Scientific Computing

Monday, March 30

Announcements

* HW 5 assigned, due Friday, April 10, 11:59pm
* No class or office hours Friday or Monday (easter break)

Office Hours:

Mon, 9:30-10:30
Fri, 2:00-3:00

Cudahy 307

Introduction to Neural Networks

Two separate questions:

(1) What is a neural network?
What does it do?

(2) How do we produce a good one for our task?

This lecture addresses (1).

Future lectures address (2).

Sources:

* Book: "Neural Networks From Scratch in Python"

  Slow and methodical, very low level

* Book: "The Welch Labs Illustrated Guide to AI"

  Less low level, but still lots of detail, very beautiful, lots of topics.

* Lots of online resources and Youtube videos that I'll share as we go.

Goals:

* Understand the foundations of neural networks.
* See examples of training NNs to accomplish a task
  ↳ "training" = "find a good NN"
* Write our own Python code to create and train NNs (not using Machine Learning libraries)

Maybe:

* Learn about Python ML libraries (pytorch, tensorflow)
* Learn about specialized kinds of NNs for certain tasks.

Strong Analogy: Linear Regression

What is it?

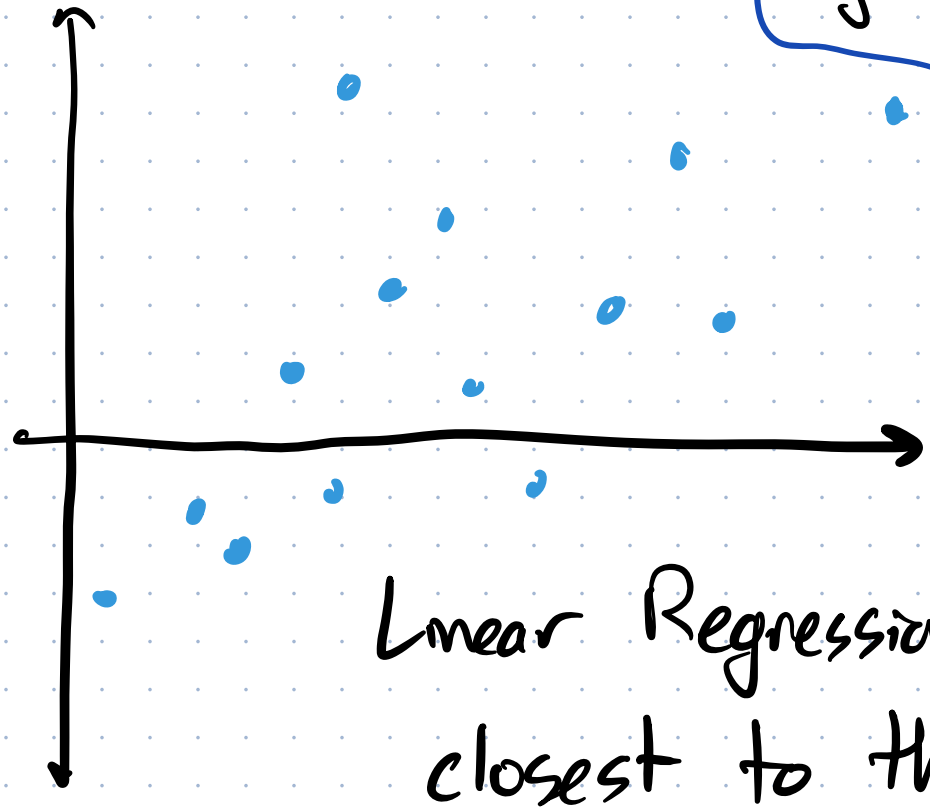
Simplest version: you have a bunch of (x,y) points and you want to find the line the best approximates them

Usually, the (x,y) points represent inputs (x) and outputs (y) of some unknown function.

x: time since Jan 1 this year
y: temperature on my outdoor thermometer

Strong Analogy: Linear Regression

x: time since Jan 1 this year
y: temperature on my outdoor thermometer



We only have sporadic readings.

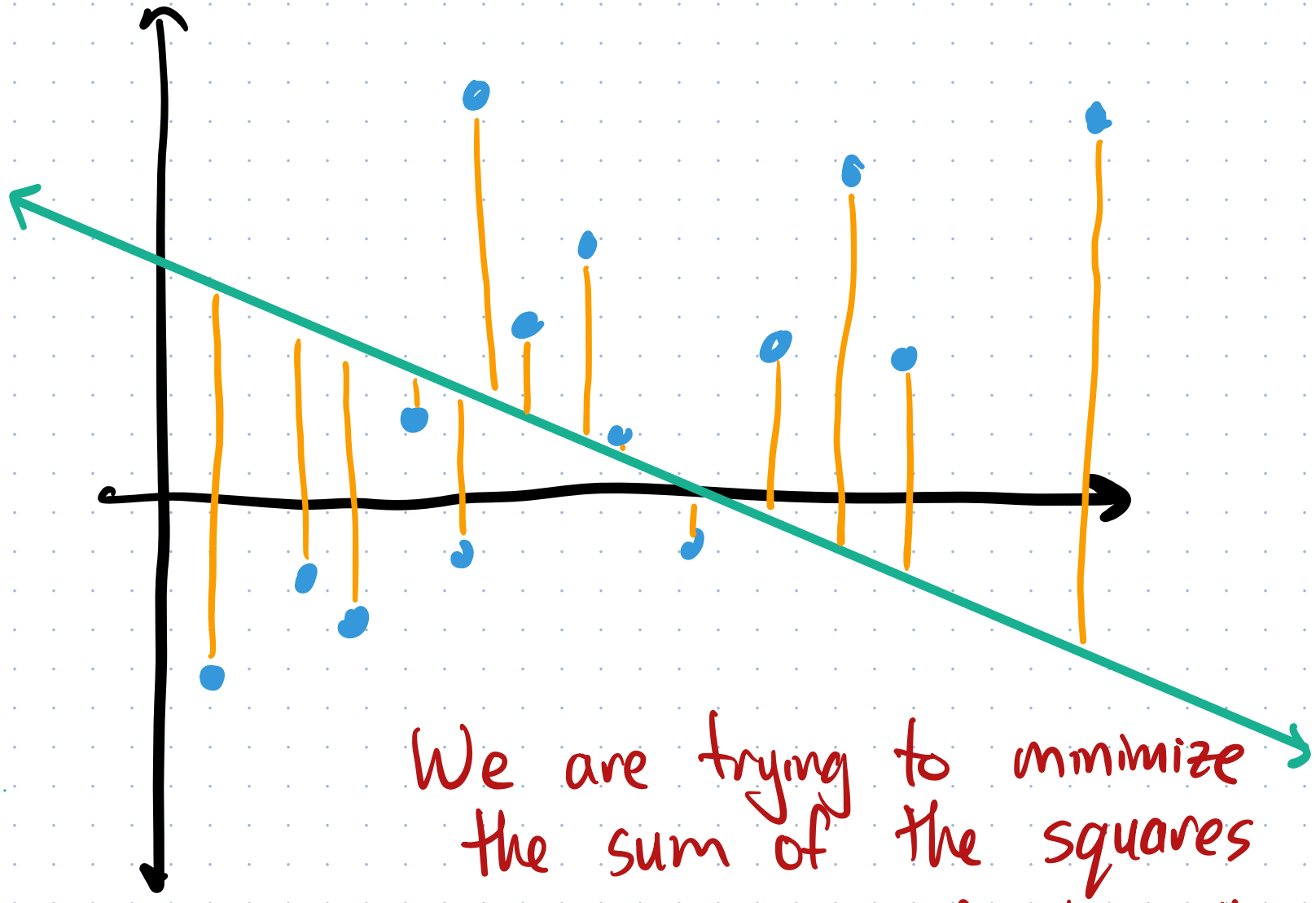
Linear Regression asks "what line is closest to these points?"

"Closest" means minimizing the sum of

$$([\text{actual y value}] - [\text{predicted y value}])^2$$

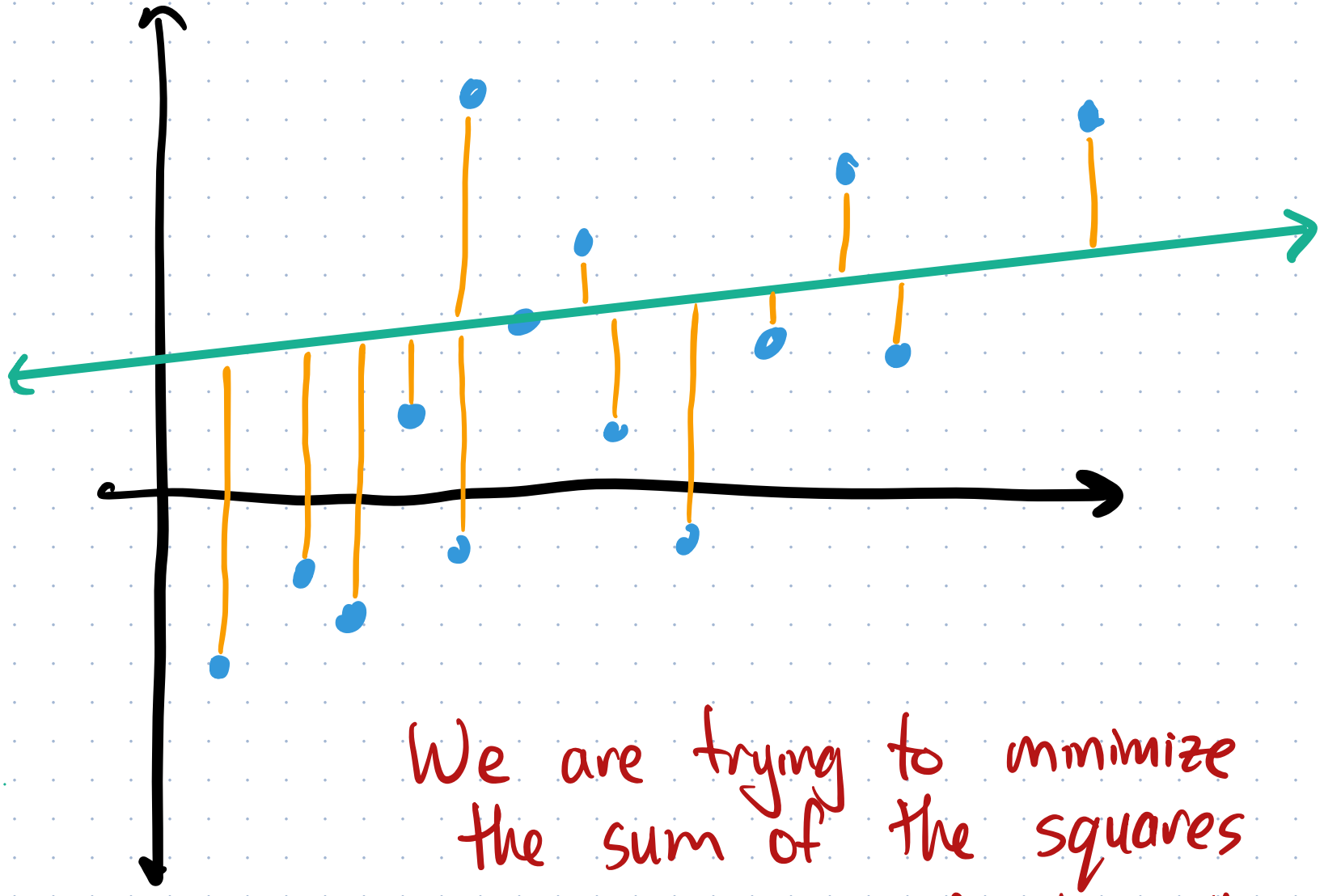
over all known points.

Strong Analogy: Linear Regression



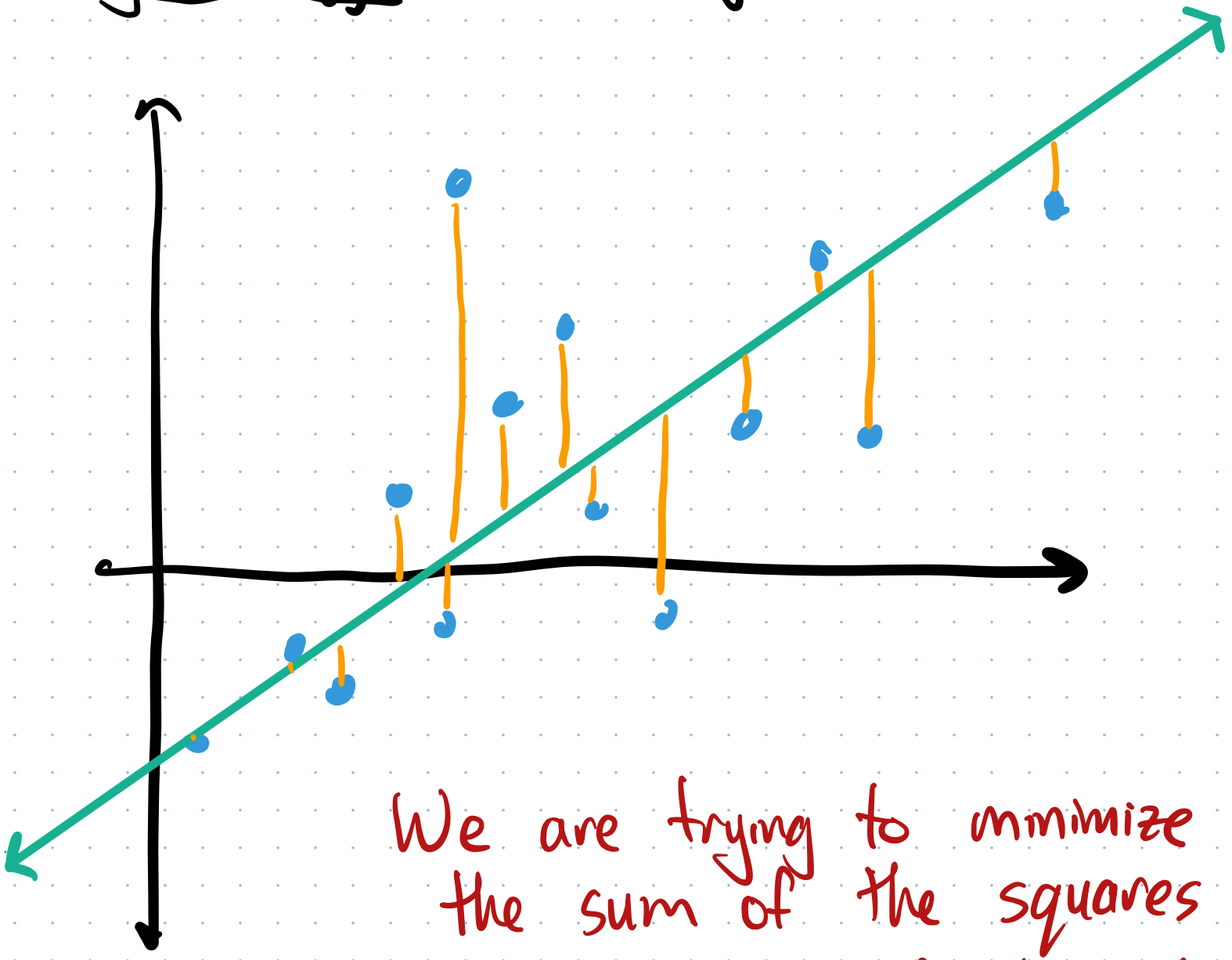
We are trying to minimize the sum of the squares of the lengths of the yellow lines

Strong Analogy: Linear Regression



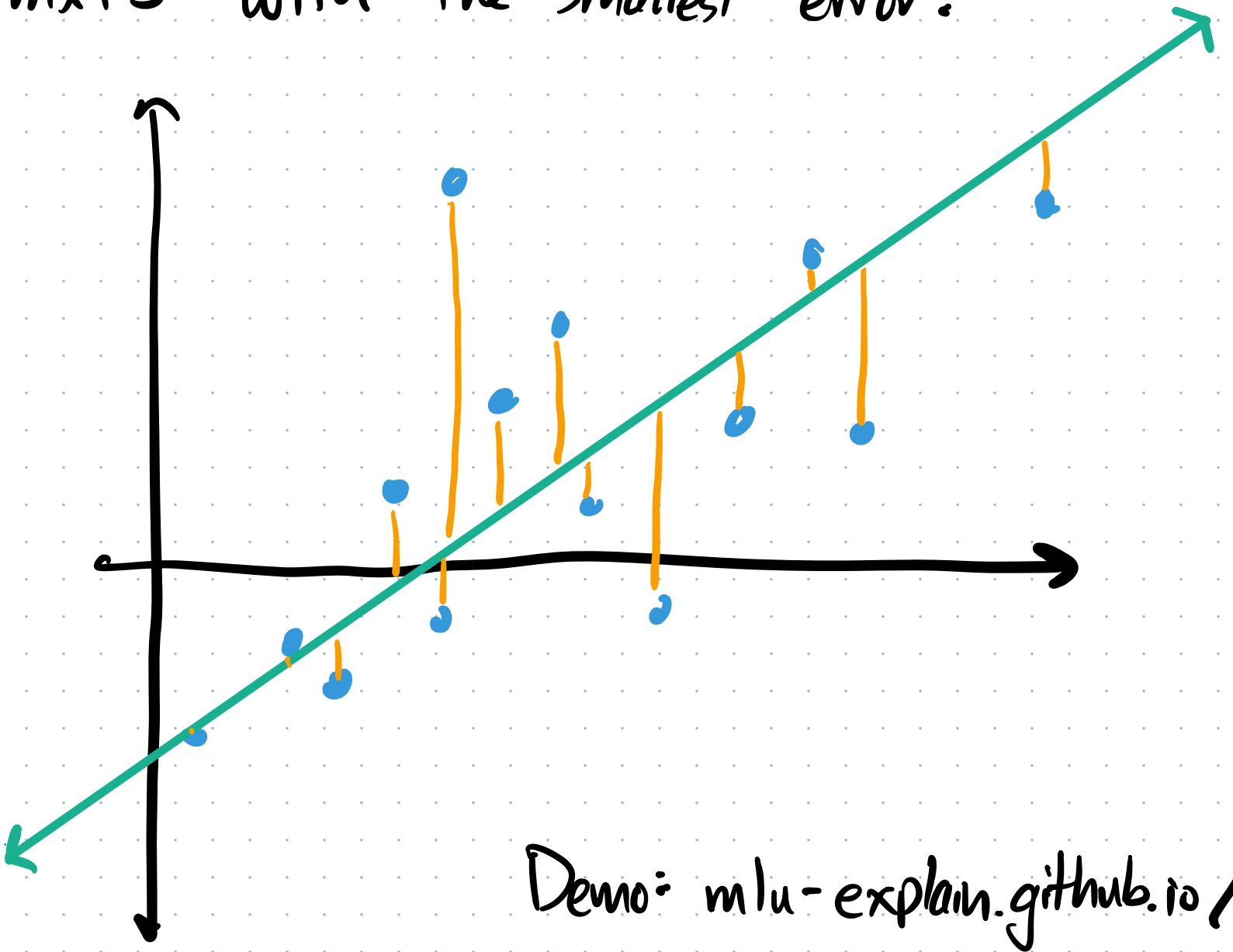
We are trying to minimize the sum of the squares of the lengths of the yellow lines

Strong Analogy: Linear Regression



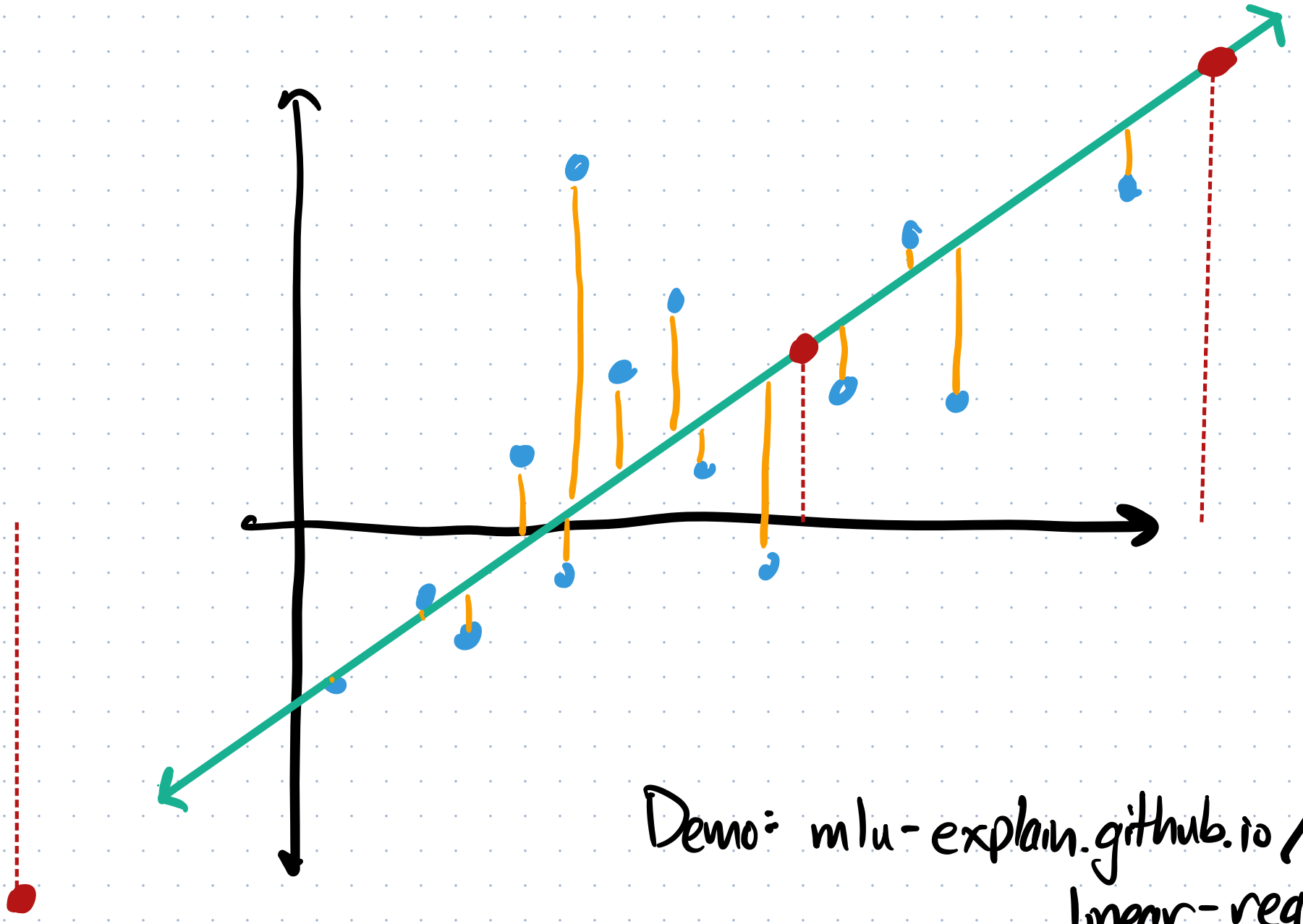
We are trying to minimize the sum of the squares of the lengths of the yellow lines

Problem: What values of m and b make the line $y = mx + b$ with the smallest error?



Demo: mlu-explain.github.io/linear-regression

Purpose: Estmate the output at new inputs.



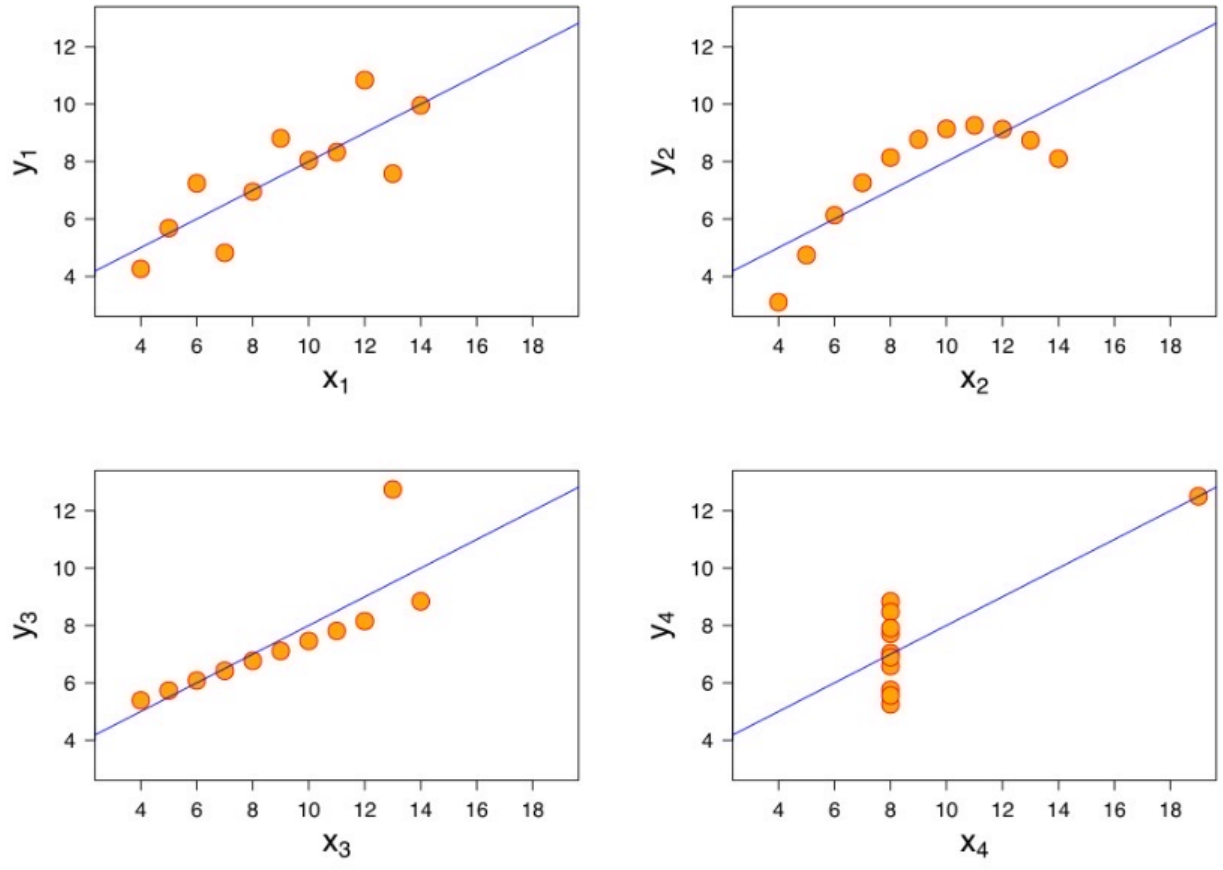
Demo: mlu-explain.github.io/linear-regression

This can be done with any # of input variables, and then you're finding planes and hyperplanes instead of lines. Same idea though.

How do you find the m, b that make the best line?

Formulas, Linear Algebra

The problem is a lot of data isn't linear.



The four datasets composing Anscombe's quartet. All four sets have identical statistical parameters, but the graphs show them to be considerably different

https://commons.m.wikimedia.org/wiki/File:Anscombe%27s_quartet_3.svg

Linear Regression: Approximate data with a line

Neural Network: Approximate data with <u>any function</u>

Pros: Can approximate data much better

Cons: Requires a lot of computation to produce

Big Picture:

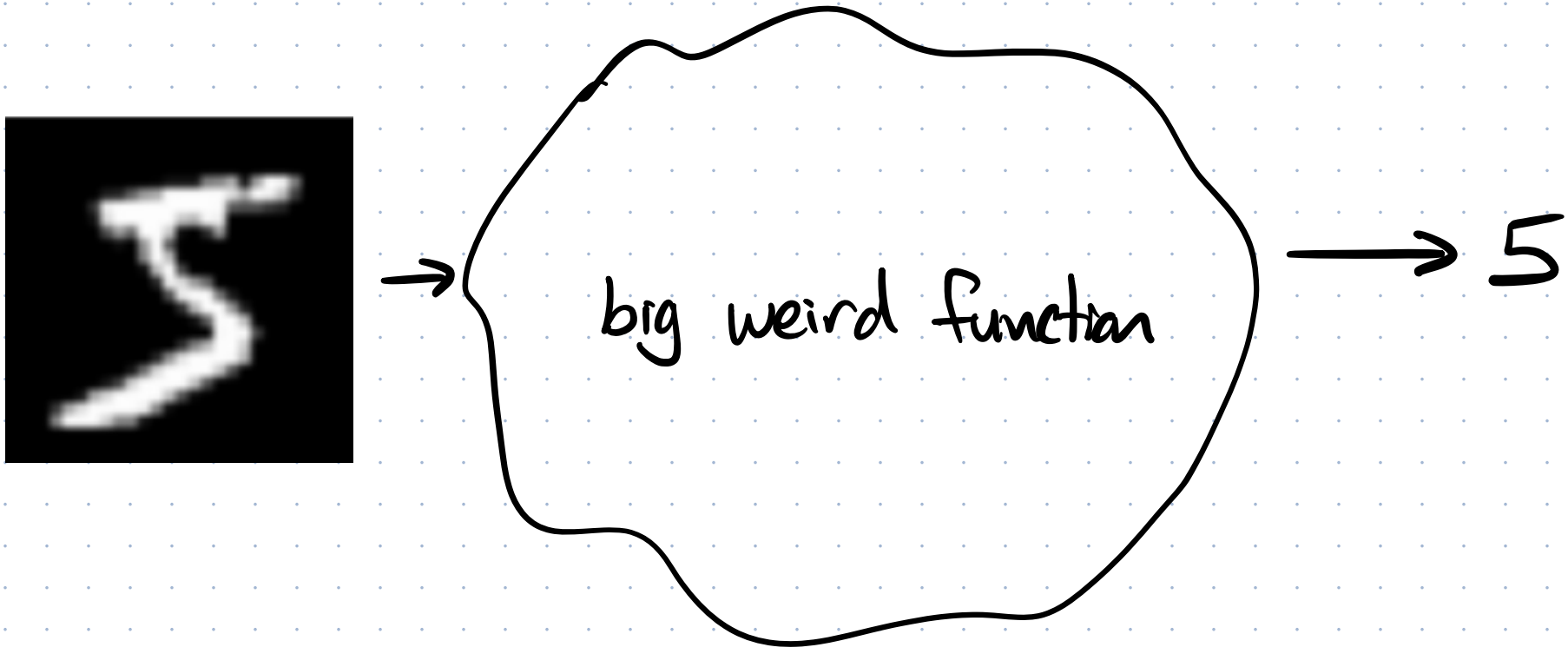
* A neural network is just a fancy function.
* It takes numbers as inputs and produces numbers as outputs, just like any function from Calculus.
* Finding a good neural network that approximates your data is hard.

Also: Lots of interesting things can be framed as a (numerical inputs) → (numerical outputs) function

Example function:

Input: a 28 × 28 grayscale image
Output: what digit it is

MNIST dataset



How is this "numeric input"?

Example function:

{ Input: a 28 × 28 grayscale image
Output: what digit it is }

* Each image is $28 \times 28 = 784$ pixels

Each pixel has a grayscale value from 0 (black) to 255 (white)

```
[[  0,   0,   0,   0,   0,   0,   0,   0,   0,   0,   0,   0,   0,   0,   0,   0,   0,   0,   0,   0,   0,   0,   0,   0,   0,   0,   0,   0],
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```

(In practice, we divide by 255 to make a decimal between 0 and 1)

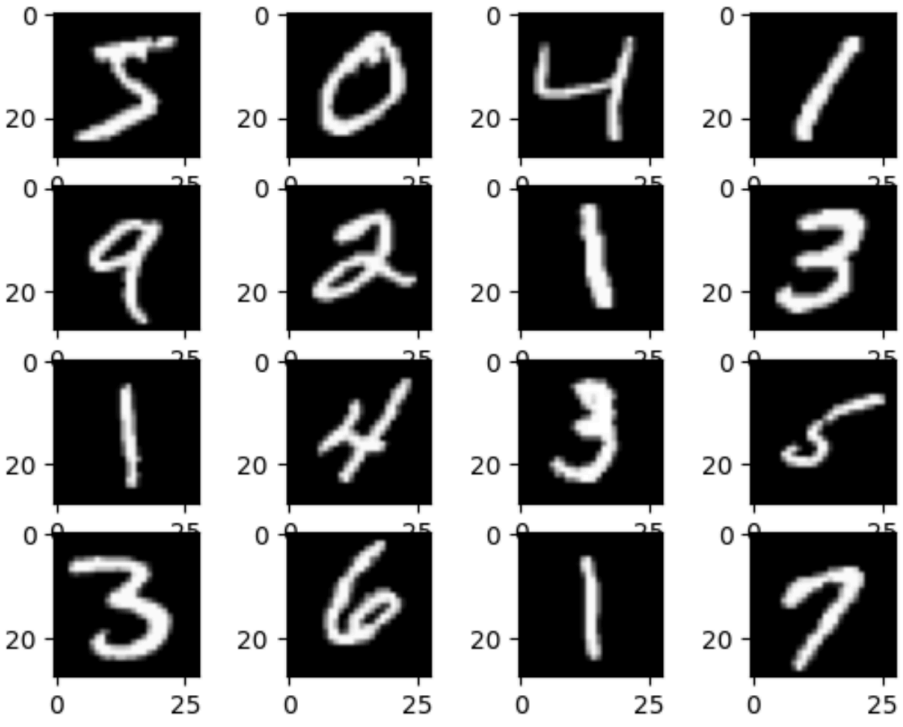
= 784 #s → big weird function → 5

* slight lie, our output will be a little different

So this is a 784-dimensional function.

And not really well-defined because many input pictures are not obviously a particular number

That's fine! We'll produce a neural network that takes 784 input #s (1 per pixel) and predicts the #.



MNIST data set

We'll use "training data", known (input, output) pairs, to build the NN.

(just like using data to find a linear regression line)

Big Picture:

* A neural network is just a fancy function.
* It takes numbers as inputs and produces numbers as outputs, just like any function from Calculus.
* Finding a good neural network that approximates your data is hard.

↳ We do this using lots of known (input, output) pairs.

Then we can use that good NN to predict new digits for us.

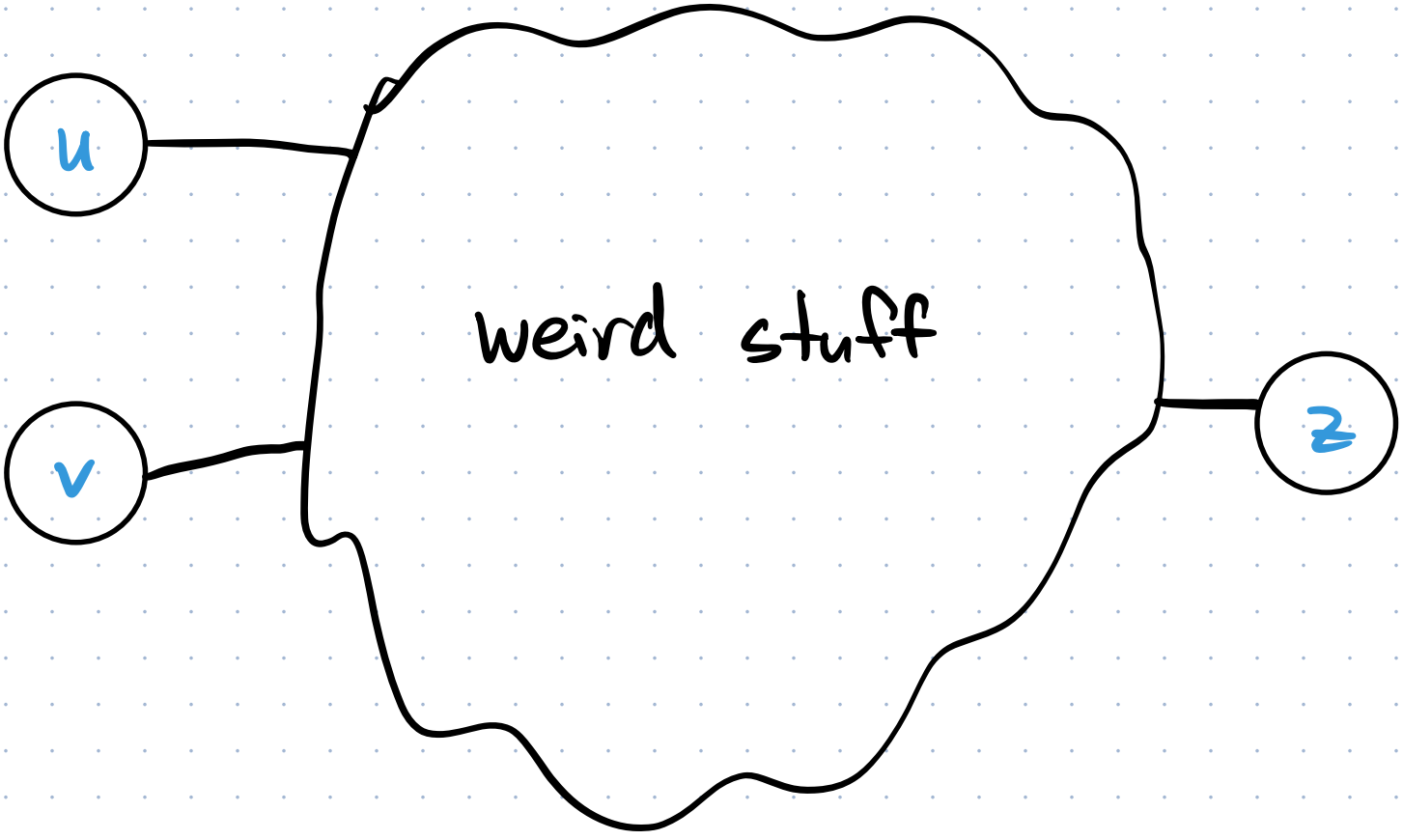
* Web applet demo

* Imagine if your job was to write an algorithm to look at the pixels manually a say what # it is! That would be so difficult.

What is a neural network?

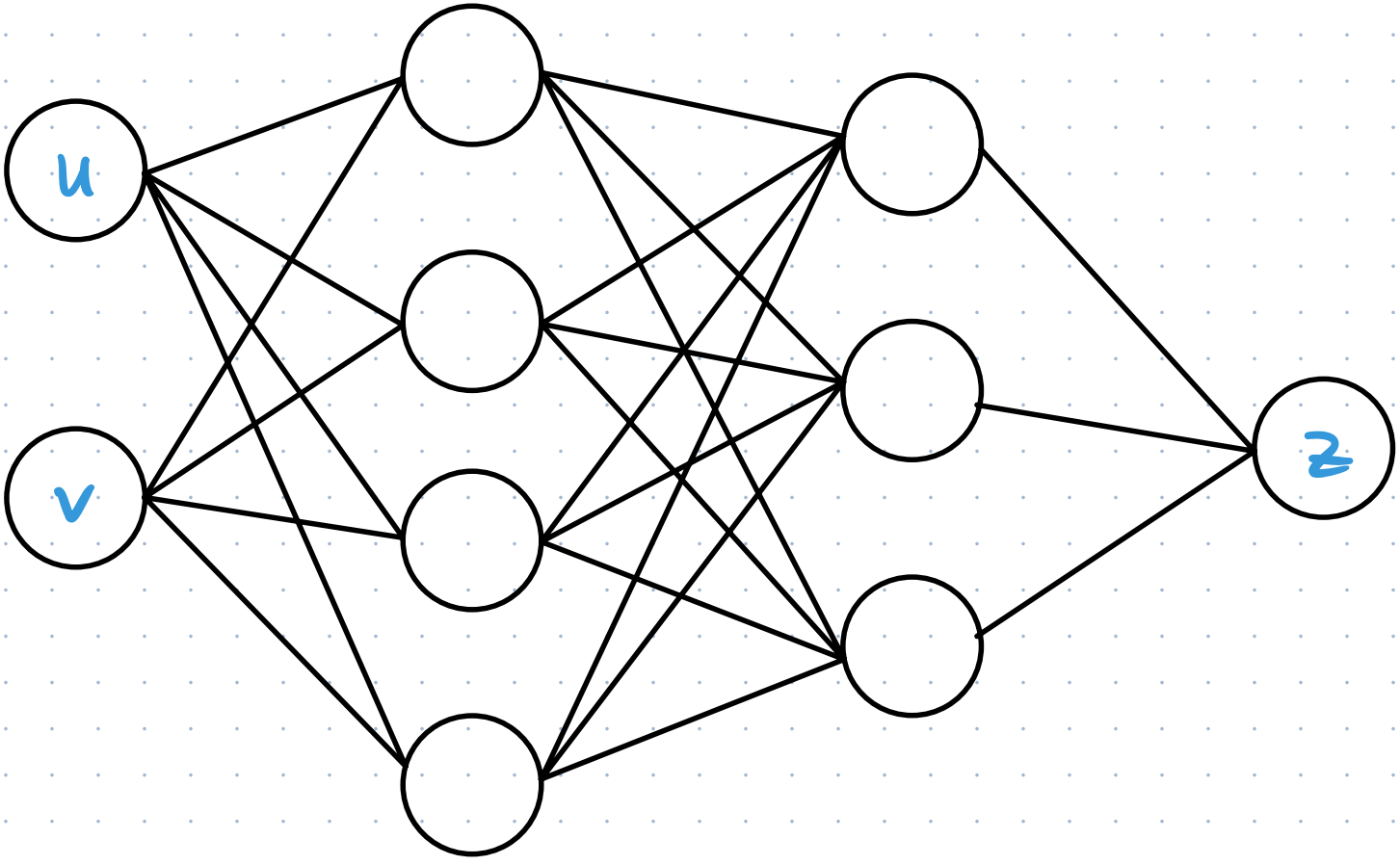
A fancy function defined in the following way.

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



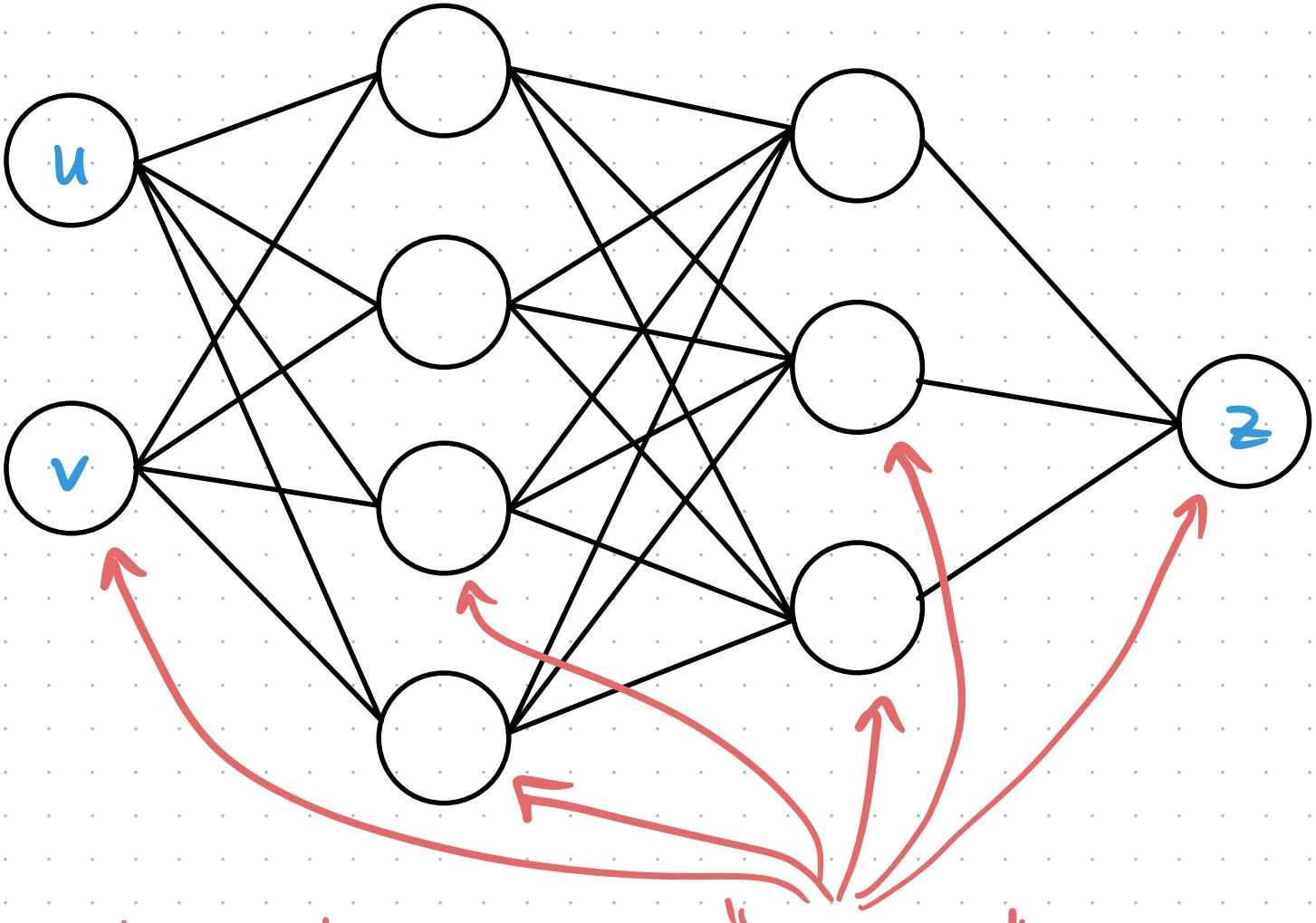
Example: A NN that takes 2 inputs and has 1 output

$f(u,v) = z$



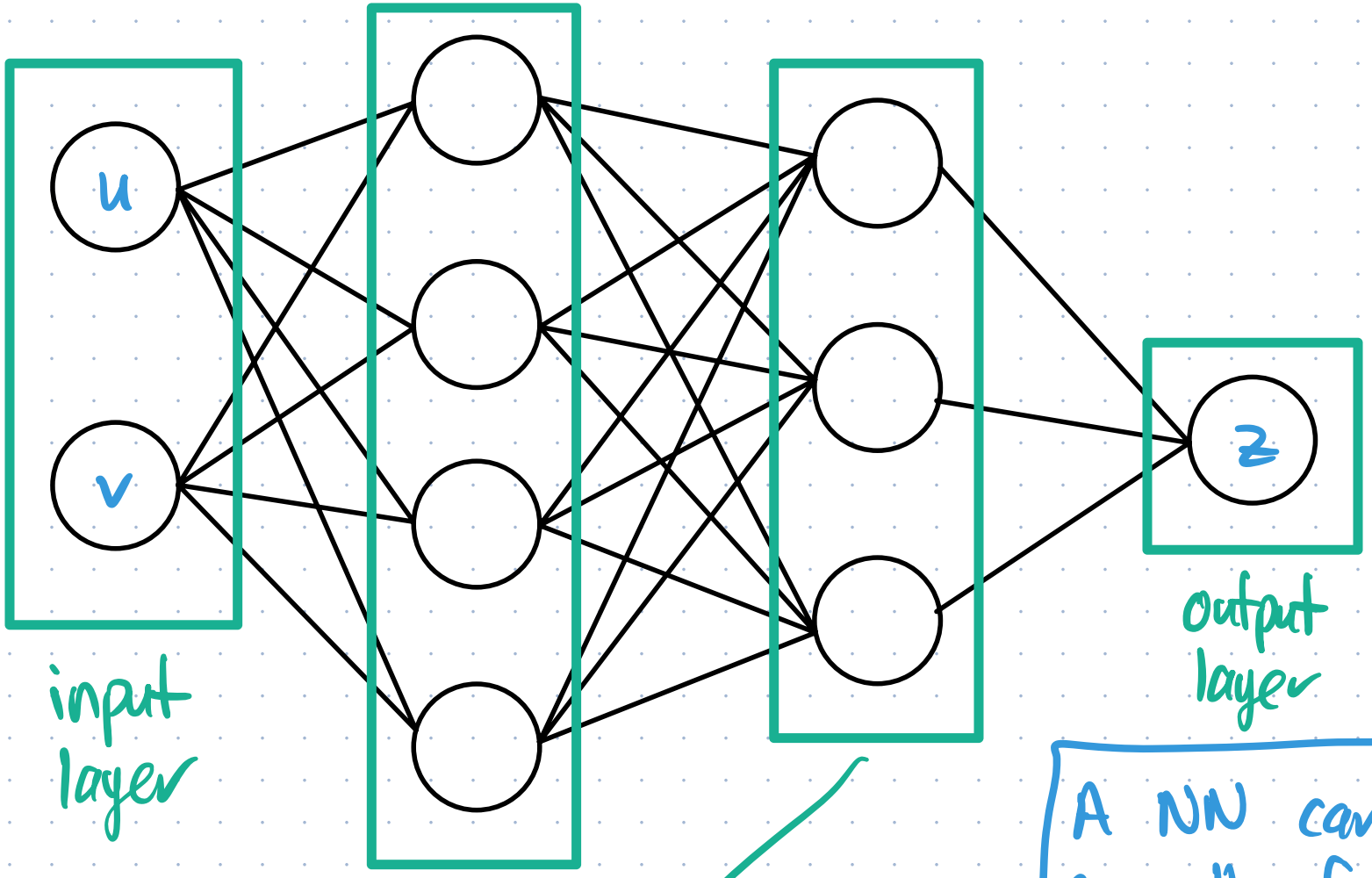
Example: A NN that takes 2 inputs and has 1 output

$f(u,v) = z$



each circle is a "neuron"

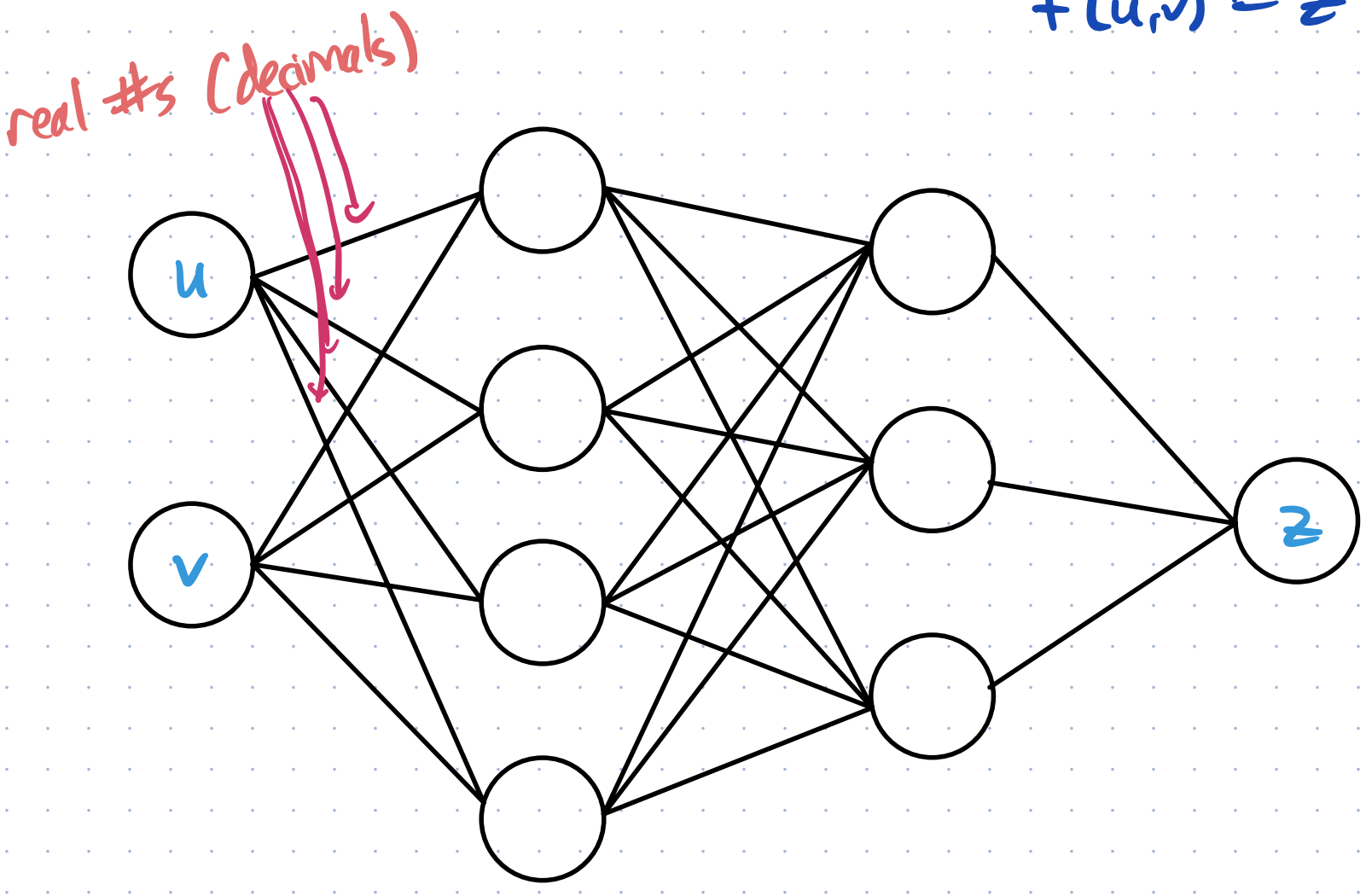
Example: A NN that takes 2 inputs and has 1 output
$f(u,v) = z$



A NN can have any # of layers, and they can be any size.

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

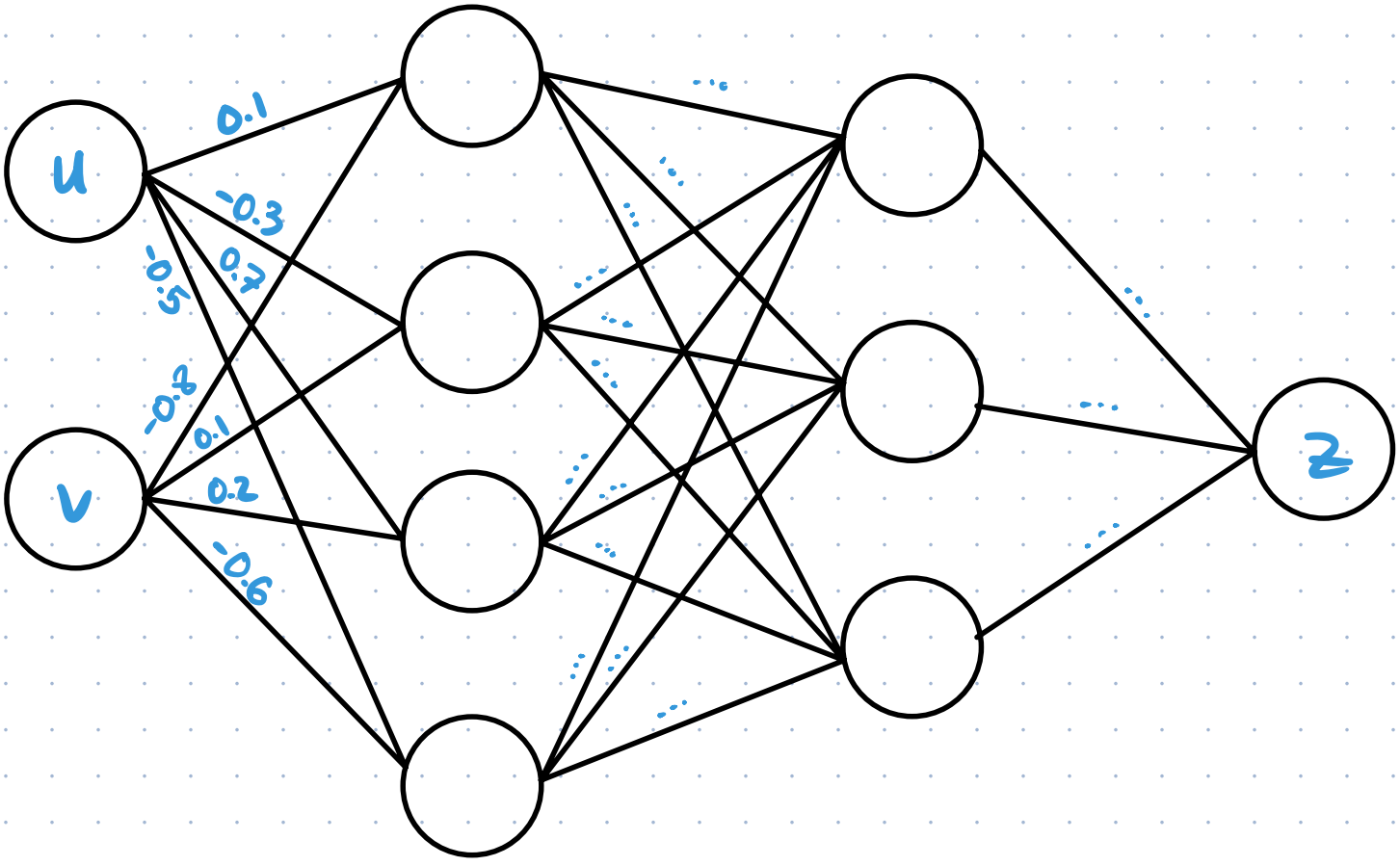
$f(u,v) = z$



Every edge between neurons has a real # attached to it called its weight

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

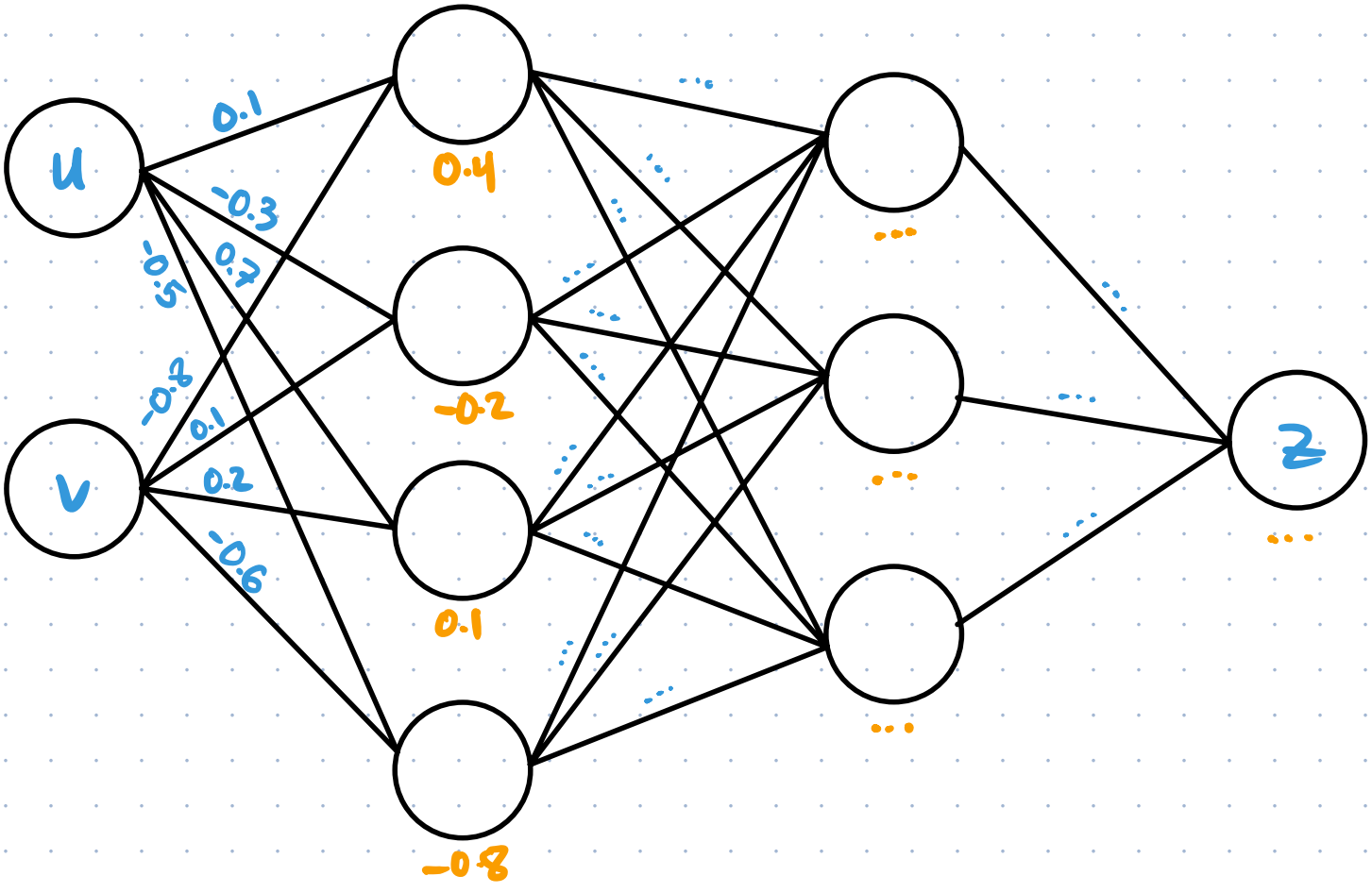
$f(u,v) = z$



I'm using #s to 1 decimal place for simplicity, but typically the are full floating point #s.

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

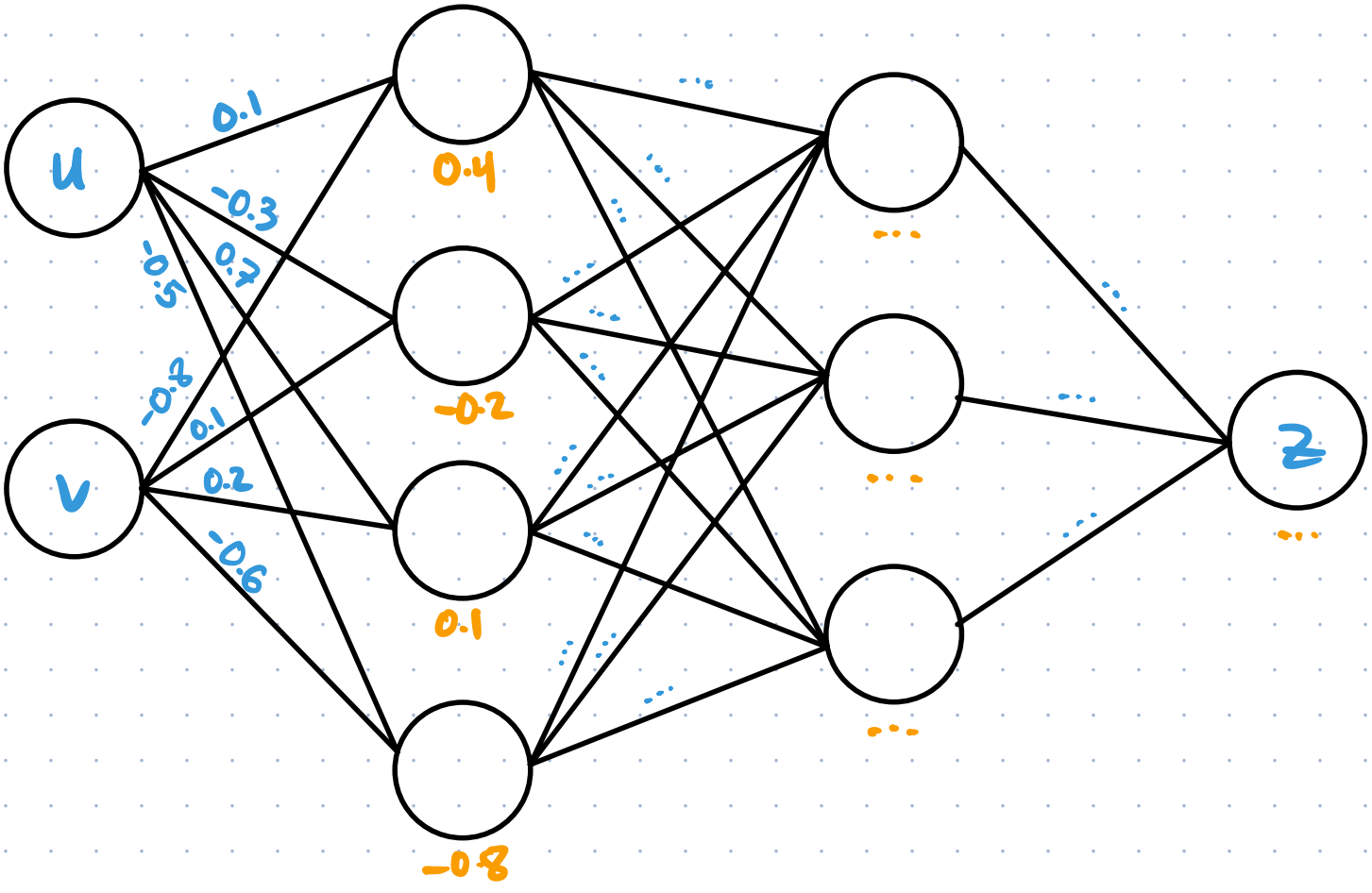
$f(u,v) = z$



Every neuron (except the input layer) has a # attached to it called its **bias**.

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

$f(u,v) = z$

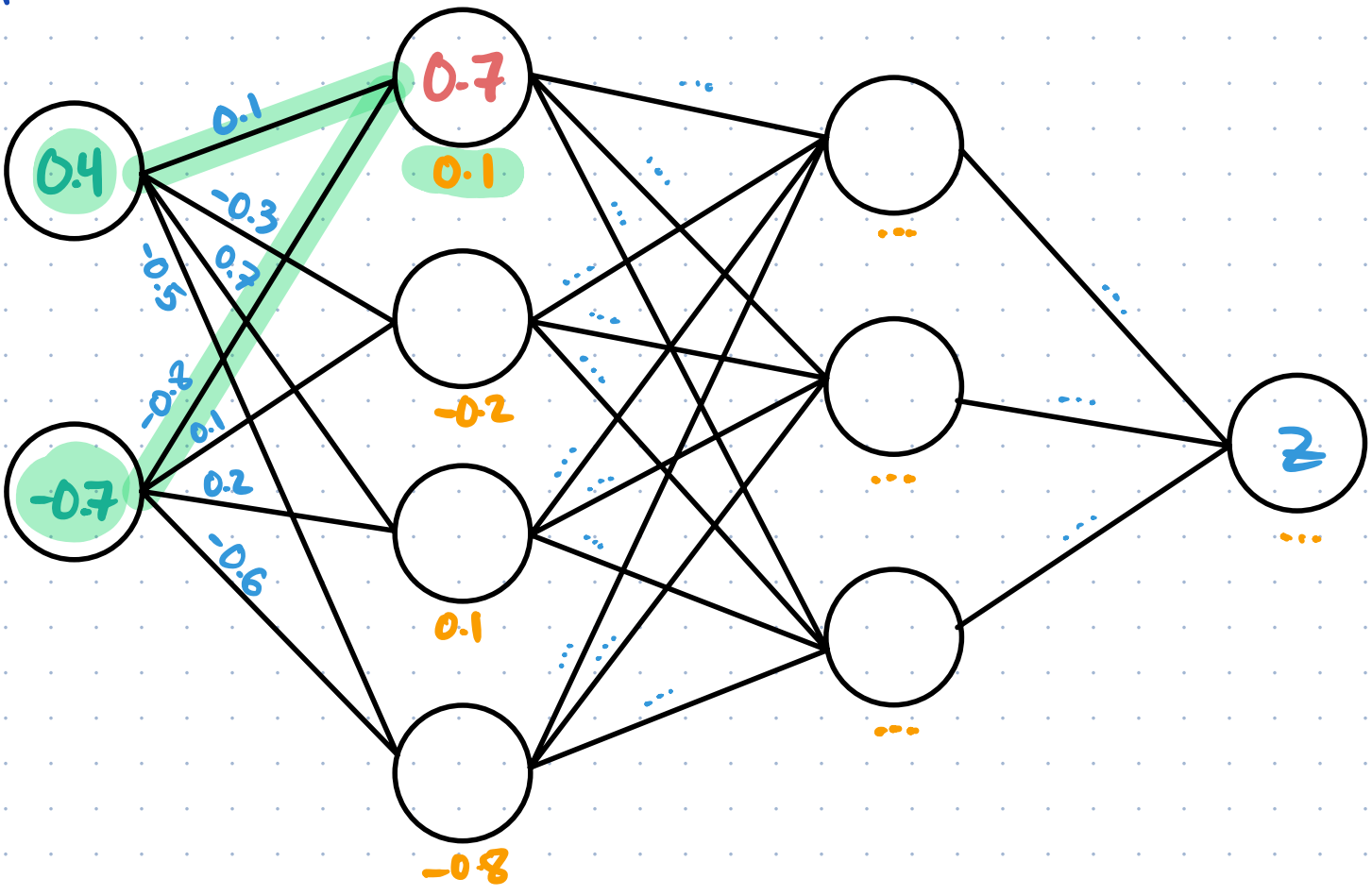


The #s u and v get "fed forward" to the neurons in the next layer.

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

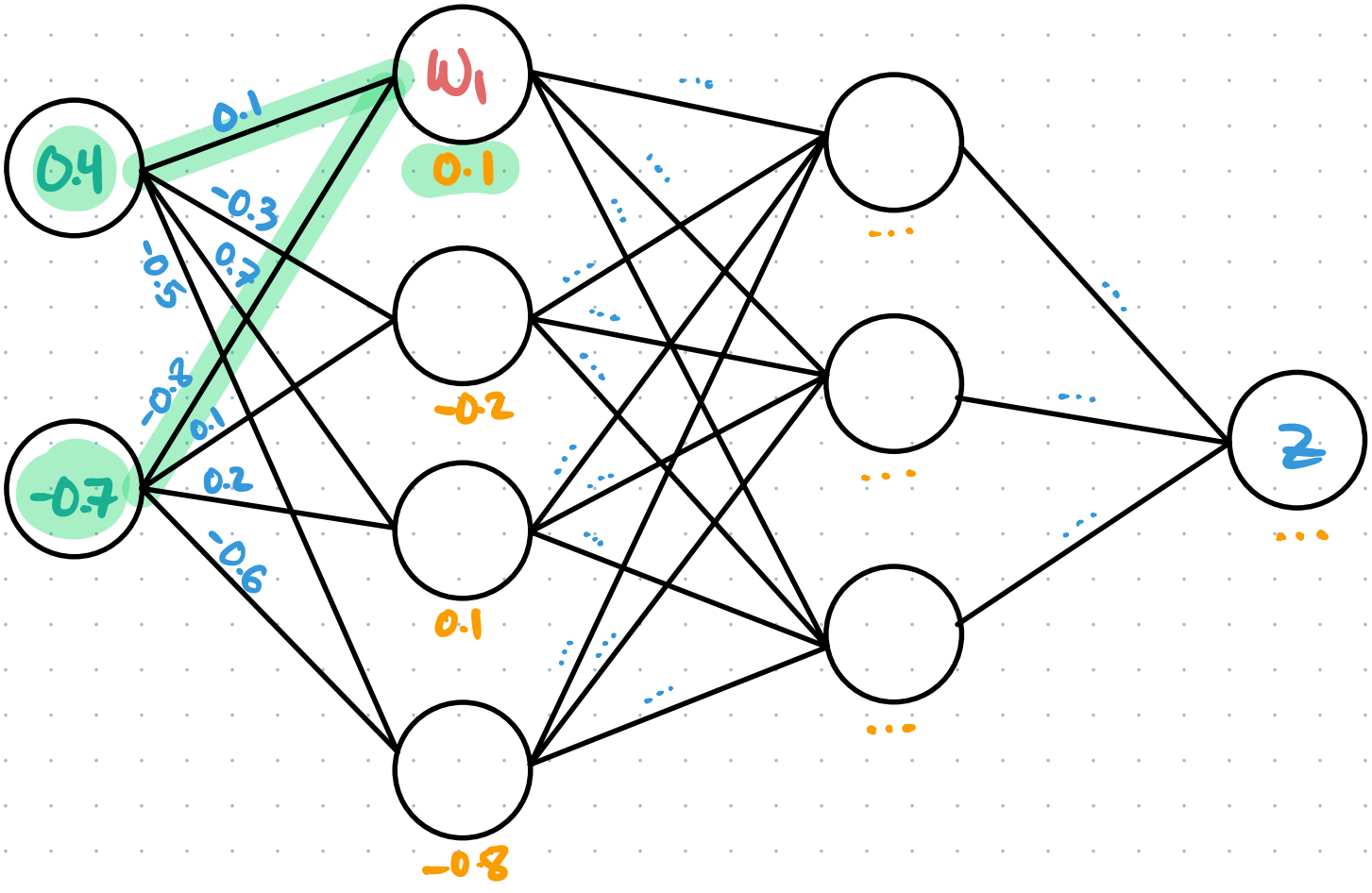
$f(u,v) = z$

$f(0.4, -0.7) = ?$



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

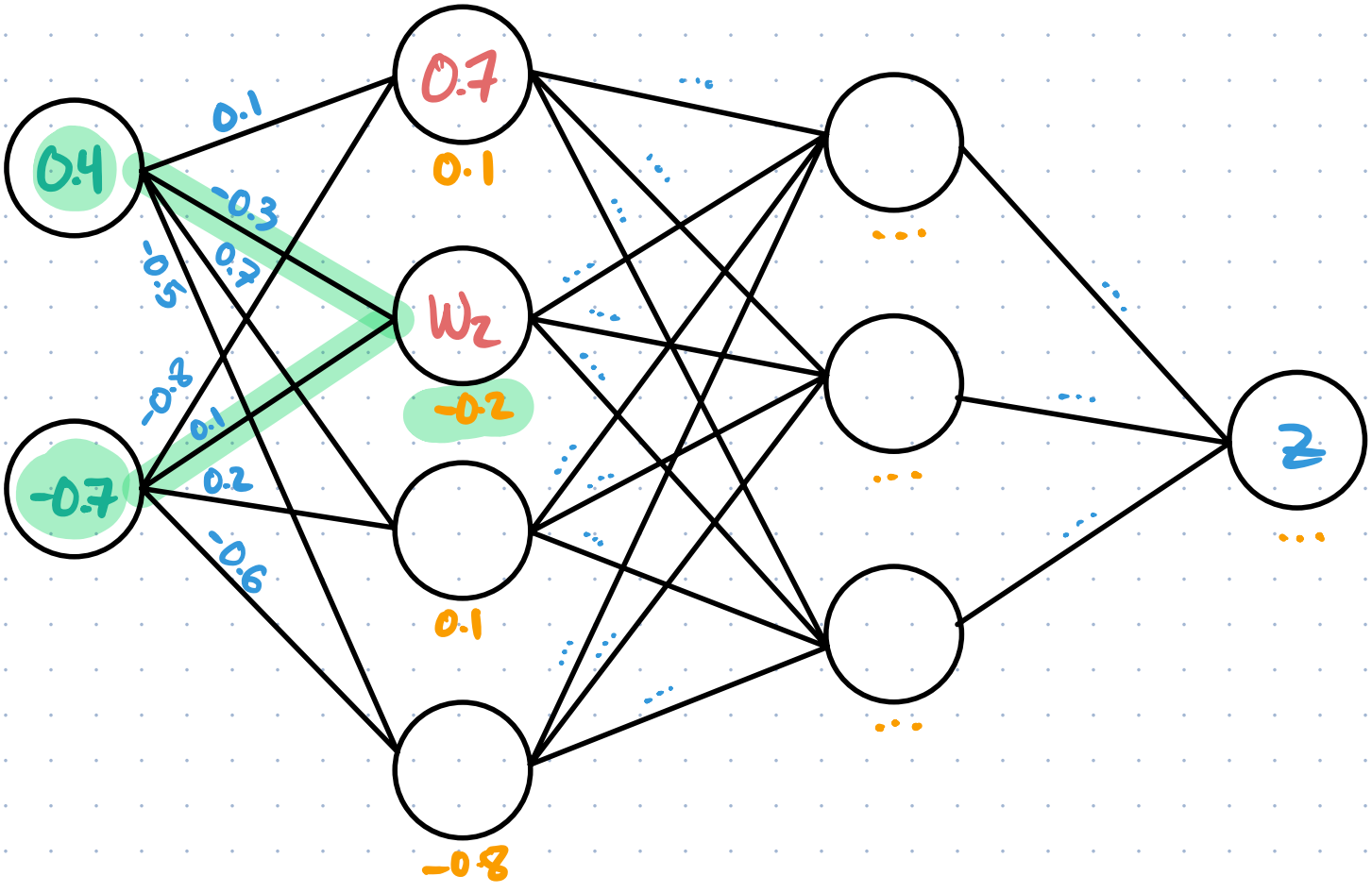
Example: A NN that takes 2 inputs and has 1 output
$f(u,v) = z$



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

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

$f(u,v) = z$

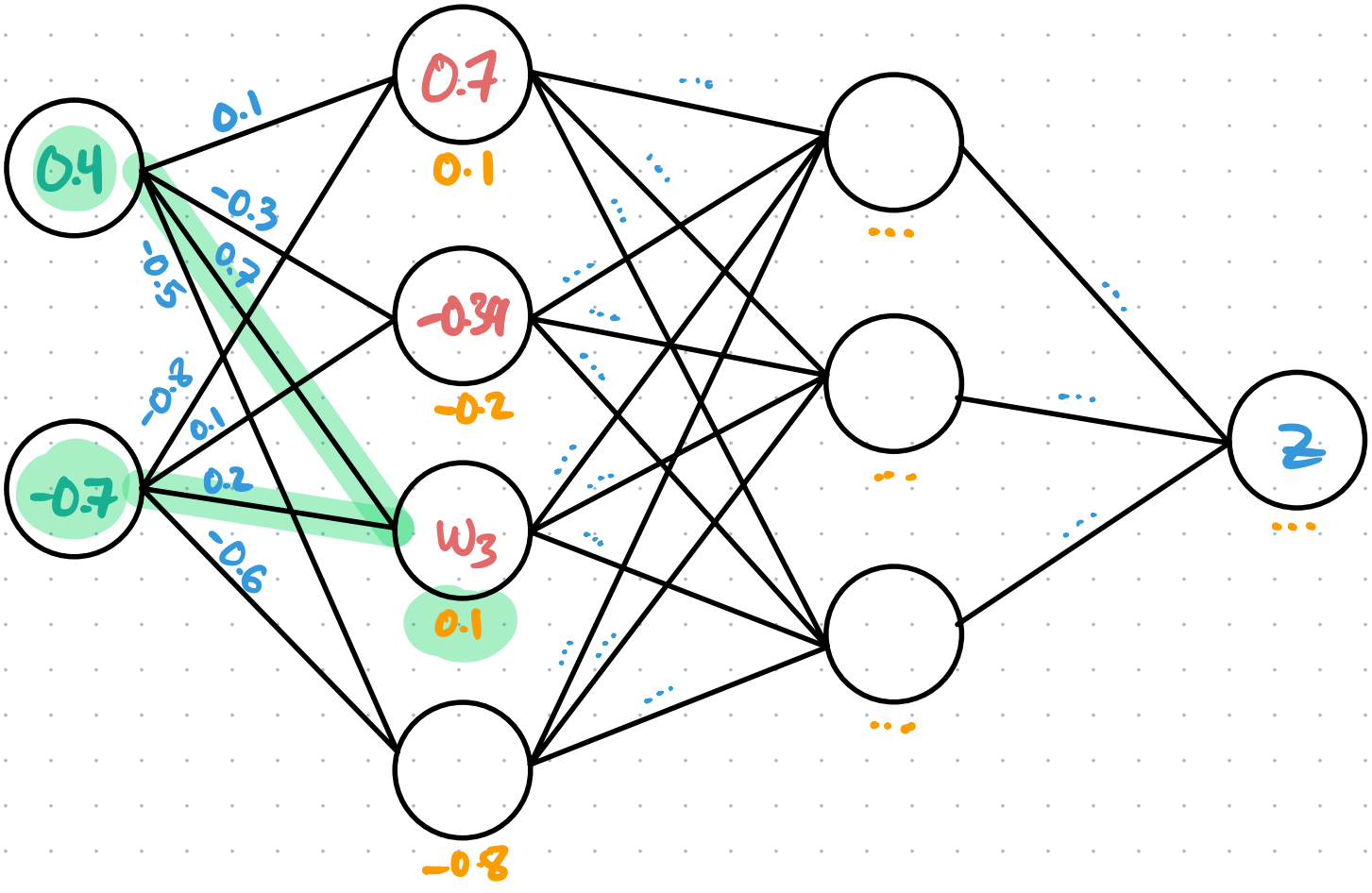


$W_2 = (0.4)(-0.3) + (-0.7)(0.1) + -0.2$

$= -0.39$

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

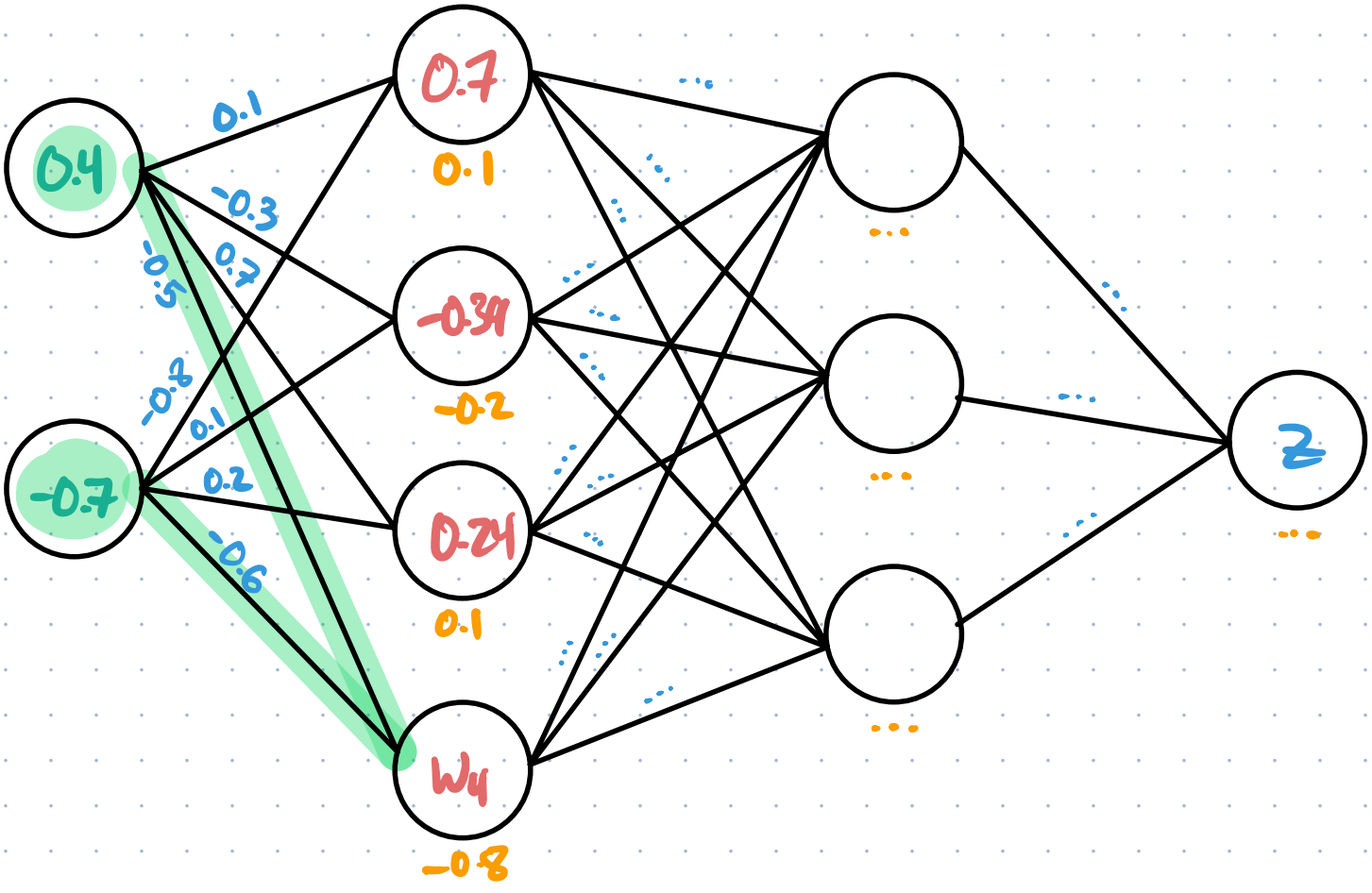
$f(u,v) = z$



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

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

$f(u,v) = z$

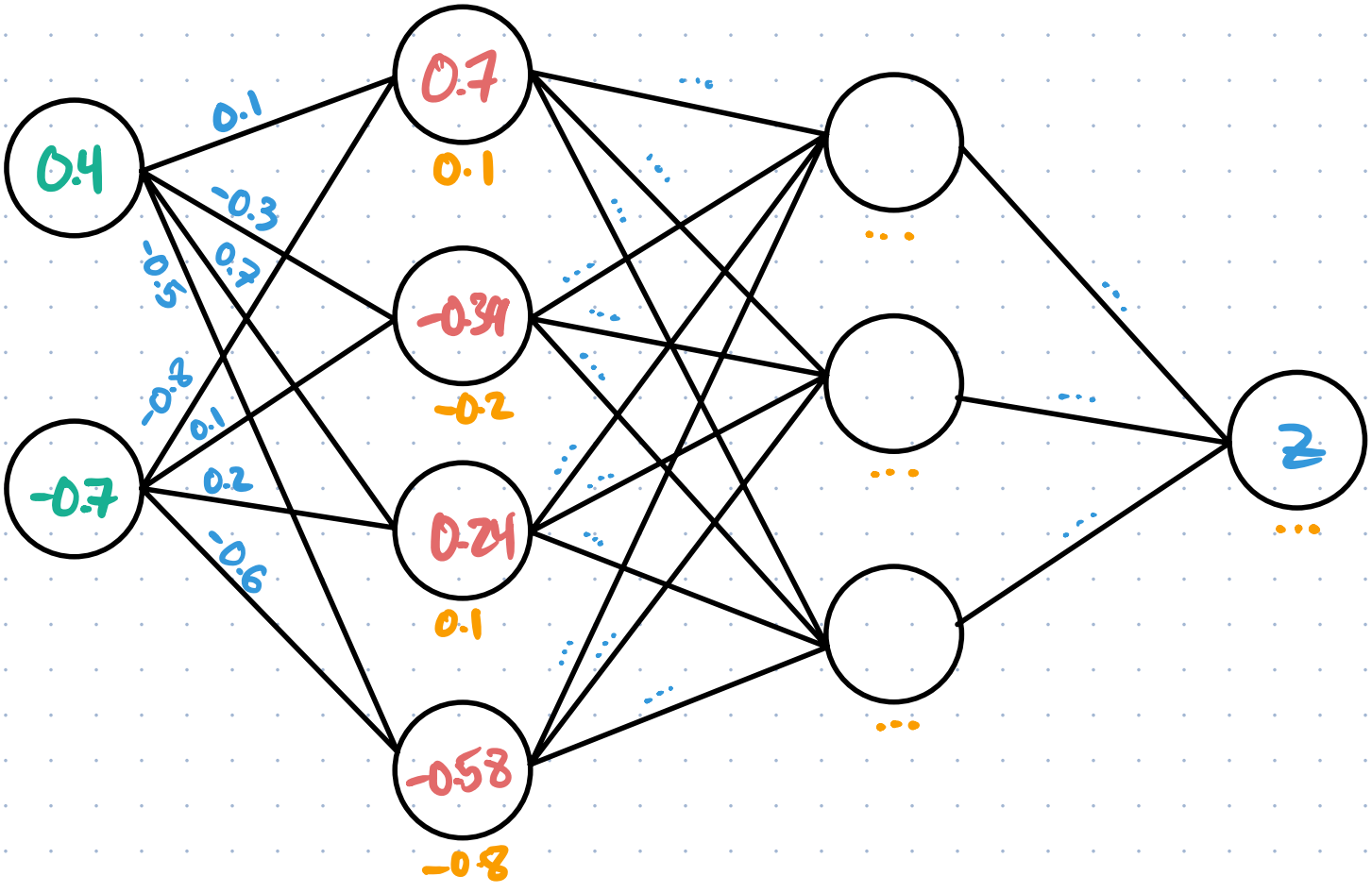


$W_4 = (0.4)(-0.5) + (-0.7)(-0.6) + -0.8$

$= -0.58$

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

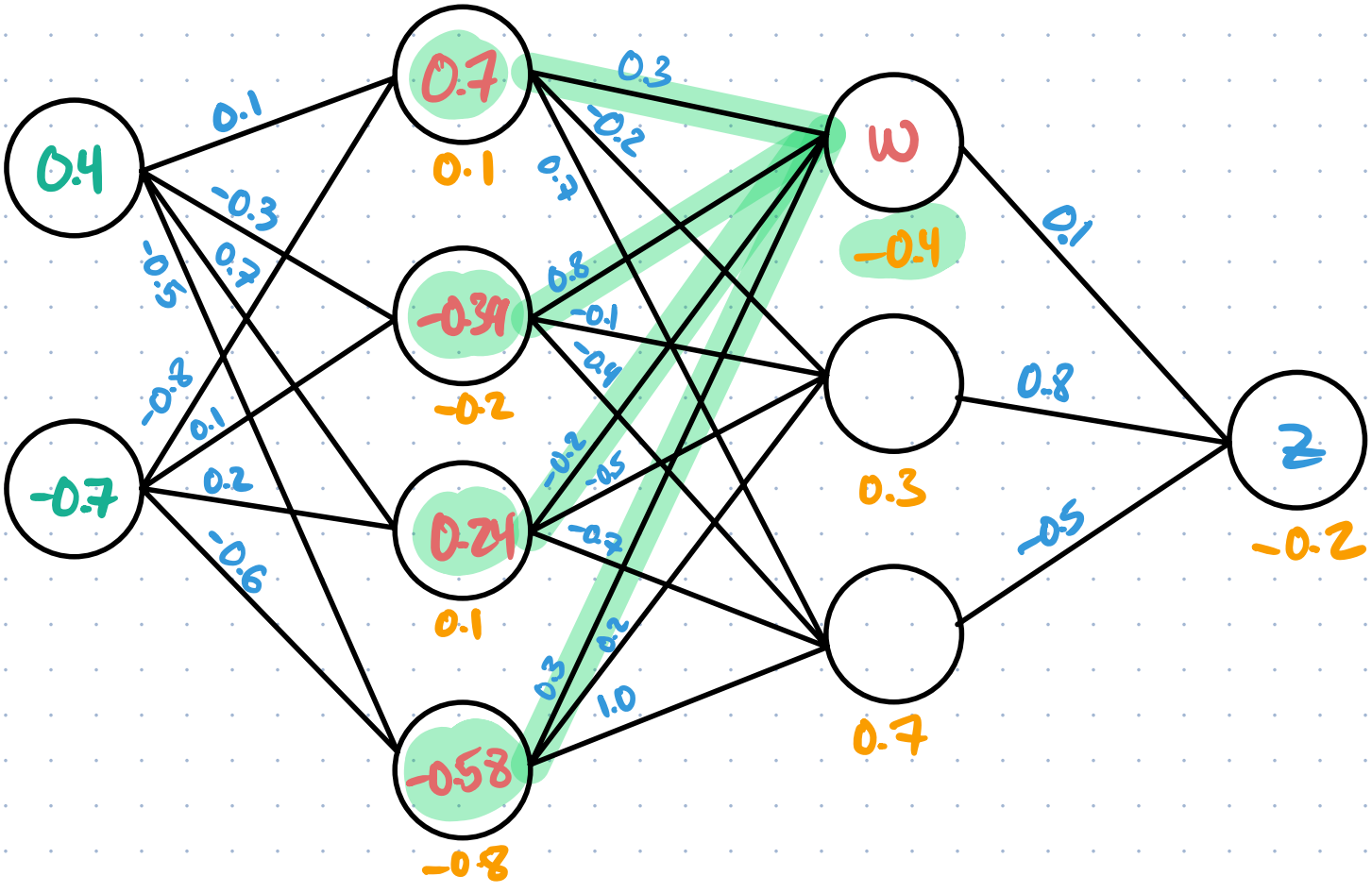
$f(u,v) = z$



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

$f(u,v) = z$

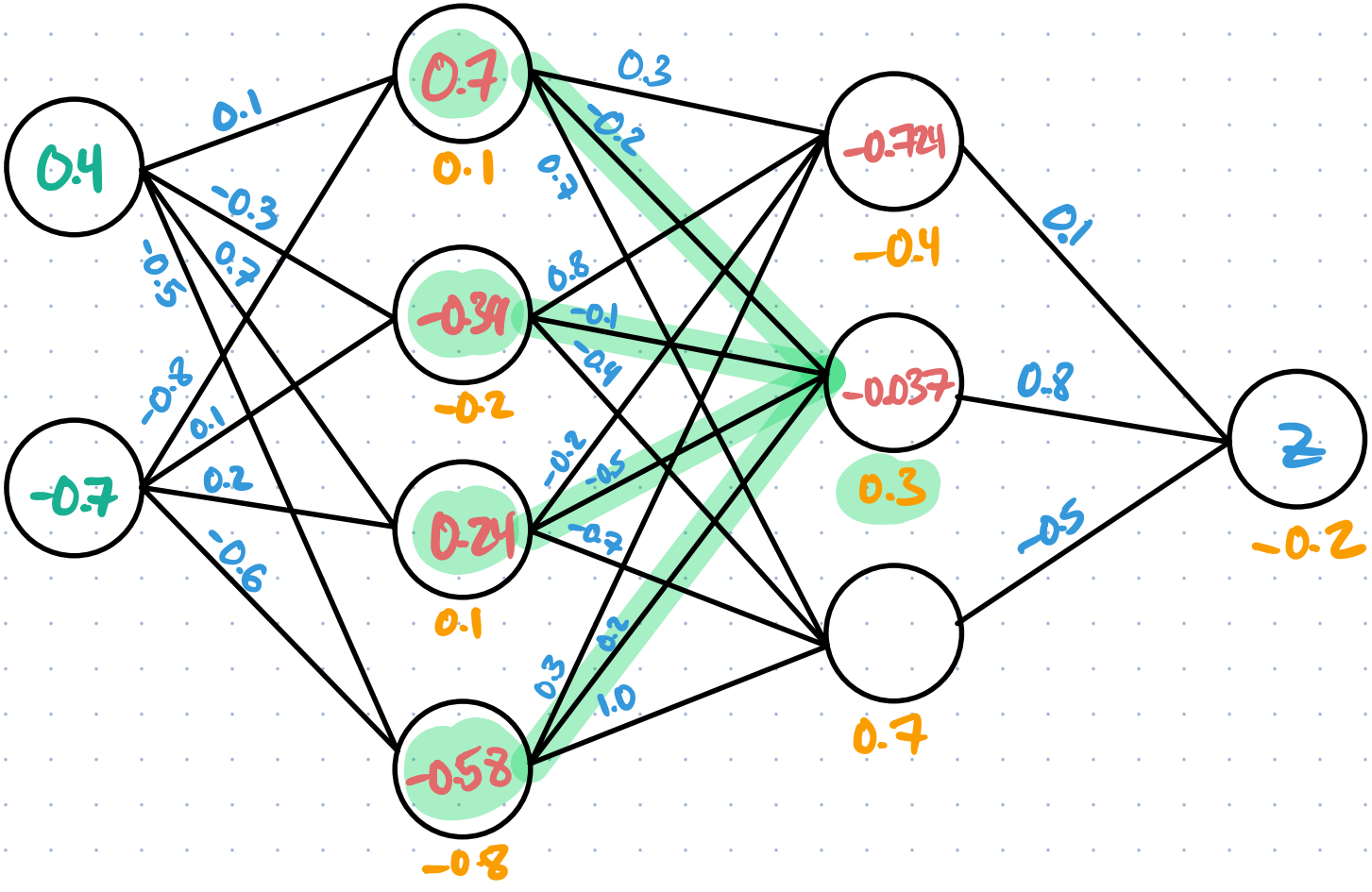


$w = (0.7)(0.3) + (-0.39)(0.8) + (0.24)(-0.2) + (-0.58)(0.3) + -0.4$

≈ -0.724

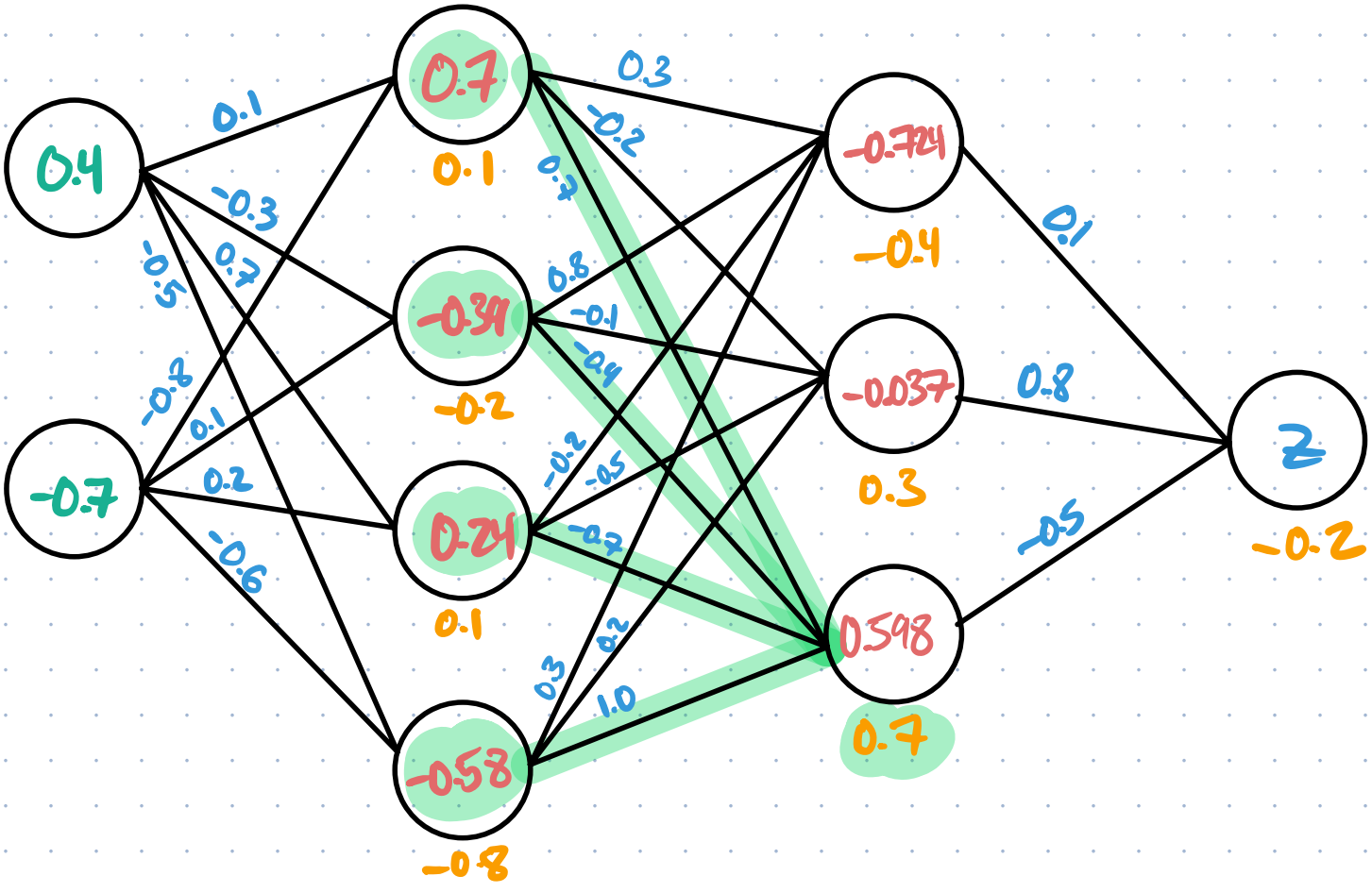
Example: A NN that takes 2 inputs and has 1 output

$f(u,v) = z$



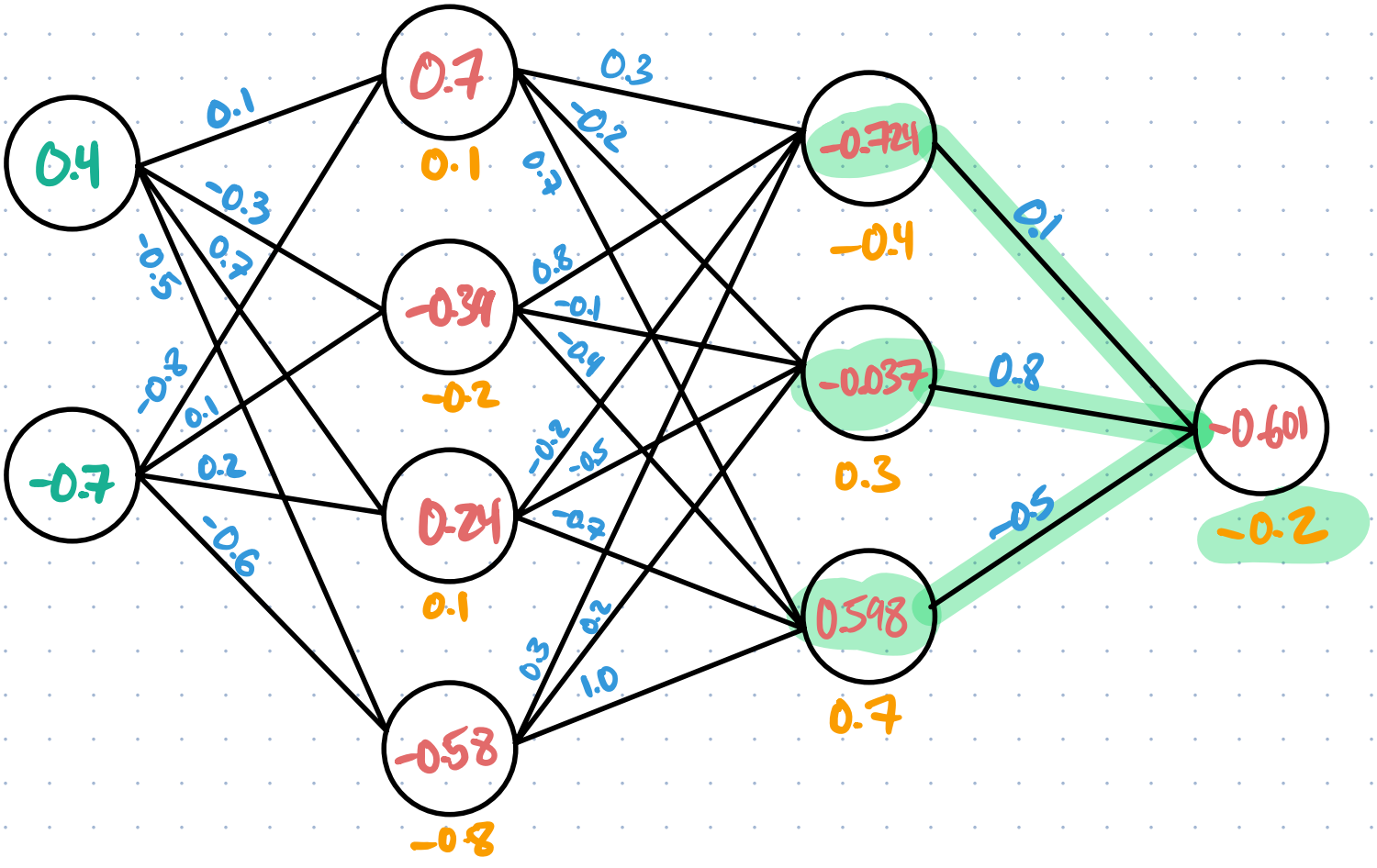
Example: A NN that takes 2 inputs and has 1 output

$f(u,v) = z$



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

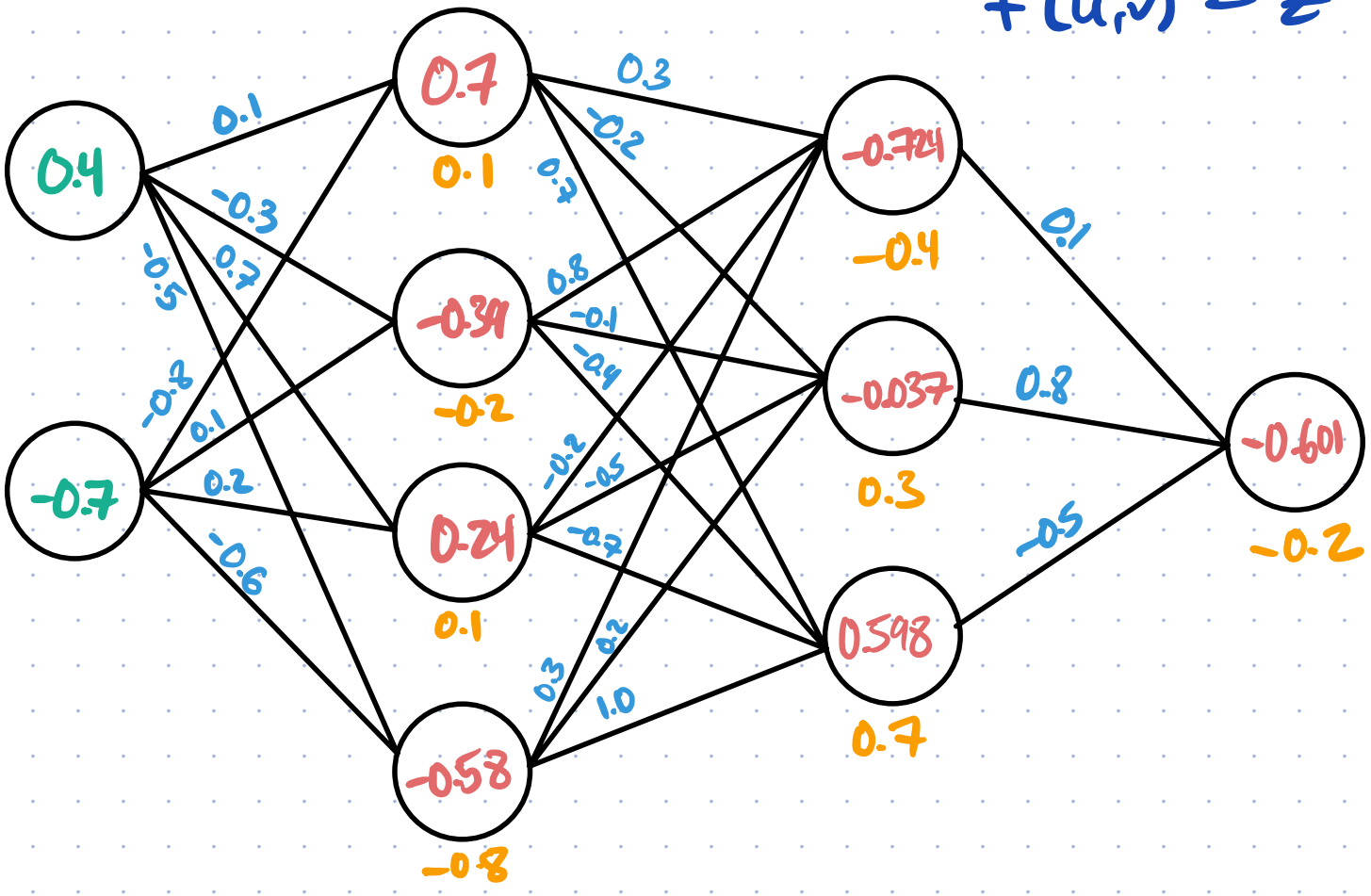
$f(u,v) = z$



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

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

$f(u,v) = z$

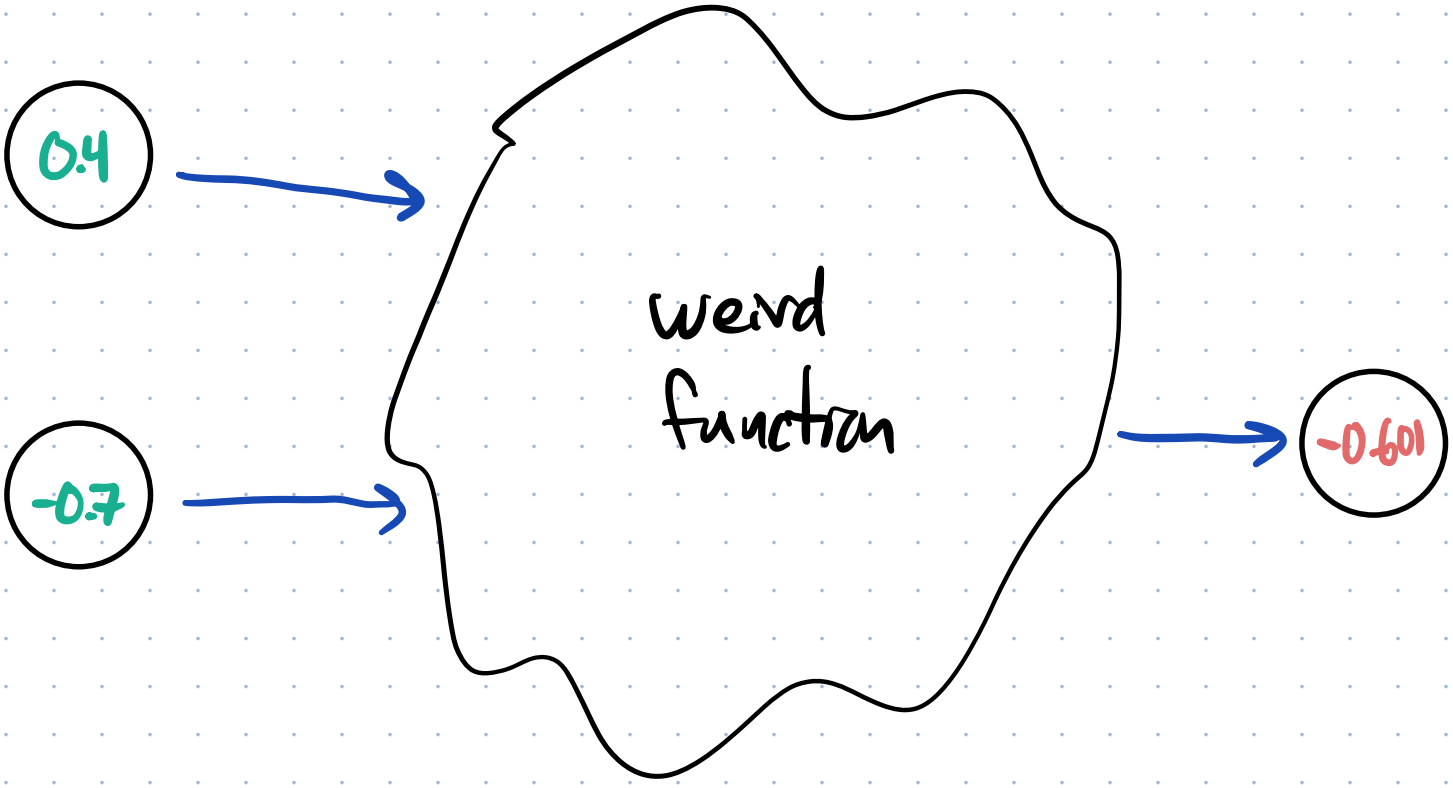


So, for this particular neural network, with these weights and biases, the inputs $(0.4, -0.7)$ produce output -0.601

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

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

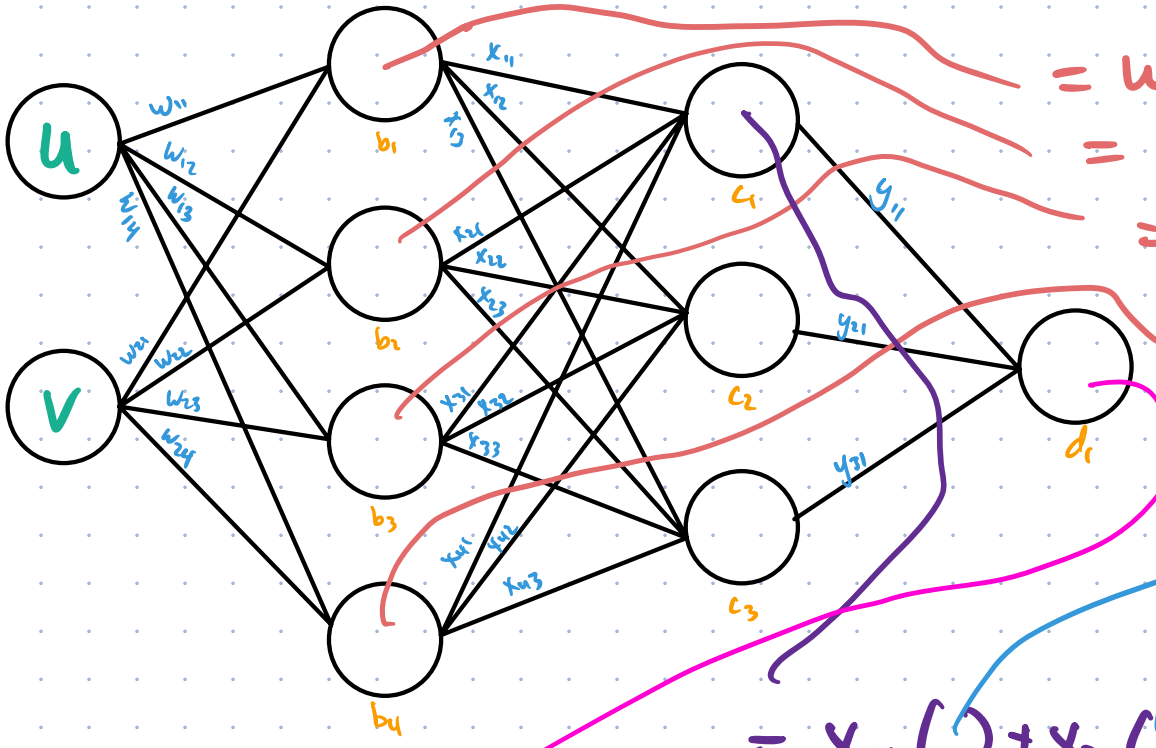
$f(u,v) = z$



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

* NNs can have any # of layers
* The layers can have any # of neurons in them
* If every neuron in a layer is connected to every neuron in the next layer, then the network is "fully connected"

* But we're missing a really key component so far.



$= w_{11}u + w_{21}v + b_1$

$= w_{12}u + w_{22}v + b_2$

$= w_{13}u + w_{23}v + b_3$

$= w_{14}u + w_{24}v + b_4$

$= x_{11}(\ ) + x_{21}(\ ) + x_{31}(\ ) + x_{41}(\ ) + c_1$

$= (x_{11}w_{11} + x_{21}w_{12} + x_{31}w_{13} + x_{41}w_{14}) \cdot u$

$+ (x_{11}w_{21} + x_{21}w_{22} + x_{31}w_{23} + x_{41}w_{24}) \cdot v$

$+ (b_1 + b_2 + b_3 + b_4)$

$=$

```
(w11*x11*y11 + w11*x12*y21 + w11*x13*y31 + w12*x21*y11 + w12*x22*y21 + w12*x23*y31 + w13*x31*y11 + w13*x32*y21 + w13*x33*y31 + w14*x41*y11 + w14*x42*y21 + w14*x43*y31) * u
 + (w21*x11*y11 + w21*x12*y21 + w21*x13*y31 + w22*x21*y11 + w22*x22*y21 + w22*x23*y31 + w23*x31*y11 + w23*x32*y21 + w23*x33*y31 + w24*x41*y11 + w24*x42*y21 + w24*x43*y31) * v
 + b1*x11*y11 + b1*x12*y21 + b1*x13*y31 + b2*x21*y11 + b2*x22*y21 + b2*x23*y31 + b3*x31*y11 + b3*x32*y21 + b3*x33*y31 + b4*x41*y11 + b4*x42*y21 + b4*x43*y31 + c1*y11 + c2*y21 + c3*y31 + d1
```

As we've built them NNs are still just (big) linear functions, so this is no better than linear regression.