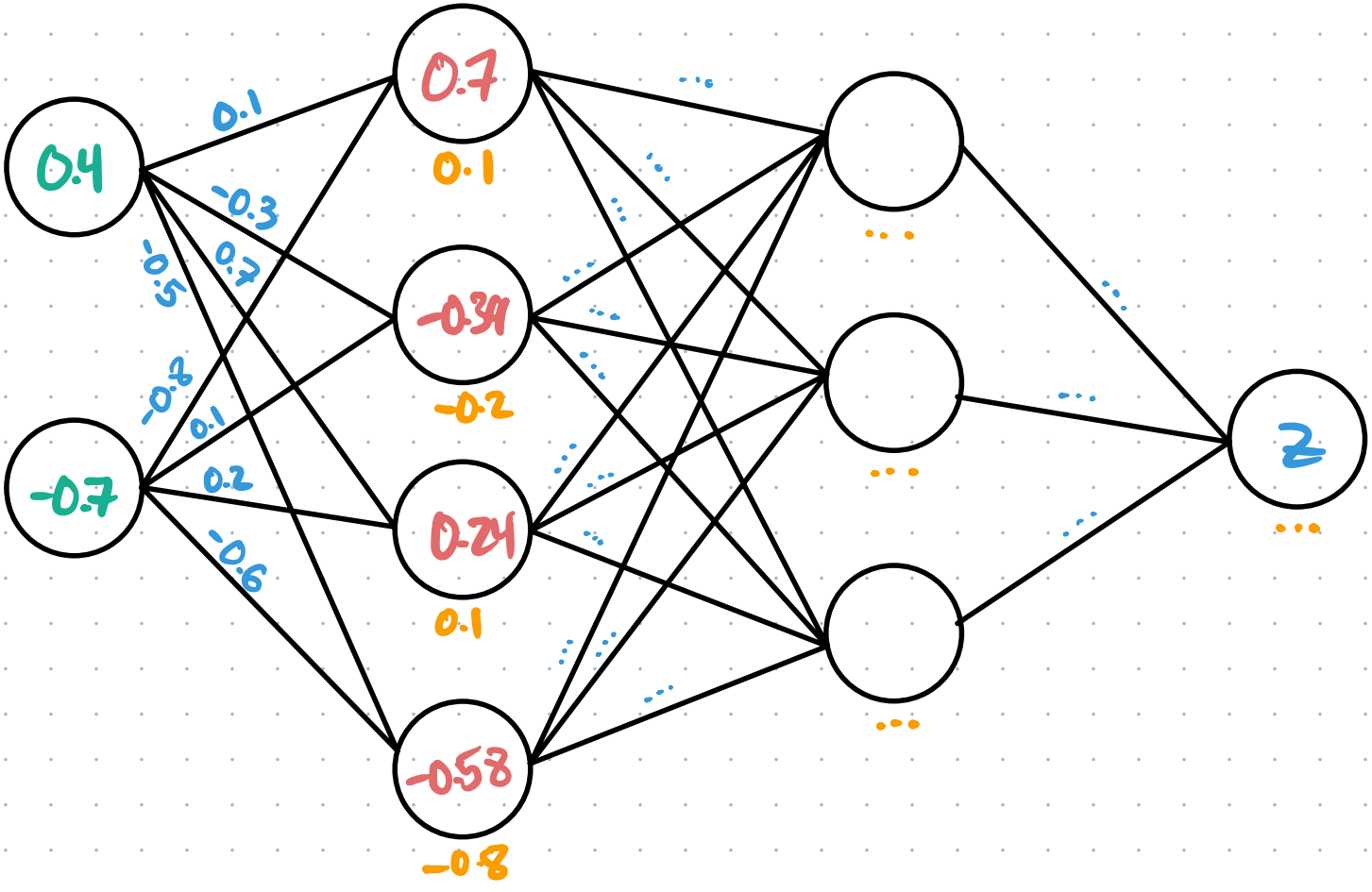
$f(u,v) = z$



$w_4 = (0.4)(-0.5) + (-0.7)(-0.6) + -0.8$

$= -0.58$

Example: A NN that takes 2 inputs and has 1 output
$f(u,v) = z$



Then, the neurons from the first hidden layer feed forward to the next hidden layer.

Example: A NN that takes 2 inputs and has 1 output

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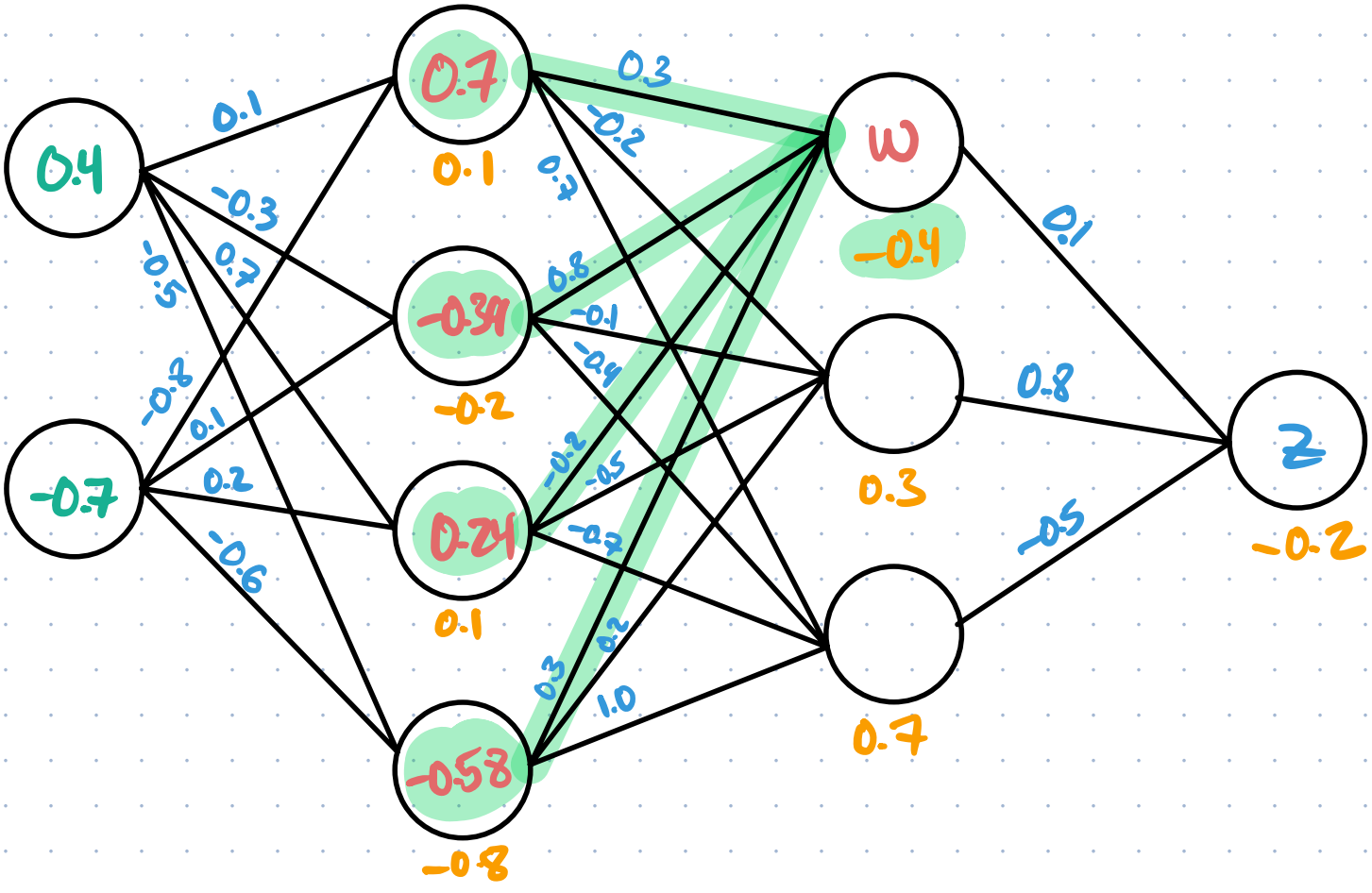
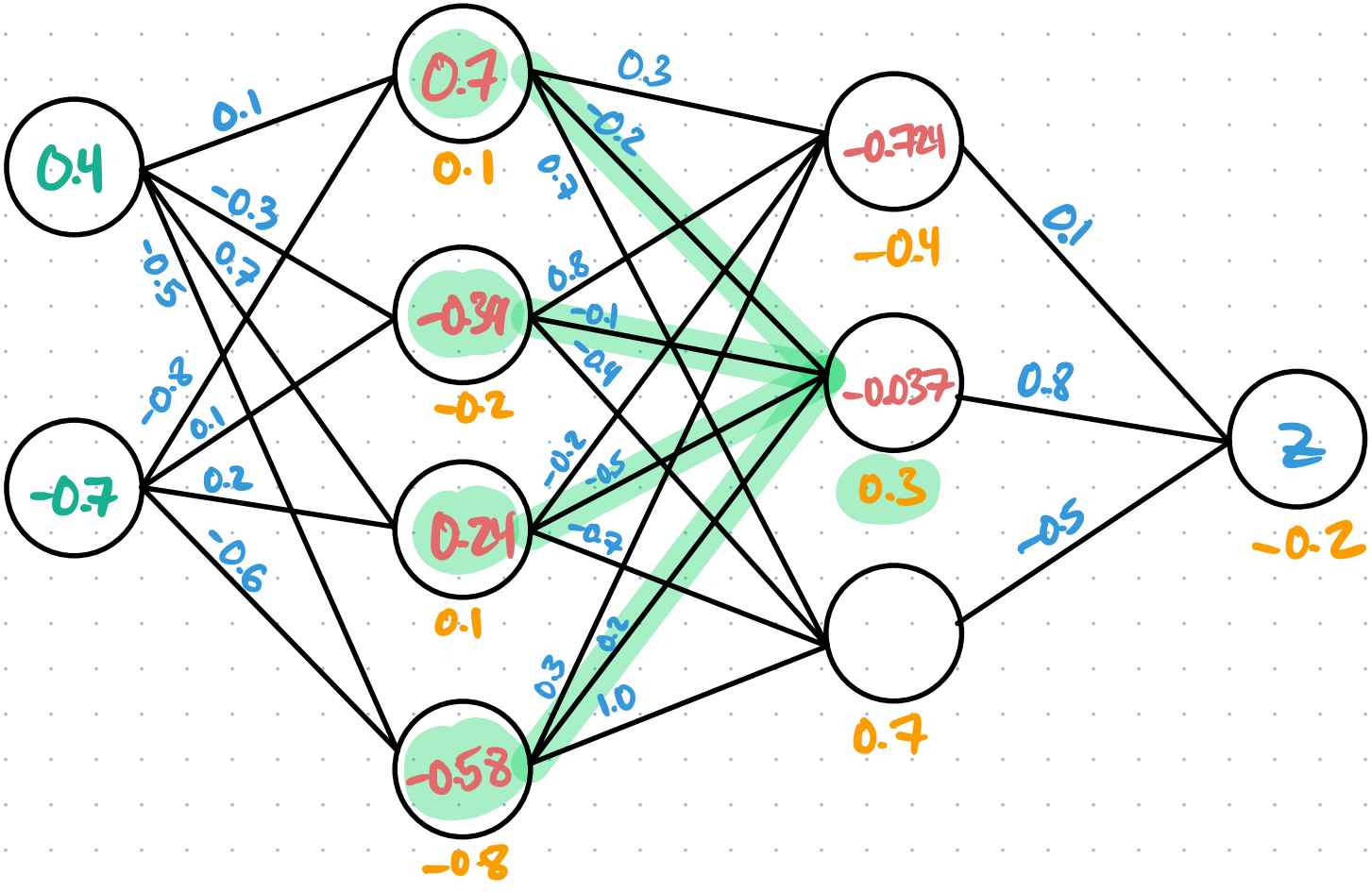


$w = (0.7)(0.3) + (-0.39)(0.8) + (0.24)(-0.2) + (-0.58)(0.3) + -0.4$

≈ -0.724

Example: A NN that takes 2 inputs and has 1 output

$f(u,v) = z$



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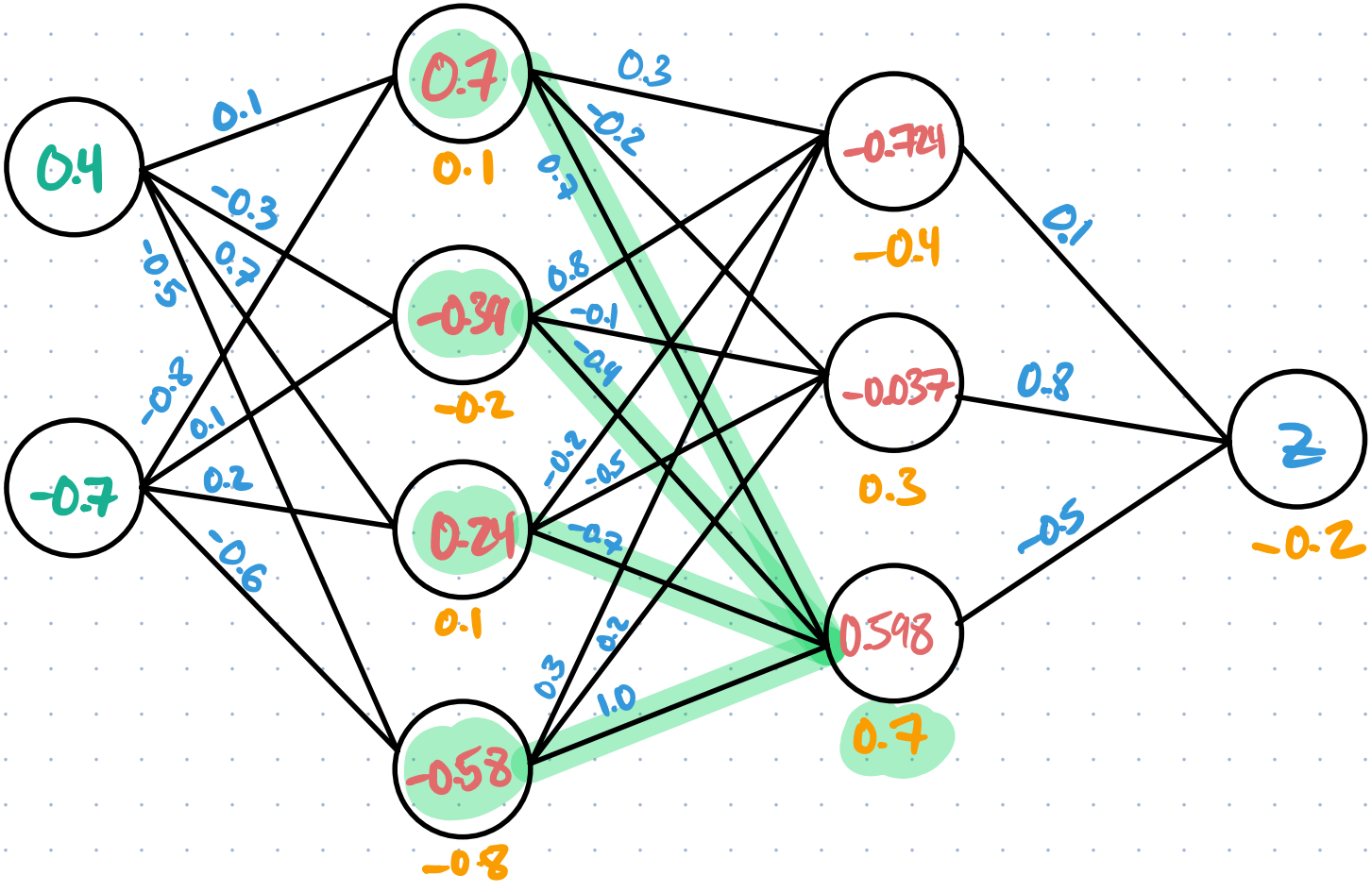

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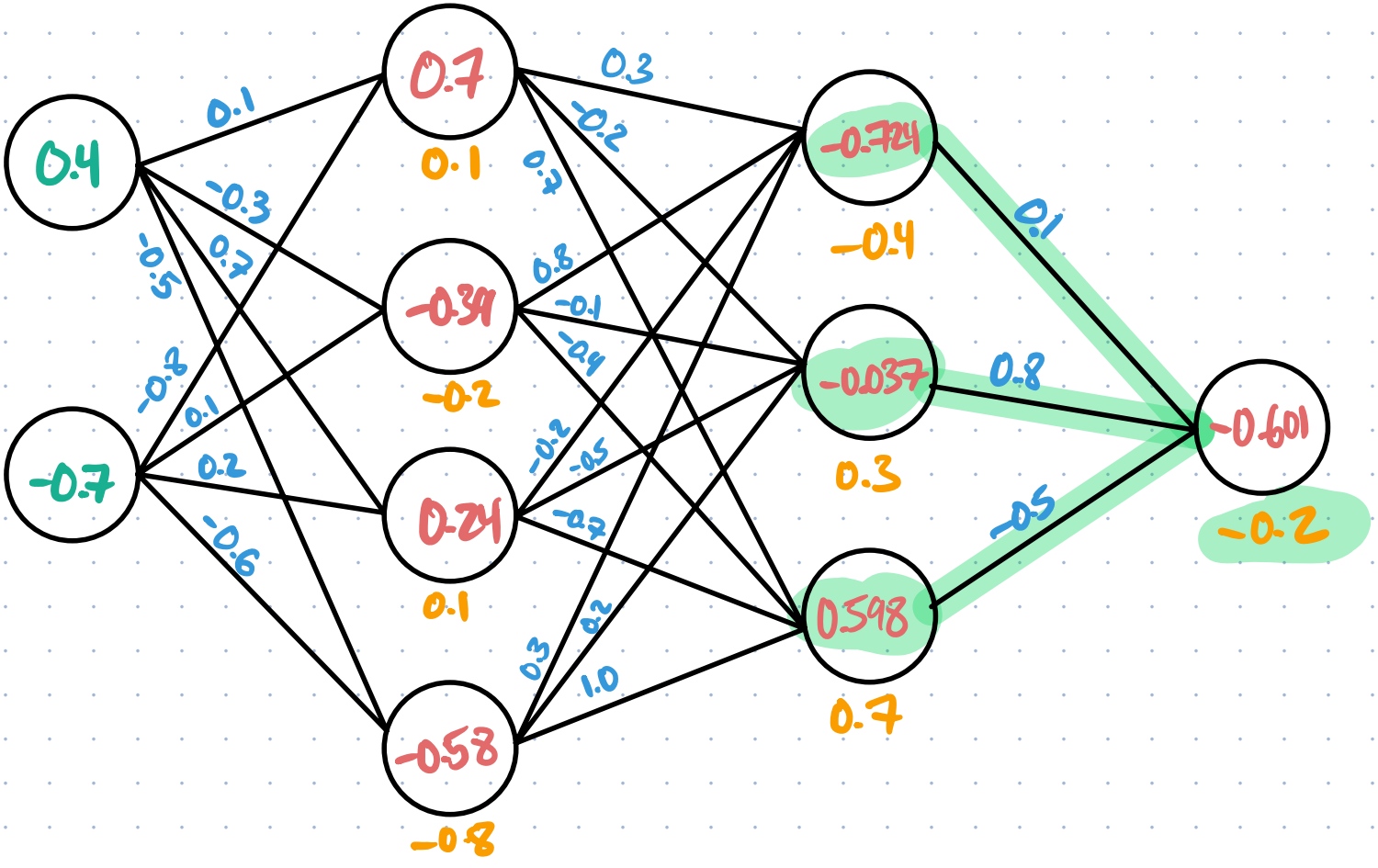

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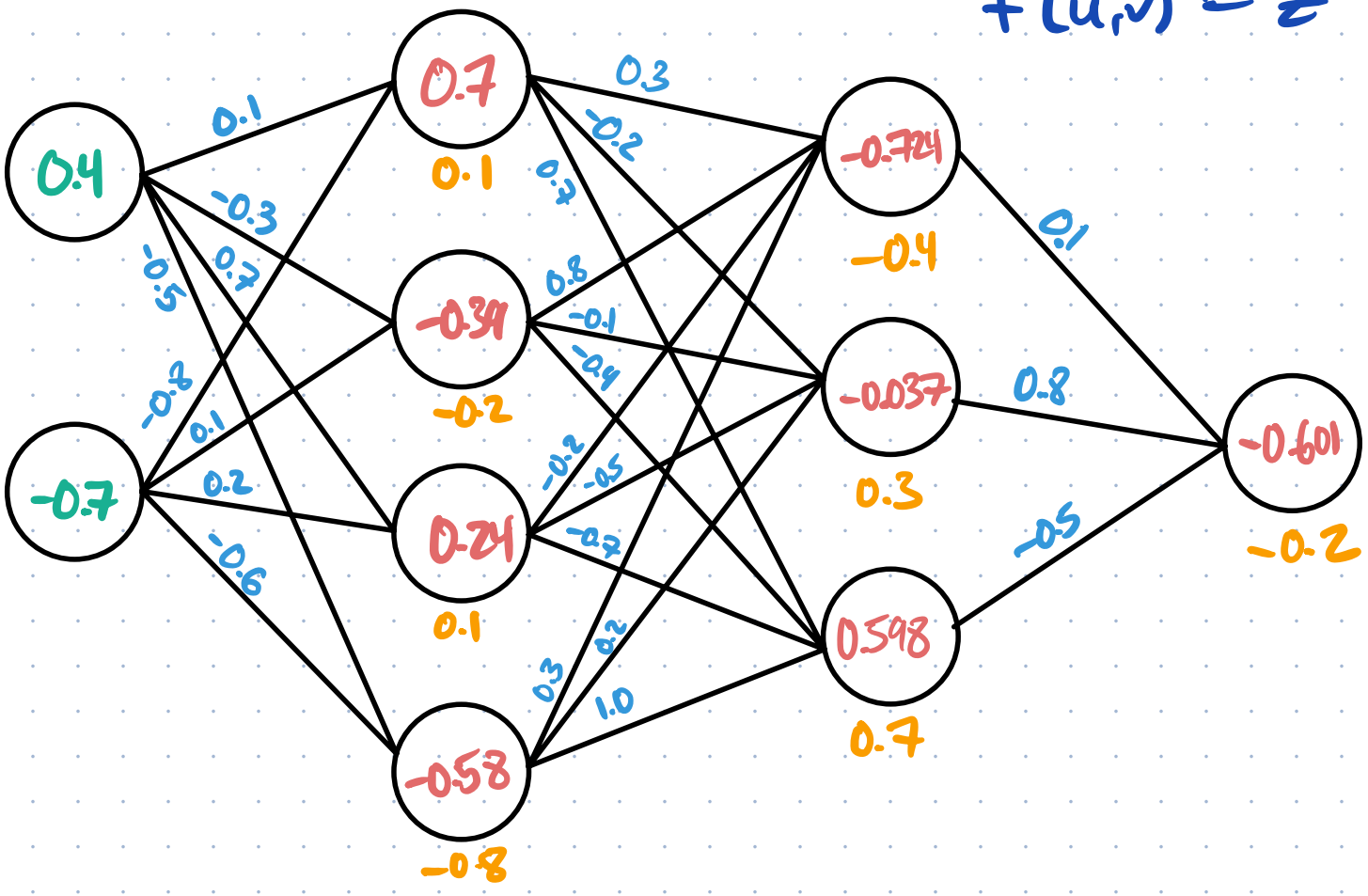


So, for this particular neural network, with these weights and biases, the inputs $(0.4, -0.7)$ produce output -0.601

$$f(0.4, -0.7) = -0.601$$

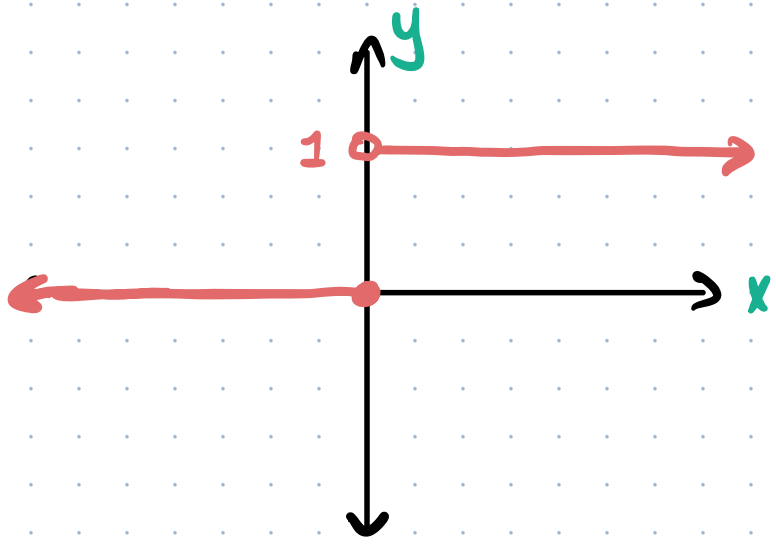
Activation Functions

In order to make NNs capable of representing non-linear functions, we pass the output of each neuron through an "activation function" before passing it on to the next layer.

The activation functions themselves are non-linear.

AF #1: Step Function (old school, not used often anymore)

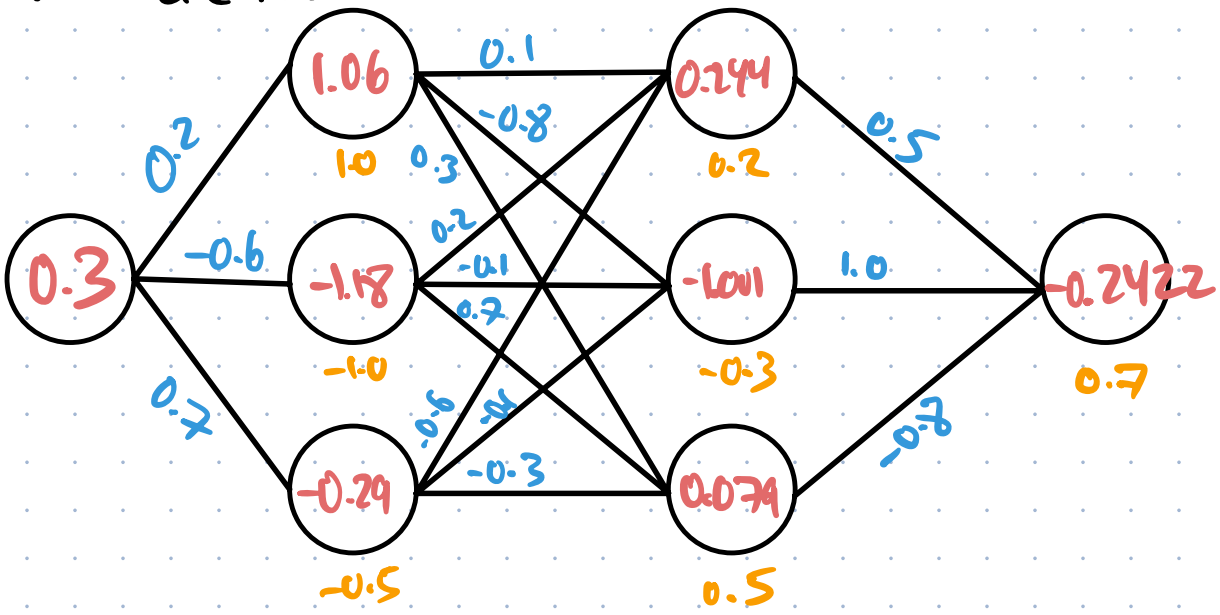
$$f(x) = \begin{cases} 1, & \text{if } x > 0 \\ 0, & \text{if } x \leq 0 \end{cases}$$

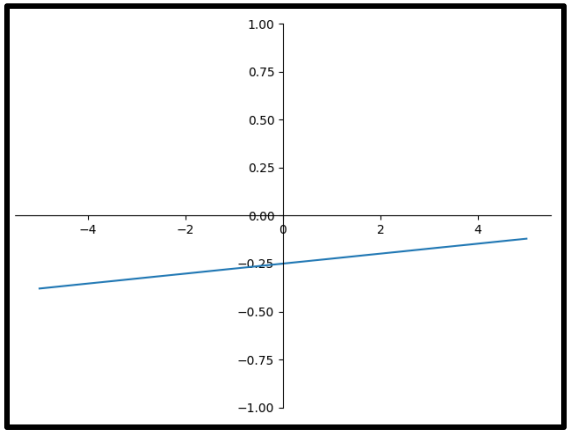


With this AF each neuron only outputs 0 or 1, not any decimal.

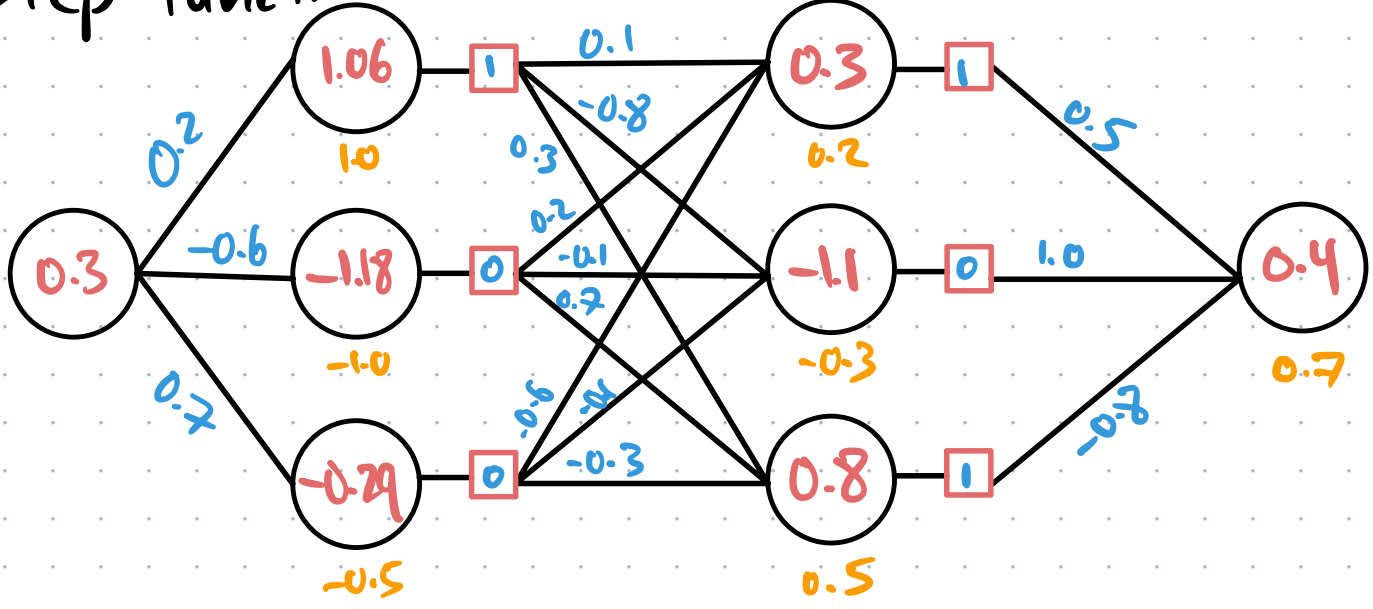
(off → 0, on → 1)

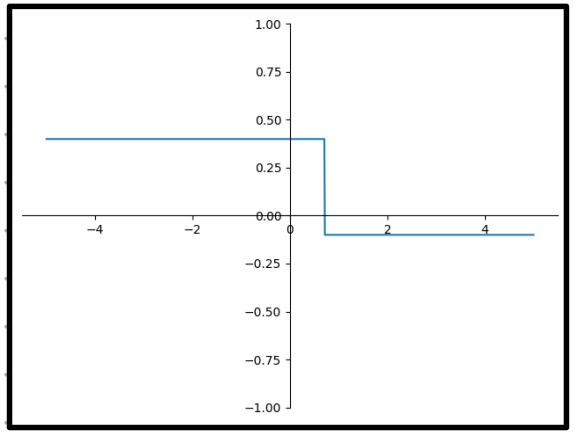
no activation:





step function:



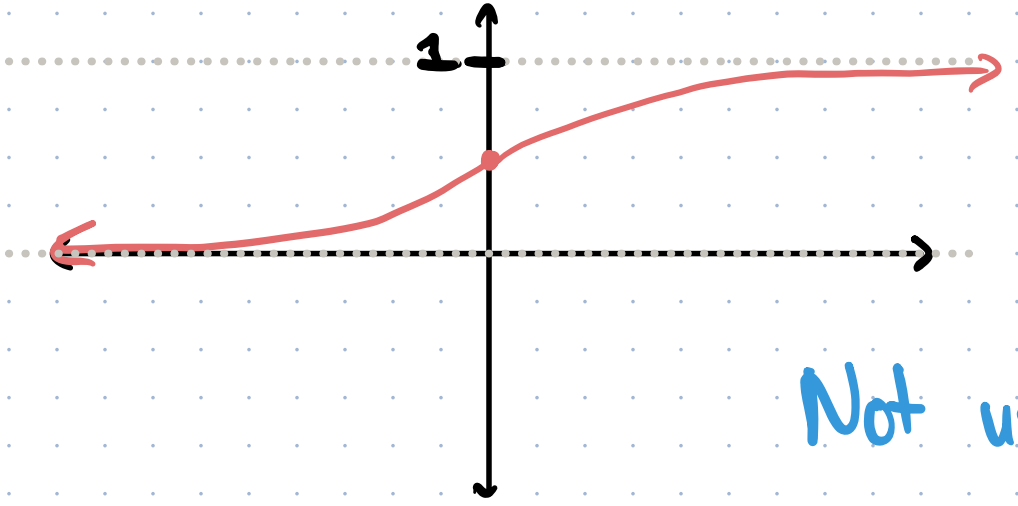


AF #2 : Sigmoid

A problem with the step function ⎍ is that it throws away a lot of information.

$f(0.001) = f(100) = 1$

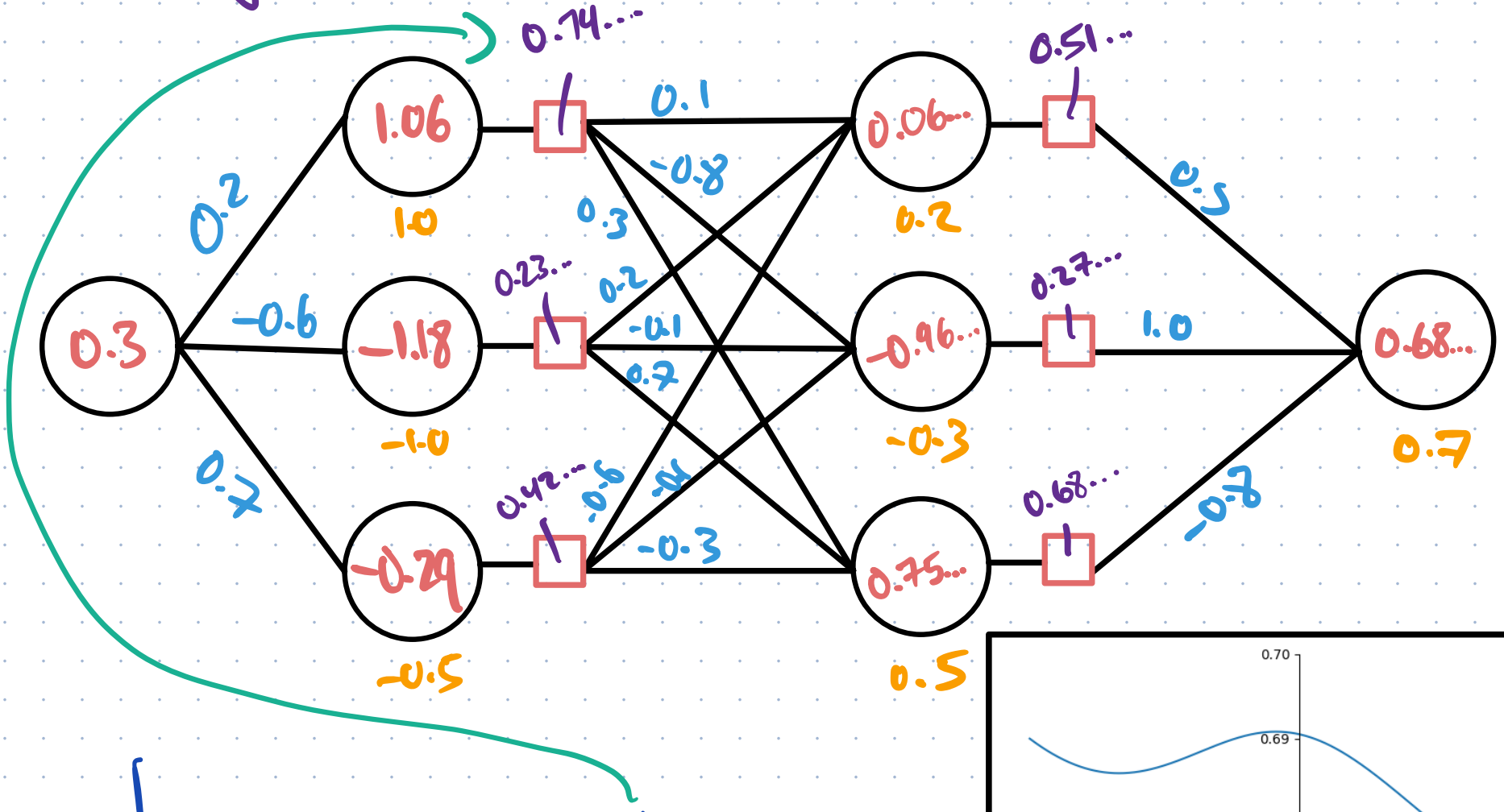
Sigmoid: $f(x) = \frac{1}{1+e^{-x}}$



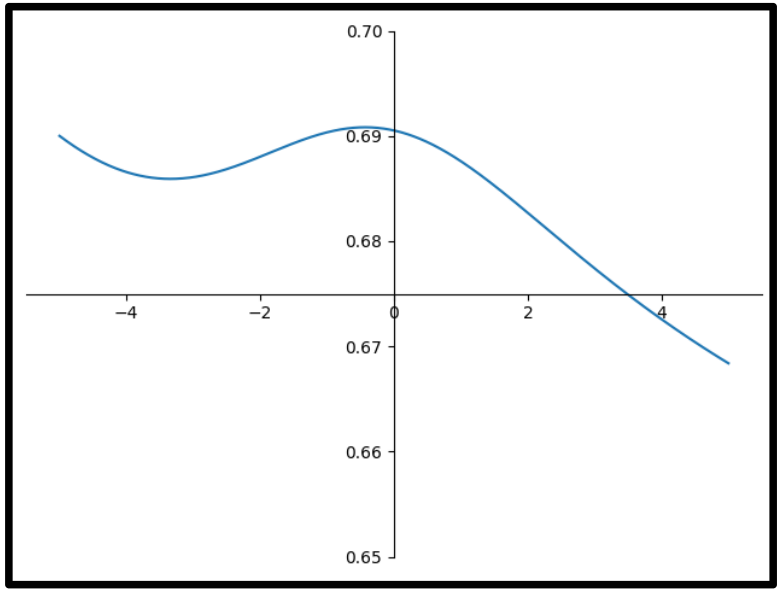
More gentle, and not as lossy.

Not used much anymore

With sigmoid activation

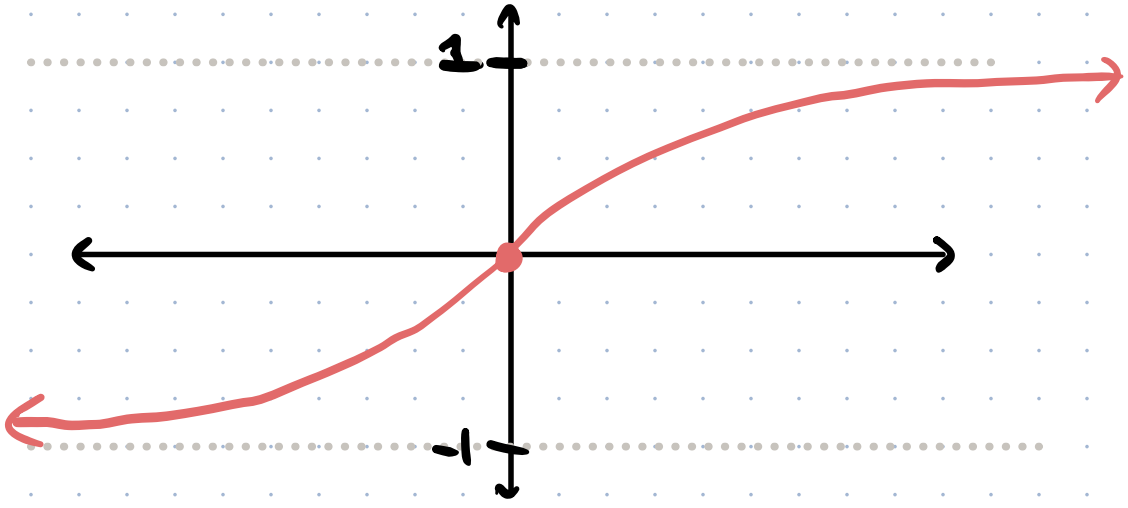


$$\frac{1}{1+e^{-1.06}} \simeq 0.74$$



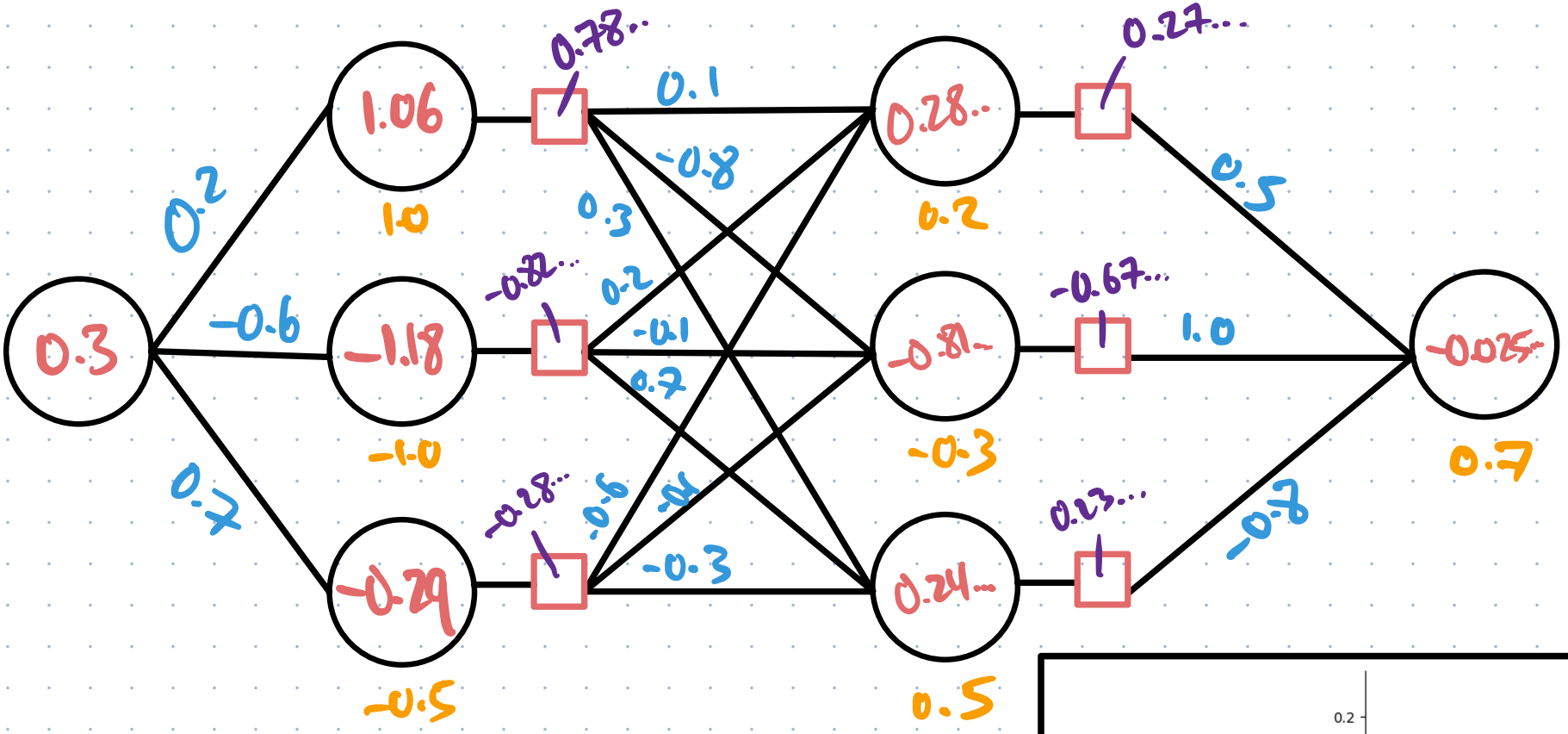
AF #3: Hyperbolic Tangent (tanh)

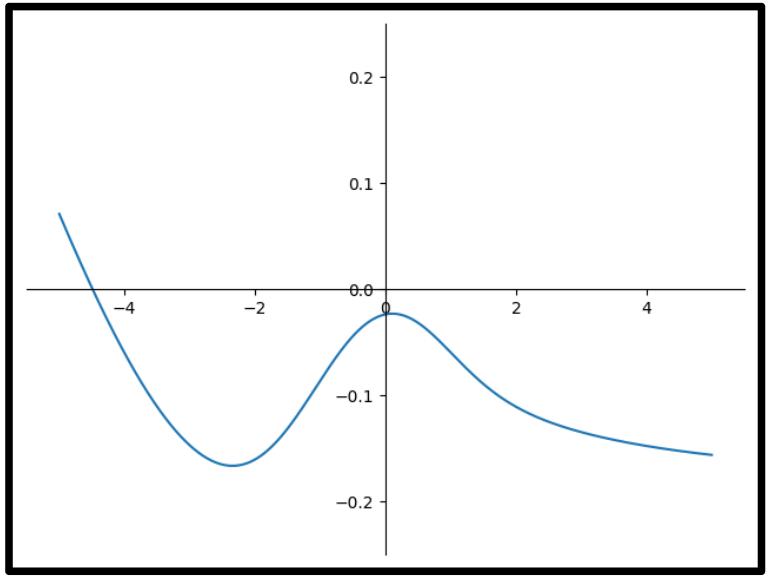
$$f(x) = \frac{e^x - e^{-x}}{e^x + e^{-x}}$$



a bit like sigmoid, but can be negative

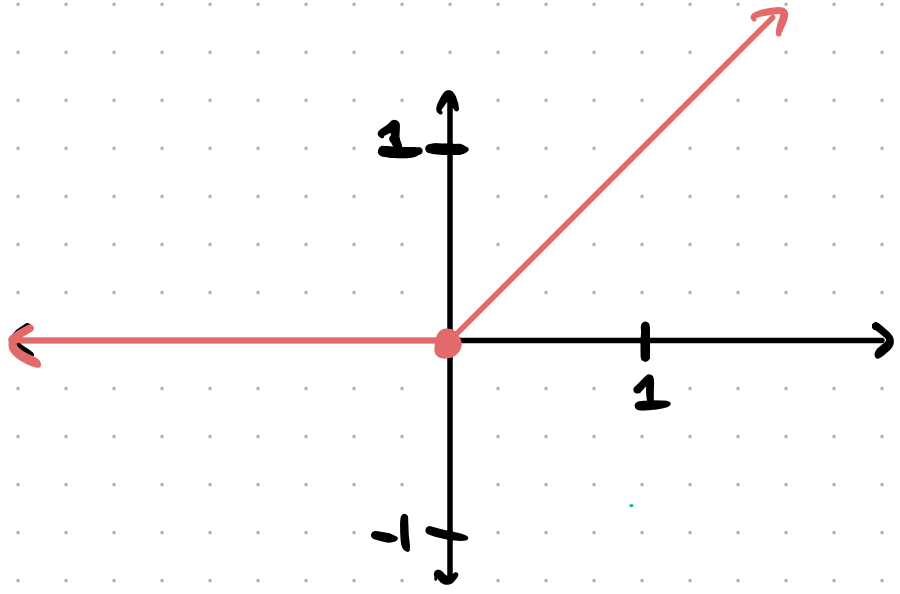
With tanh activation





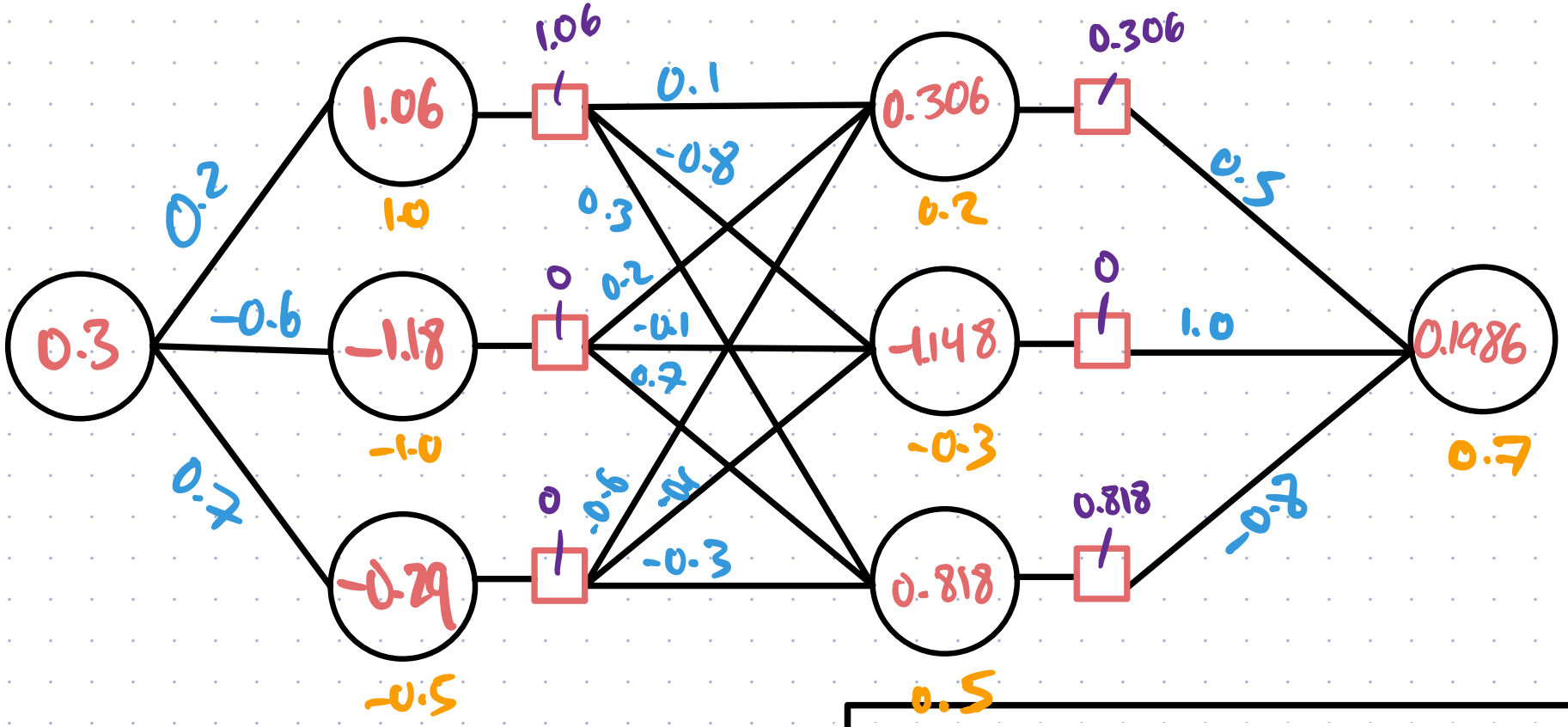
AF #4: Rectified Linear Unit (ReLU)

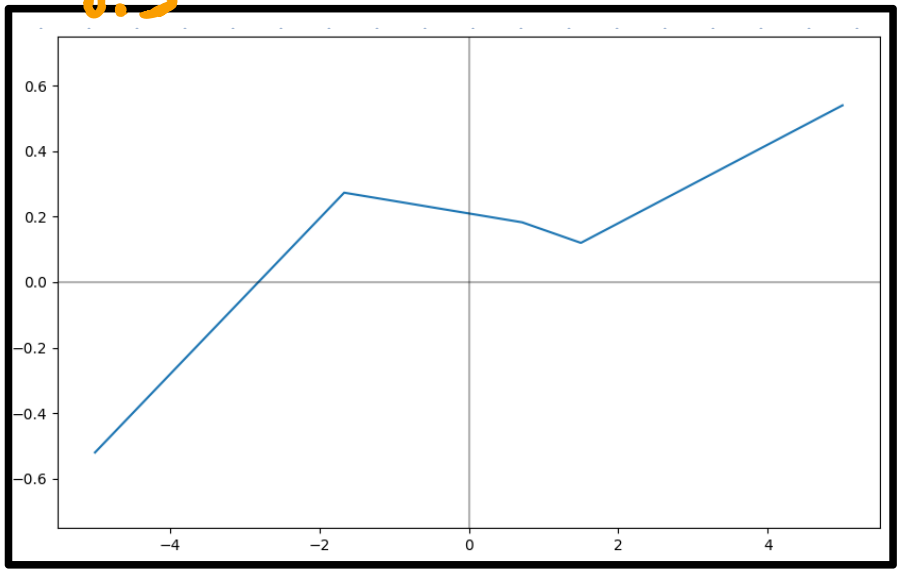
$$f(x) = \begin{cases} x, & \text{if } x \geq 0 \\ 0, & \text{if } x < 0 \end{cases}$$

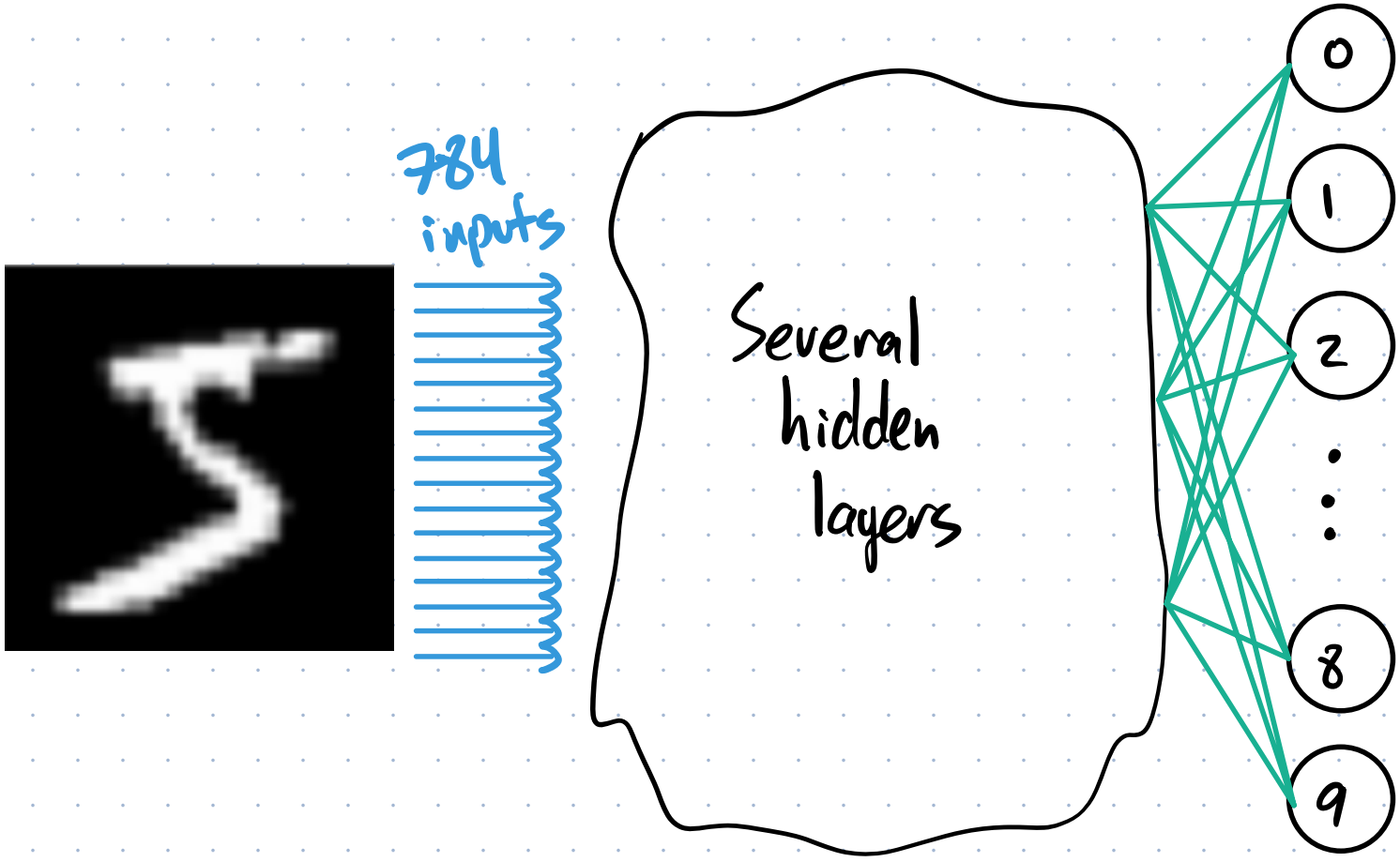


Neuron is "on" if ≥ 0, and keeps its value, and "off" if < 0, and returns no value

With ReLU activation







output neuron i represents how confident we are that the input digit is i.

This is a classification problem. We are deciding which category the input belongs to. More on this later.

Linear Algebra

* You may have noticed that the operations done during the forward pass feel like dot products and matrix multiplications.

* This is why GPUs work so well with NNs.

* Let's explore.

Useful to us: we'll use a python package called "numpy"

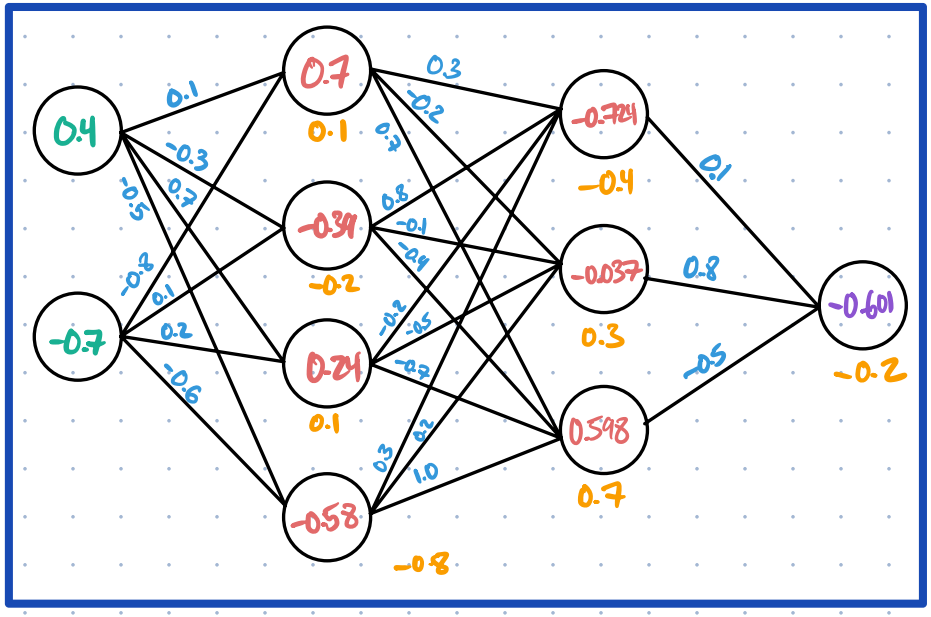
Think of each layer as a vector of values.

$$\begin{bmatrix} 0.4 \\ -0.7 \end{bmatrix} \quad \begin{bmatrix} 0.7 \\ -0.39 \\ 0.24 \\ -0.58 \end{bmatrix} \quad \begin{bmatrix} -0.724 \\ -0.037 \\ 0.598 \end{bmatrix} \quad \begin{bmatrix} -0.601 \end{bmatrix}$$

How is each layer computed from the previous one?
Make matrices for the weights between each layer and vectors for the biases.

$$M_1 = \begin{bmatrix} 0.1 & -0.8 \\ -0.3 & 0.1 \\ 0.7 & 0.2 \\ -0.5 & -0.6 \end{bmatrix} \qquad b_1 = \begin{bmatrix} 0.1 \\ -0.2 \\ 0.1 \\ -0.8 \end{bmatrix}$$

$$\begin{bmatrix} 0.1 & -0.3 & \cdots \\ -0.8 & 0.1 & \end{bmatrix}$$

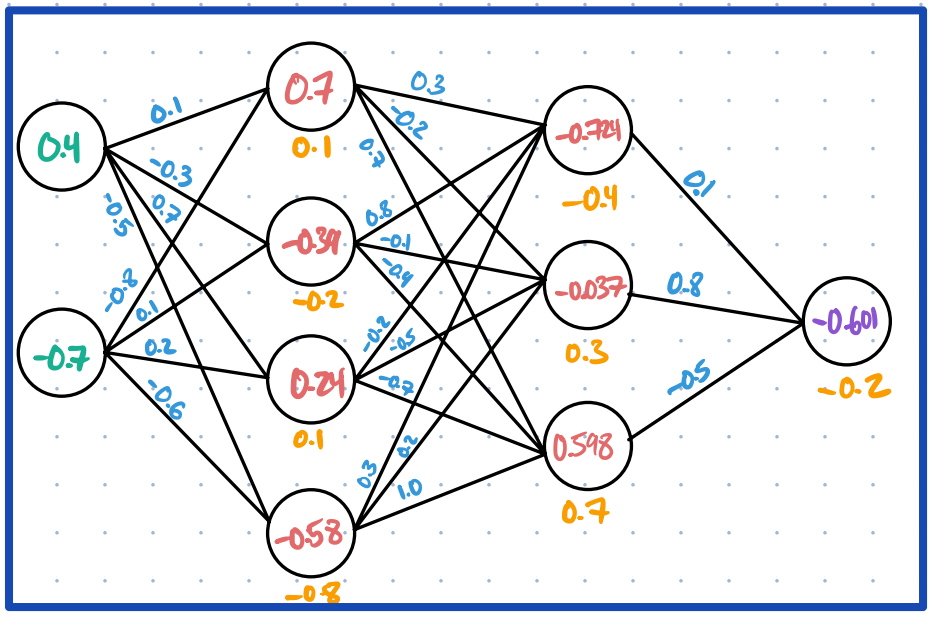


Rearrange!

(ignoring activation functions!)

$$\begin{bmatrix} 0.1 & -0.8 \\ -0.3 & 0.1 \\ 0.7 & 0.2 \\ -0.5 & -0.6 \end{bmatrix} \begin{bmatrix} 0.4 \\ -0.7 \end{bmatrix} + \begin{bmatrix} 0.1 \\ -0.2 \\ 0.1 \\ -0.8 \end{bmatrix} = \begin{bmatrix} 0.7 \\ -0.39 \\ 0.24 \\ -0.58 \end{bmatrix}$$

$$= \begin{bmatrix} 0.6 \\ - \\ - \\ \end{bmatrix} + \begin{bmatrix} 0.1 \\ -0.2 \\ 0.1 \\ -0.8 \end{bmatrix} = \checkmark \begin{bmatrix} 0.7 \\ \vdots \\ \end{bmatrix}$$



$$\begin{bmatrix} 0.1 & -0.8 \\ -0.3 & 0.1 \\ 0.7 & 0.2 \\ -0.5 & -0.6 \end{bmatrix} \begin{bmatrix} 0.4 \\ -0.7 \end{bmatrix} + \begin{bmatrix} 0.1 \\ -0.2 \\ 0.1 \\ -0.8 \end{bmatrix} = \begin{bmatrix} 0.7 \\ -0.39 \\ 0.24 \\ -0.58 \end{bmatrix}$$

(ignoring activation functions!)

$$(0.1)(0.4) + (-0.8)(-0.7) + (0.1)$$

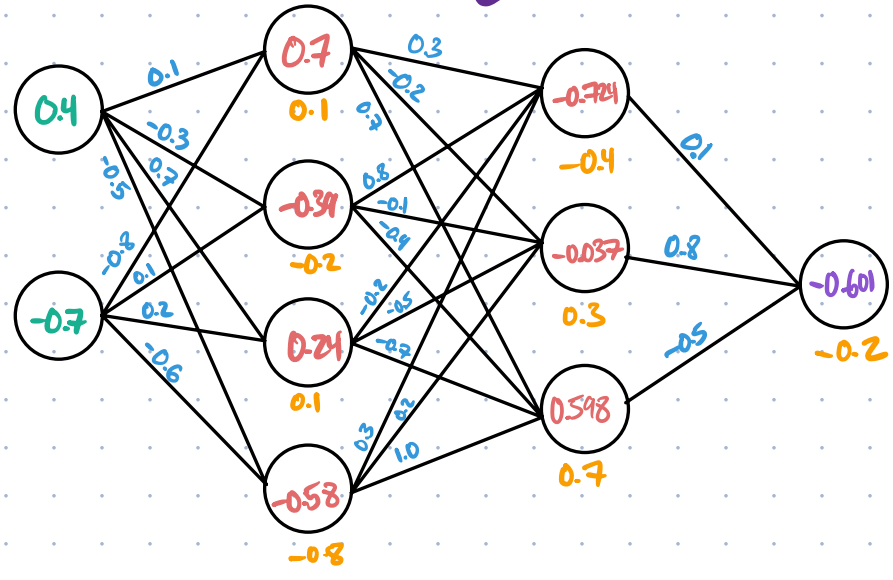
$$= 0.04 + 0.56 + 0.1$$

$$= 0.6$$

$$\begin{bmatrix} 0.3 & 0.8 & -0.2 & 0.3 \\ -0.2 & -0.1 & -0.5 & 0.2 \\ 0.7 & -0.4 & -0.7 & 1.0 \end{bmatrix} \begin{bmatrix} 0.7 \\ -0.39 \\ 0.24 \\ -0.58 \end{bmatrix} + \begin{bmatrix} -0.4 \\ 0.3 \\ 0.7 \end{bmatrix} = \begin{bmatrix} -0.724 \\ -0.037 \\ 0.598 \end{bmatrix}$$

$$\begin{bmatrix} 0.1 & 0.8 & -0.5 \end{bmatrix} \begin{bmatrix} -0.724 \\ -0.037 \\ 0.598 \end{bmatrix} + [-0.2]$$

$$= [-0.601]$$



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$$Wx_1 + b = x_2$$

What about activation function?

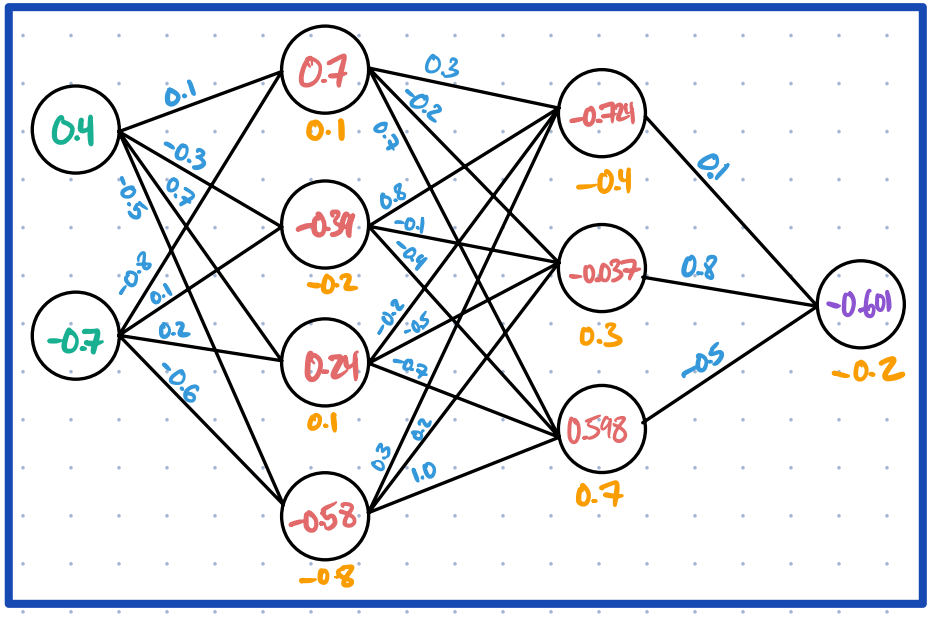
$$x_1^T W^T + b^T = x_2^T$$

Suppose our activation function is σ.

We'll use the notation

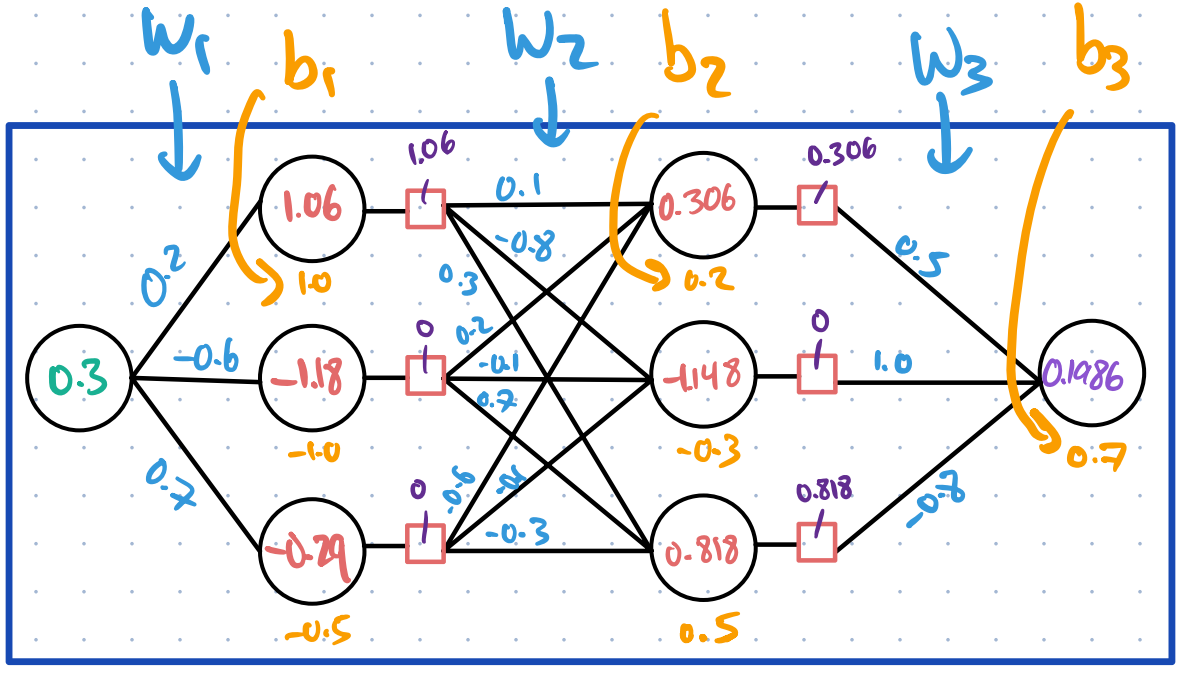
$$\sigma\left(\begin{bmatrix} v_1 \\ v_2 \\ \vdots \\ v_k \end{bmatrix}\right) = \begin{bmatrix} \sigma(v_1) \\ \sigma(v_2) \\ \vdots \\ \sigma(v_k) \end{bmatrix}.$$

$$\sigma(Wx_1 + b) = x_2$$



So this neural network, with activation function σ for each layer, is the function:

$$f(x) = \sigma(W_3\sigma(W_2\sigma(W_1[x] + b_1) + b_2) + b_3)$$



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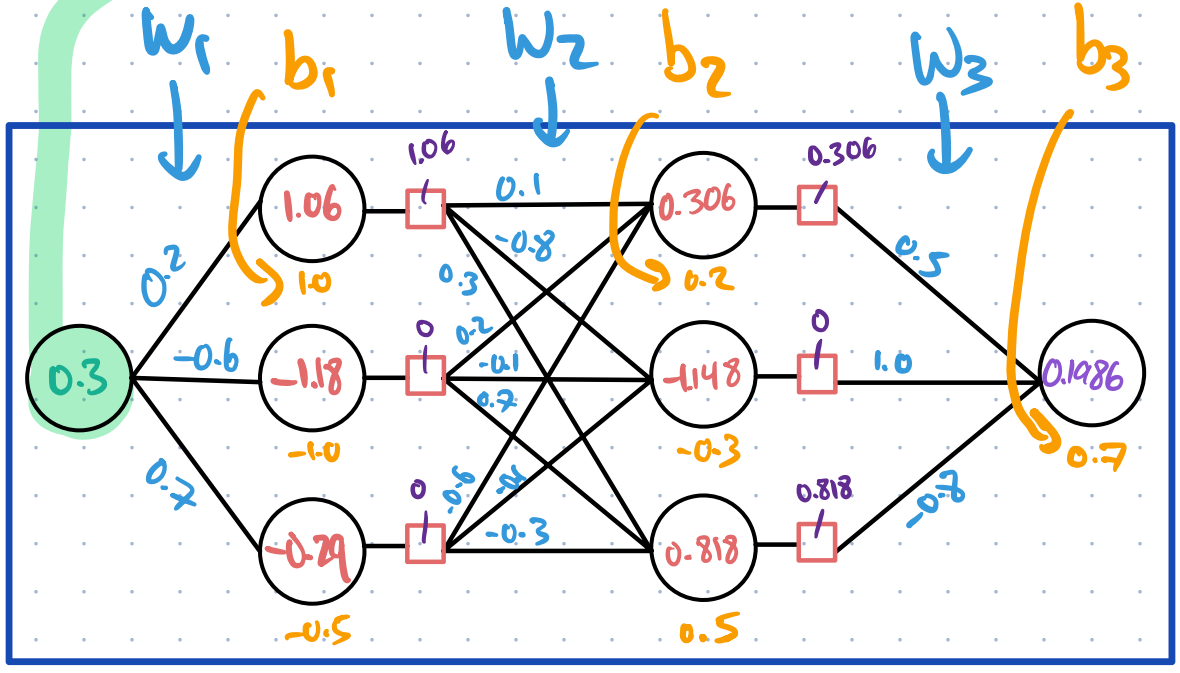

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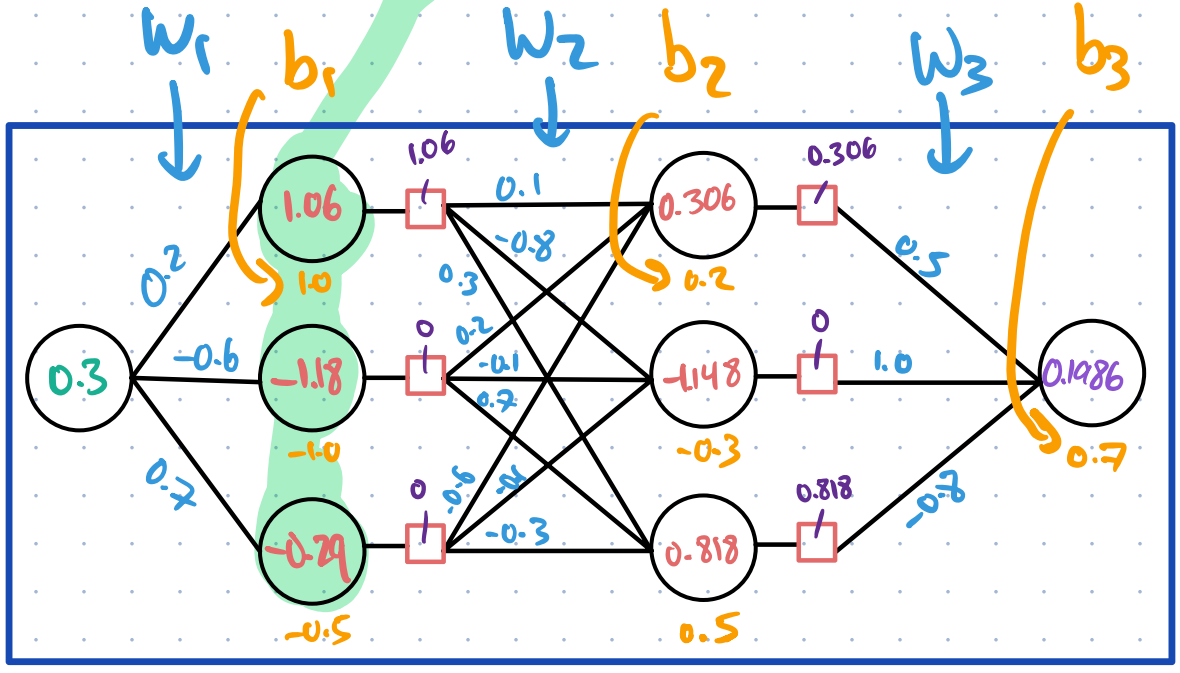

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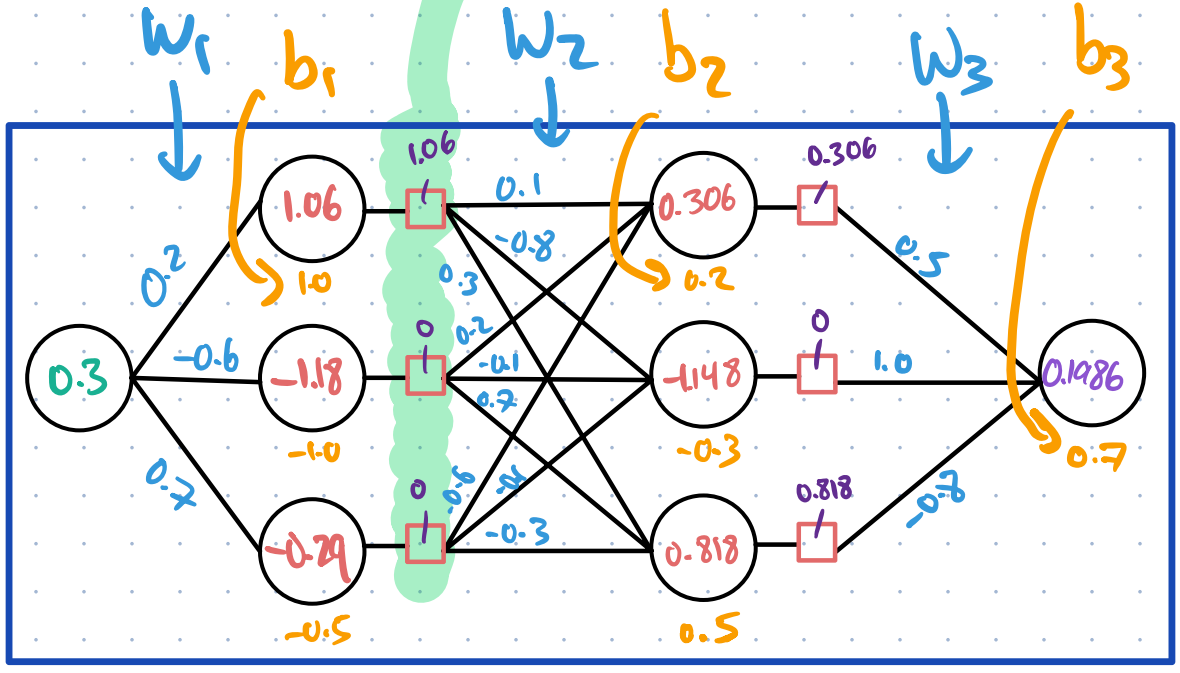

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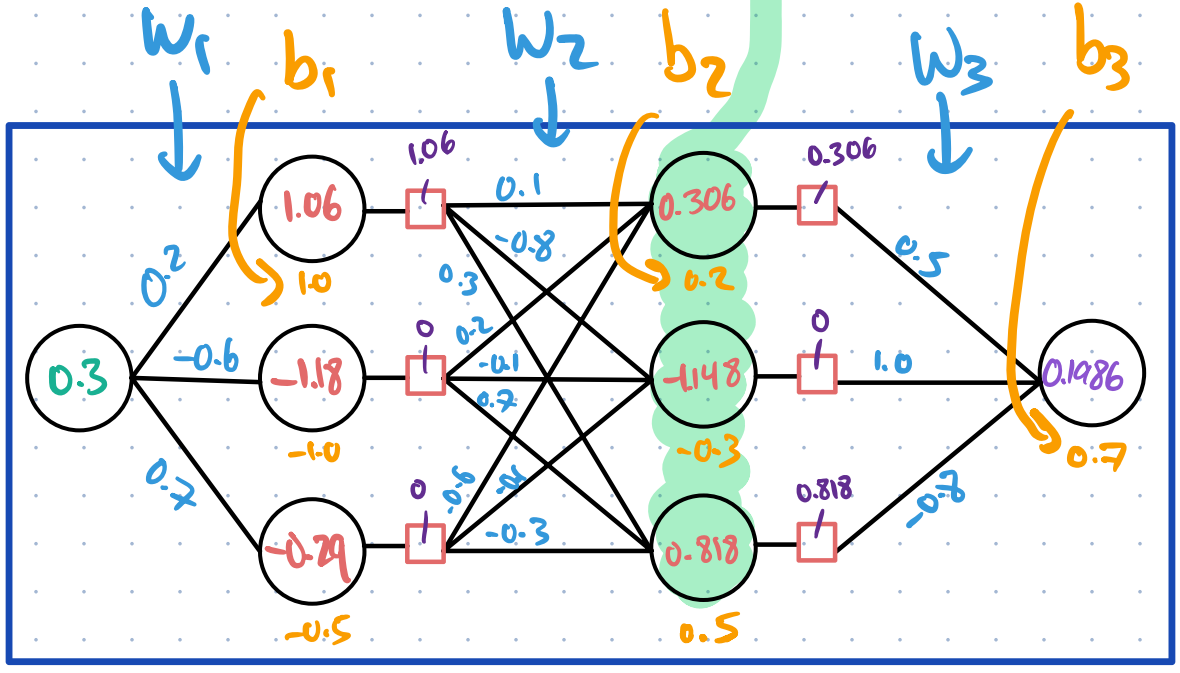

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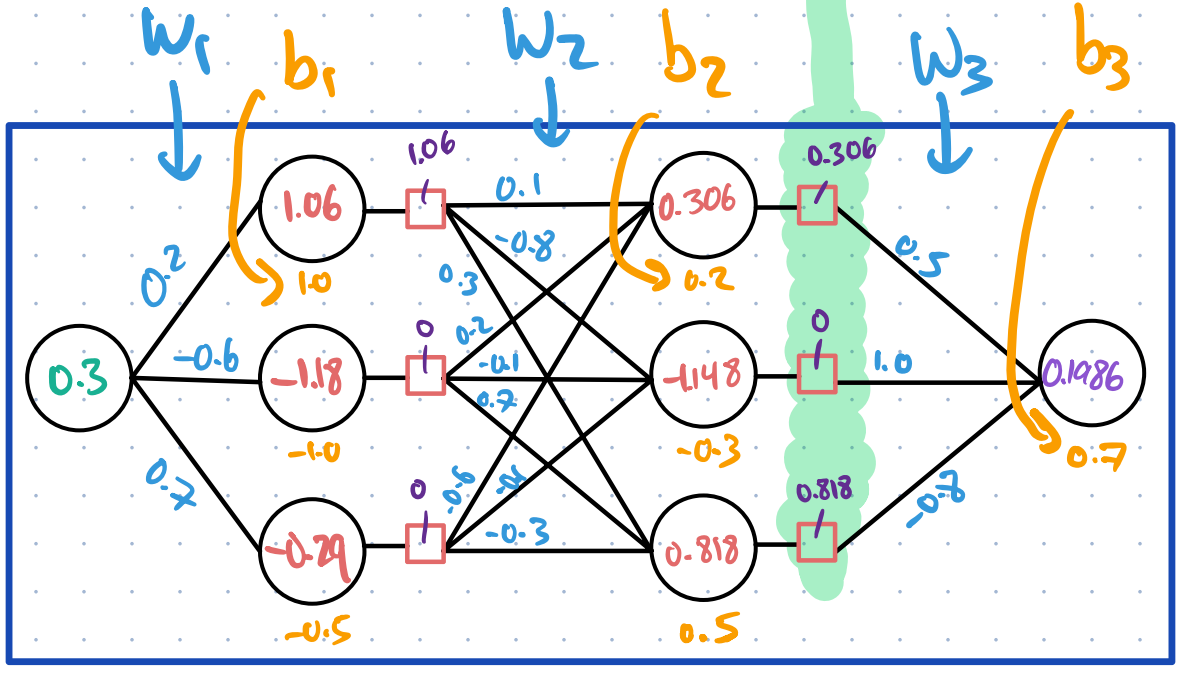

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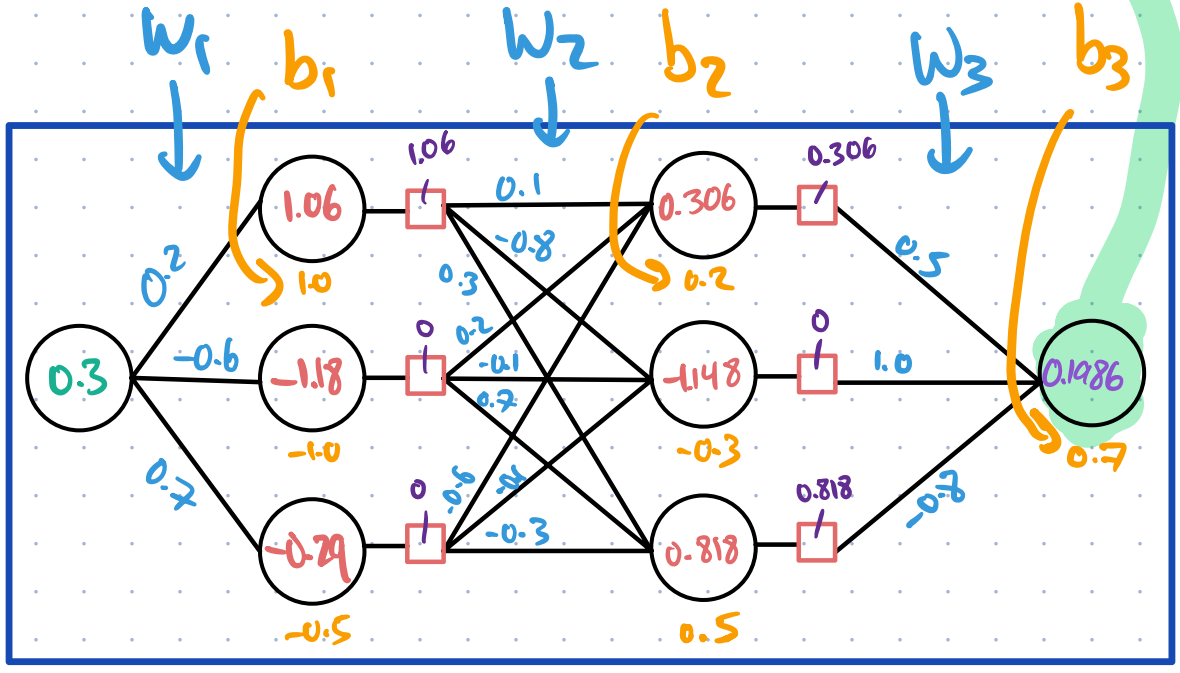

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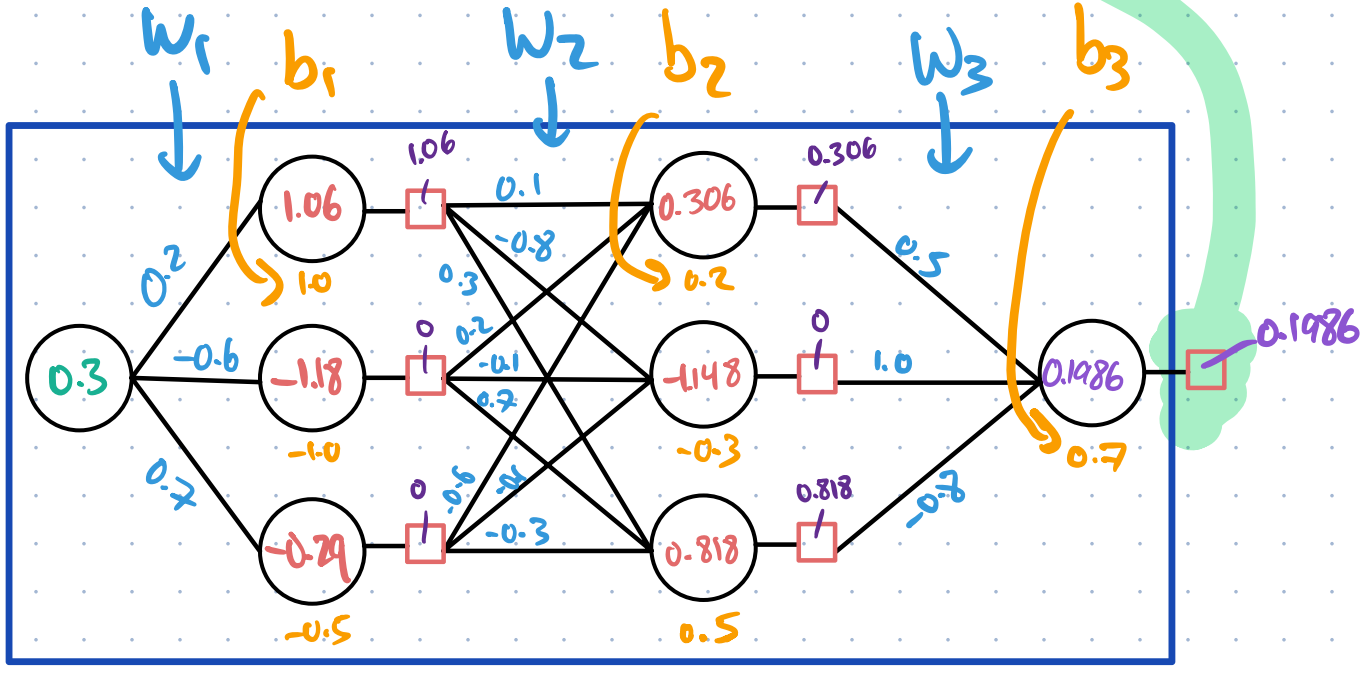


* Sometimes the output layer has a different activation function, or no AF.

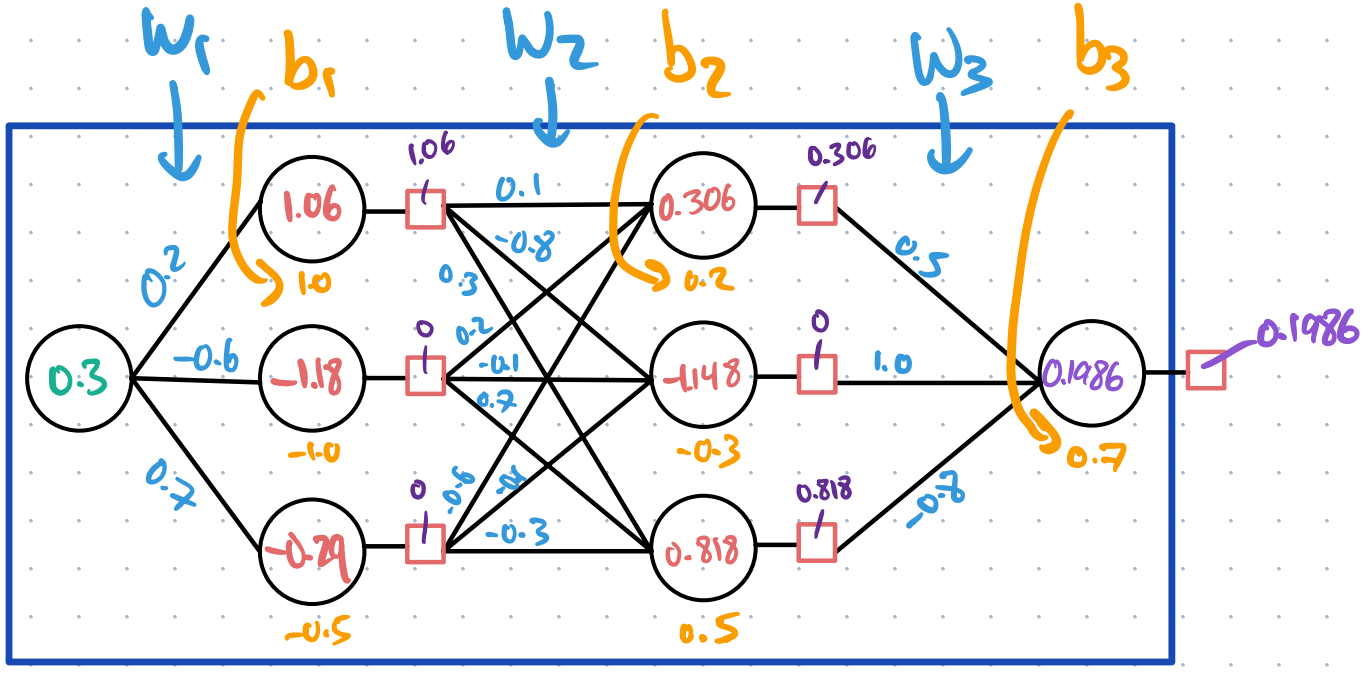
$$W_1 = \begin{bmatrix} 0.2 \\ -0.6 \\ 0.7 \end{bmatrix} \quad W_2 = \begin{bmatrix} 0.1 & -0.8 & 0.3 \\ 0.2 & -0.1 & 0.7 \\ -0.6 & -0.1 & -0.3 \end{bmatrix} \quad W_3 = \begin{bmatrix} 0.5 & 1.0 & -0.8 \end{bmatrix}$$

each row of a W is the weights coming out of one neuron

$$b_1 = \begin{bmatrix} 1.0 \\ -1.0 \\ -0.5 \end{bmatrix}, \quad b_2 = \begin{bmatrix} 0.2 \\ -0.3 \\ 0.5 \end{bmatrix}, \quad b_3 = \begin{bmatrix} 0.7 \end{bmatrix}$$

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

ReLU



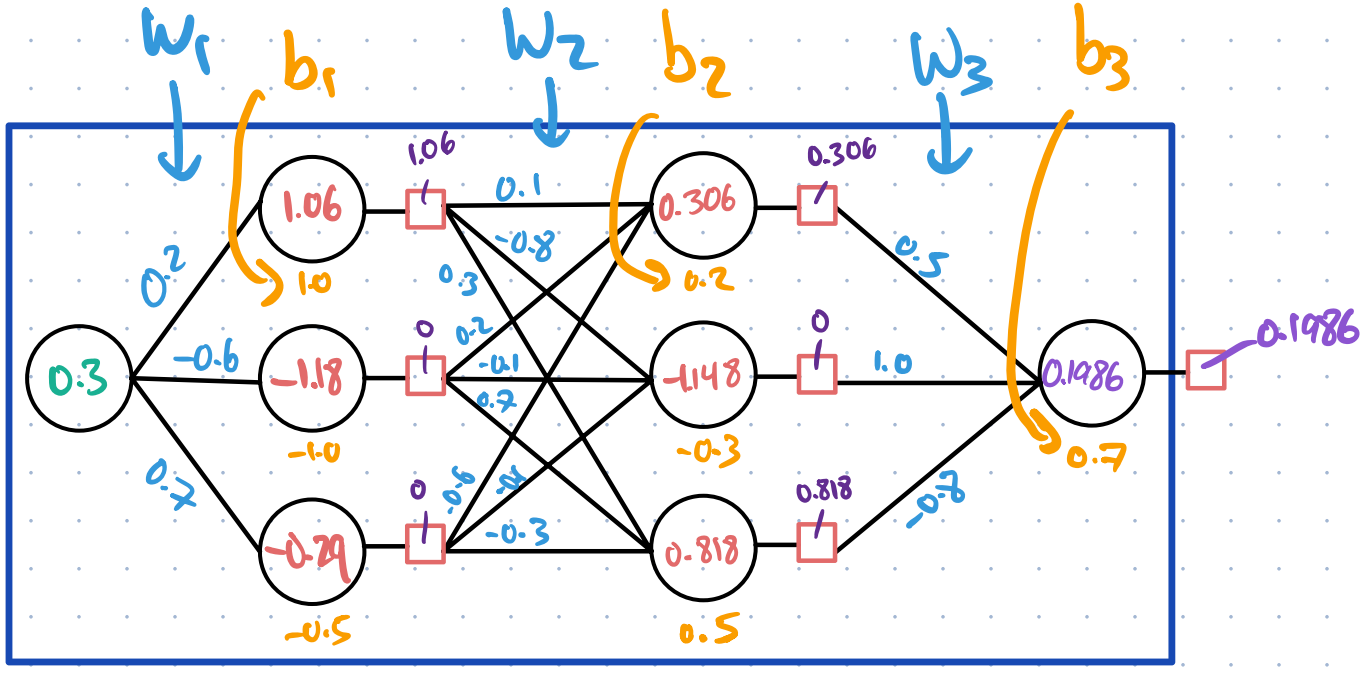
$$W_1 = \begin{bmatrix} 0.2 \\ -0.6 \\ 0.7 \end{bmatrix} \quad W_2 = \begin{bmatrix} 0.1 & -0.8 & 0.3 \\ 0.2 & -0.1 & 0.7 \\ -0.6 & -0.1 & -0.3 \end{bmatrix} \quad W_3 = \begin{bmatrix} 0.5 & 1.0 & -0.8 \end{bmatrix}$$

$$b_1 = \begin{bmatrix} 1.0 \\ -1.0 \\ -0.5 \end{bmatrix}, \quad b_2 = \begin{bmatrix} 0.2 \\ -0.3 \\ 0.5 \end{bmatrix}, \quad b_3 = \begin{bmatrix} 0.7 \end{bmatrix}$$

each row of a W is the weights coming out of one neuron

$$f([0.3]) = \max(0, [0.5 \ 1.0 \ -0.8] \max(0, \begin{bmatrix} 0.1 & -0.8 & 0.3 \\ 0.2 & -0.1 & 0.7 \\ -0.6 & -0.1 & -0.3 \end{bmatrix} \max(0, \begin{bmatrix} 0.2 \\ -0.6 \\ 0.7 \end{bmatrix} [0.3] + \begin{bmatrix} 1.0 \\ -1.0 \\ -0.5 \end{bmatrix}) + \begin{bmatrix} 0.2 \\ -0.3 \\ 0.5 \end{bmatrix}) + [0.7])$$

$$= 0.1986$$



Now you understand exactly what a neural network is:

a fancy way to define a function

But not yet:

* How to find a good one (training)
* How NNs accomplish different tasks (what good is a fancy function?)

Next topic: Coding our first NN, and batching the forward pass

Topic 14 - Implementing our first NN and Batching

* Goal: Write code to perform the forward pass of a NN, with activation functions

The purpose of writing this code is to understand the topic.

If you needed a fast NN for research, you would probably use a Python library like PyTorch