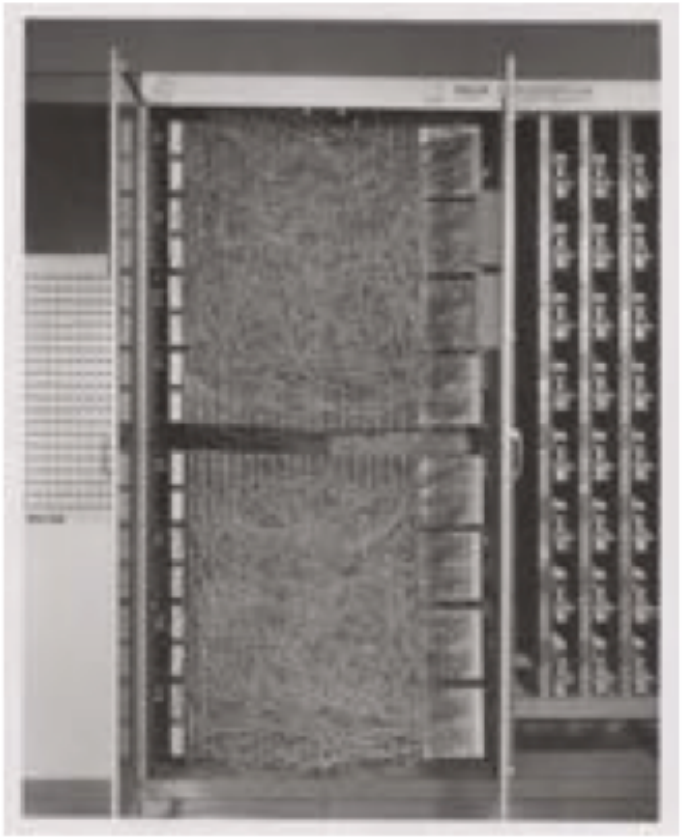
PART II: FOUNDATIONS OF "SHALLOW" NEURAL NETWORKS

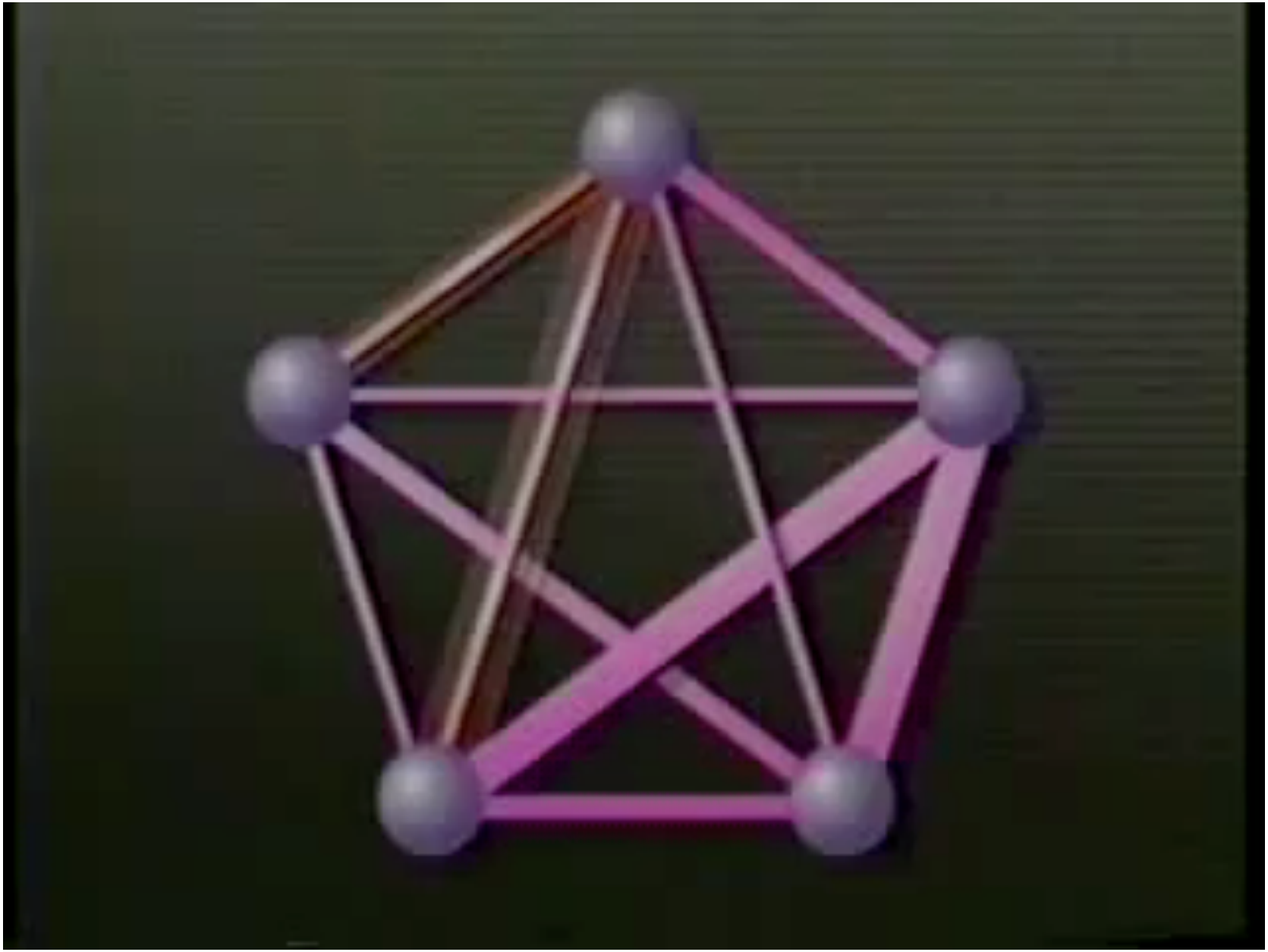
Rosenblatt Perceptron

FIRST IMPLEMENTATION OF NEURAL NETWORK [Rosenblatt, **1957!**]

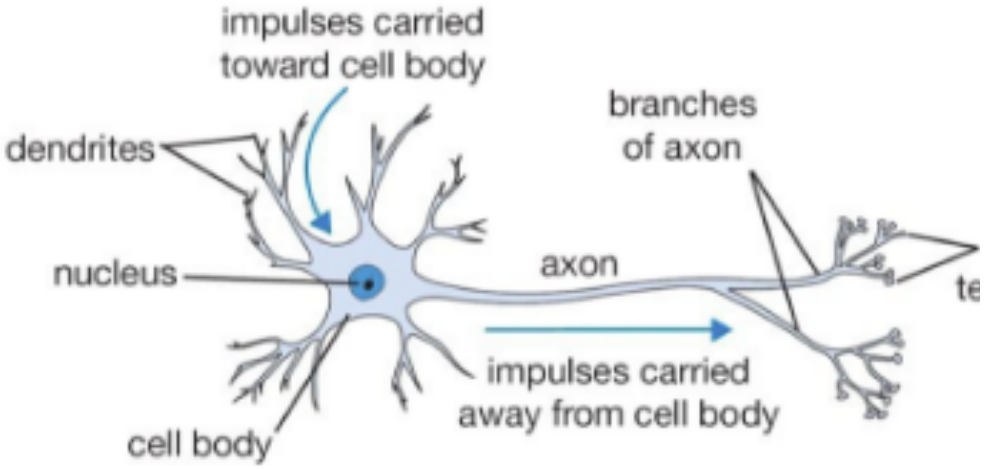
INTENDED TO BE A MACHINE (NOT AN ALGORITHM)



it had an array of 400 photocells, randomly connected to the "neurons". Weights were encoded in potentiometers, and weight updates during learning were performed by electric motors



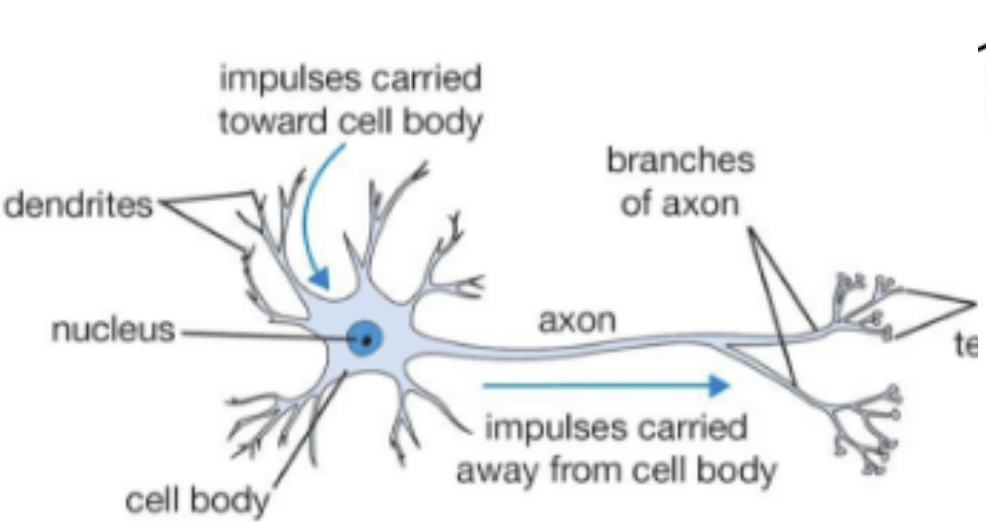
THE NEURON

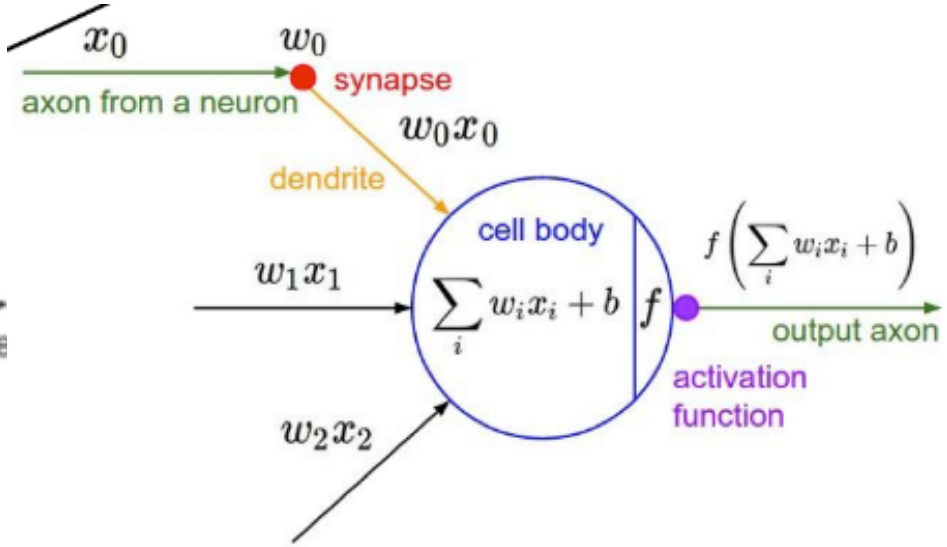


INSPIRED BY NEURO - SCIENCE?

Credit: Karpathy

THE NEURON

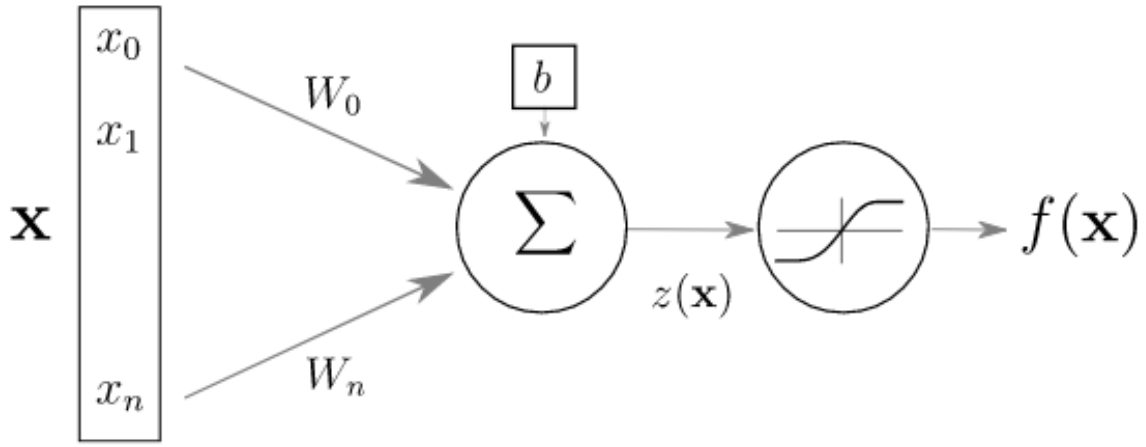




INSPIRED BY NEURO - SCIENCE?

Credit: Karpathy

TODAY'S ARTIFICIAL NEURON



$$z(\vec{x}) = \vec{W}.\vec{x} + b \qquad f(\vec{x}) = g(\vec{W}.\vec{x} + b)$$

Pre-Activation

Weights

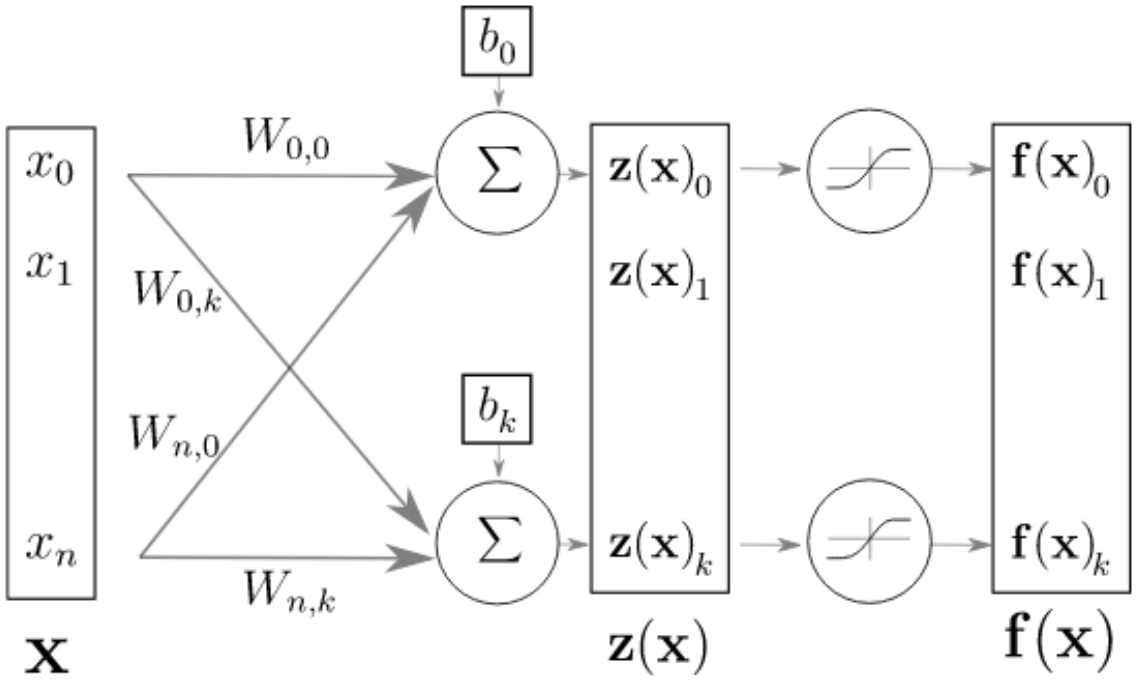
Input

Bias

Output

Activation Function

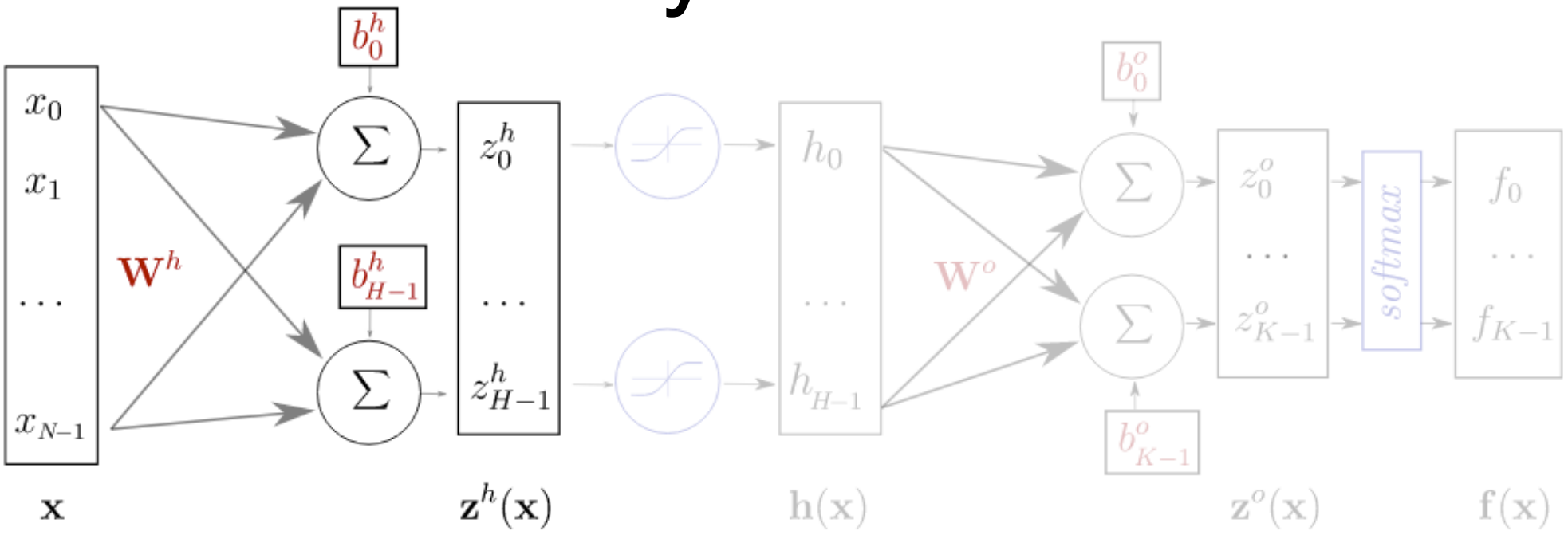
LAYER OF NEURONS



$$f(\vec{x}) = g(\mathbf{W}.\vec{x} + \vec{b})$$

SAME IDEA. NOW **W** becomes a matrix and **b** a vector

Hidden Layers of Neurons

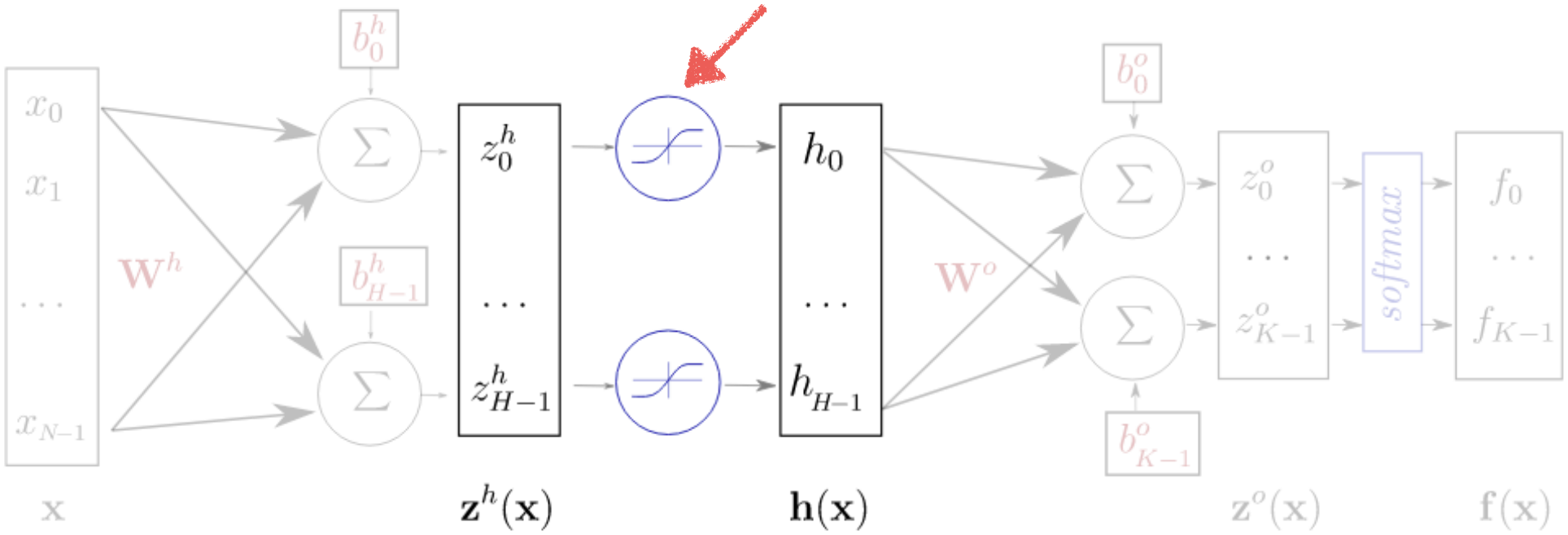


FIRST LAYER

INPUT

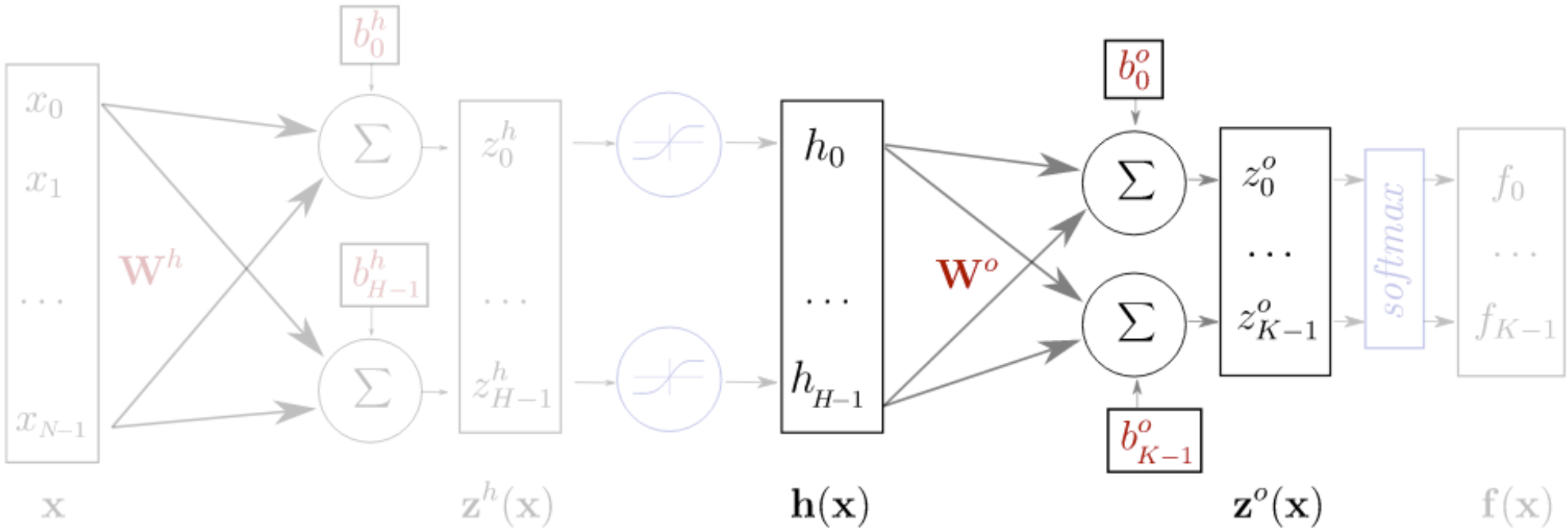
$$z^h(x) = W^h x + b^h$$

ACTIVATION FUNCTION



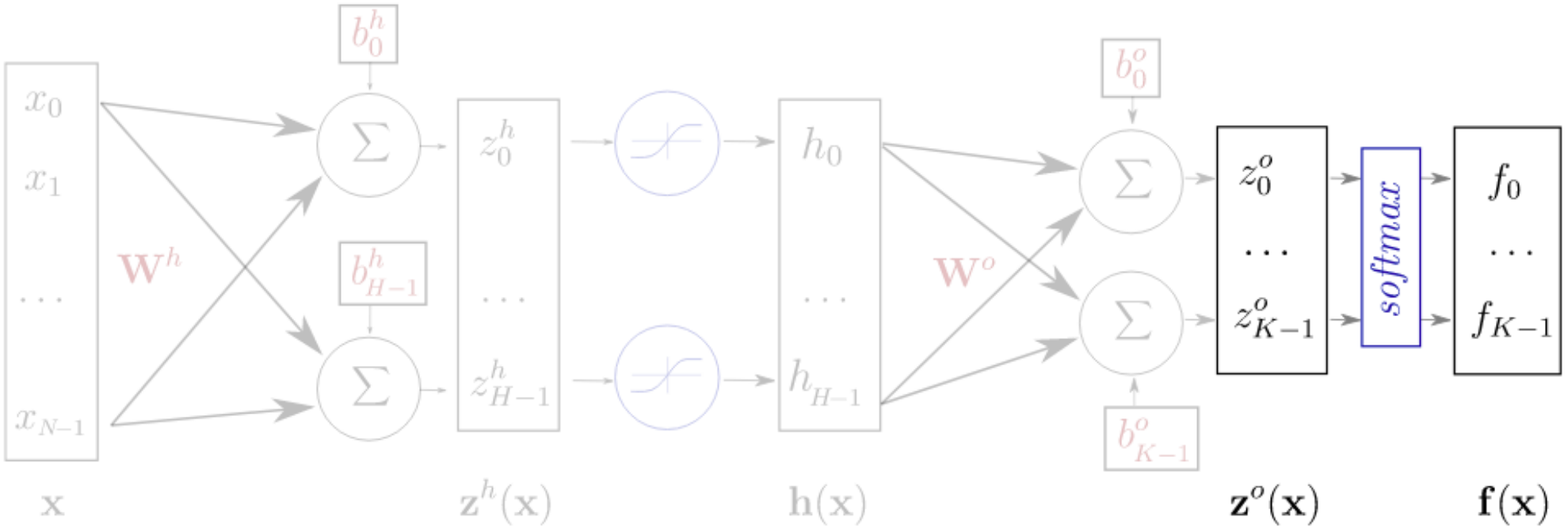
HIDDEN LAYER

$$h(x) = g(z^h(x)) = g(W^h x + b^h)$$



OUTPUT LAYER

$$z^0(\mathbf{x}) = W^0 h(\mathbf{x}) + b^0$$



PREDICTION LAYER

$$f(\mathbf{x}) = softmax(\mathbf{z^0})$$

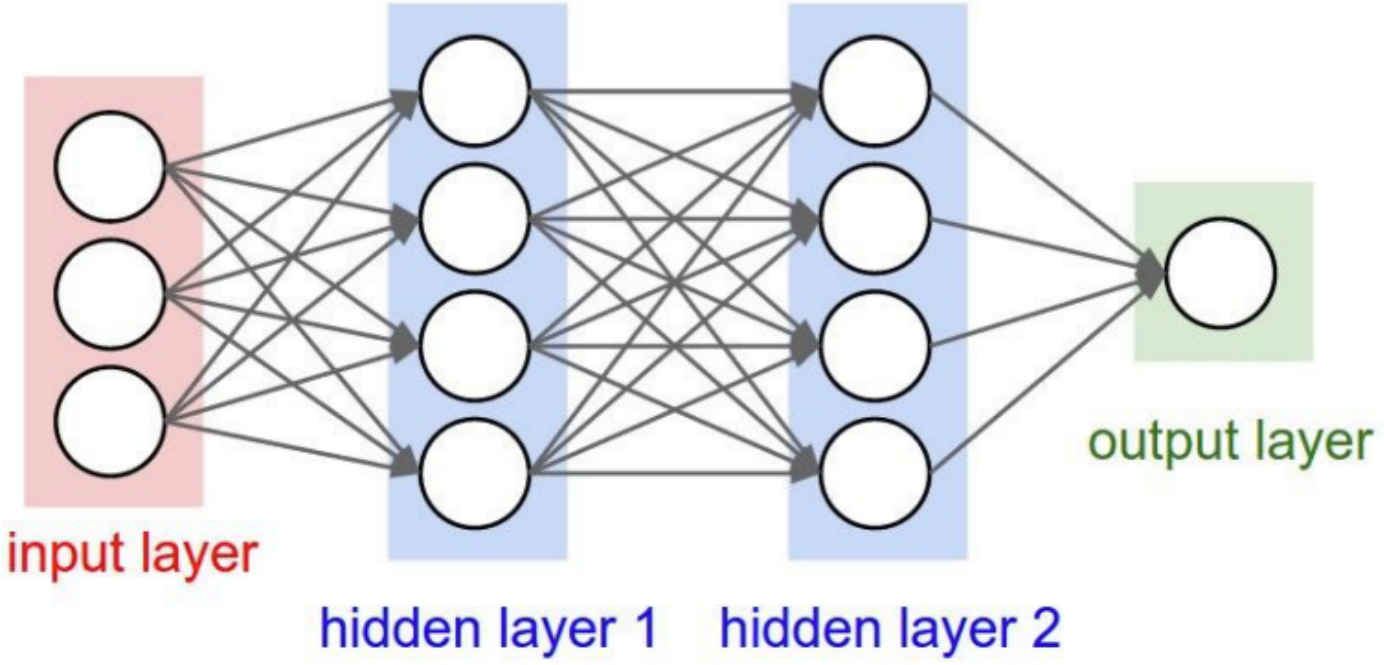
“CLASSICAL” MACHINE LEARNING

$$f_{\vec{W}}(\vec{x}) = \vec{y}$$

LABEL

Q , SF

REPLACE THIS BY A GENERAL NON LINEAR FUNCTION WITH SOME PARAMETERS W



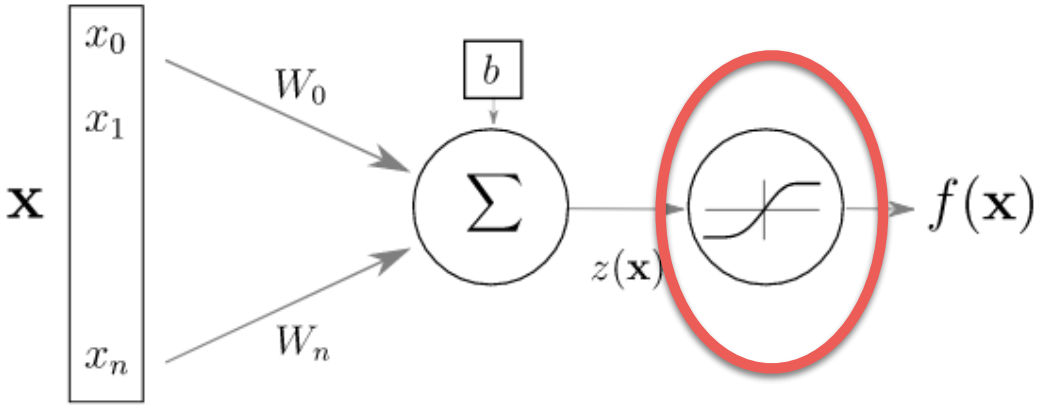
$$p = g_3(W_3 g_2(W_2 g_1(W_1 \vec{x}_0)))$$

NETWORK FUNCTION

SO LET’S GO DEEPER AND DEEPER!

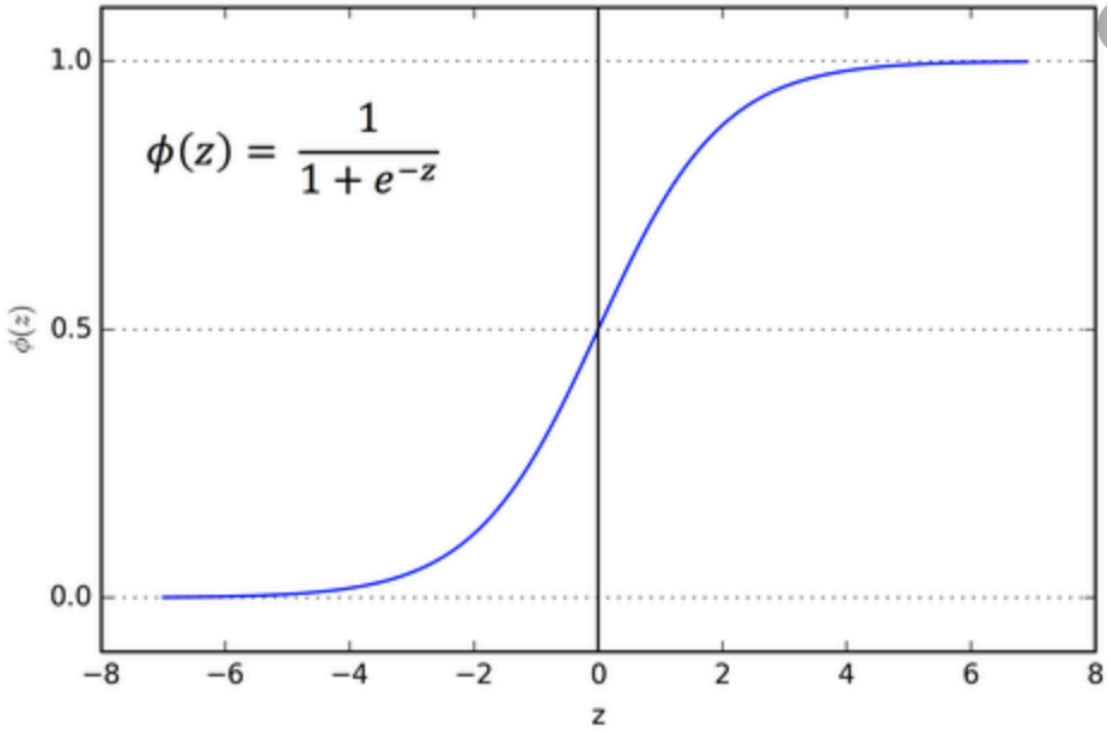
LET’S FIRST EXAMINE IN MORE DETAIL HOW SIMPLE “SHALLOW” NETWORKS WORK

ACTIVATION FUNCTIONS?

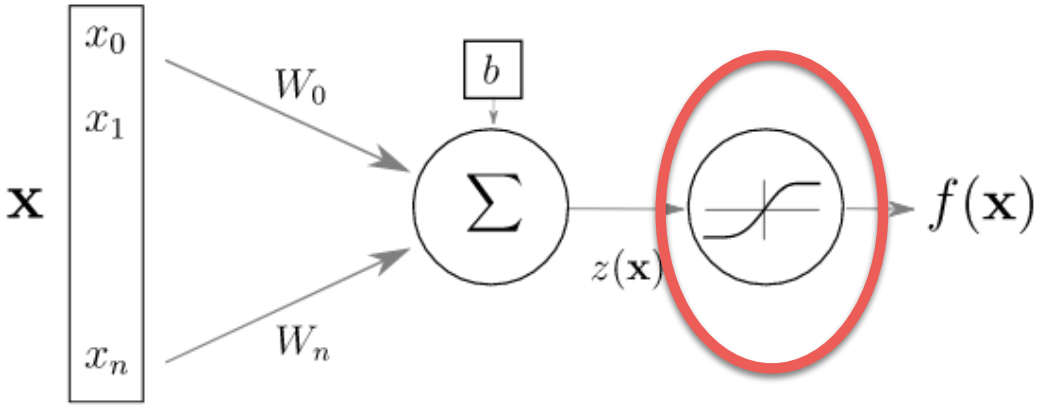


ADD NON LINEARITIES TO THE PROCESS

ACTIVATION FUNCTIONS?

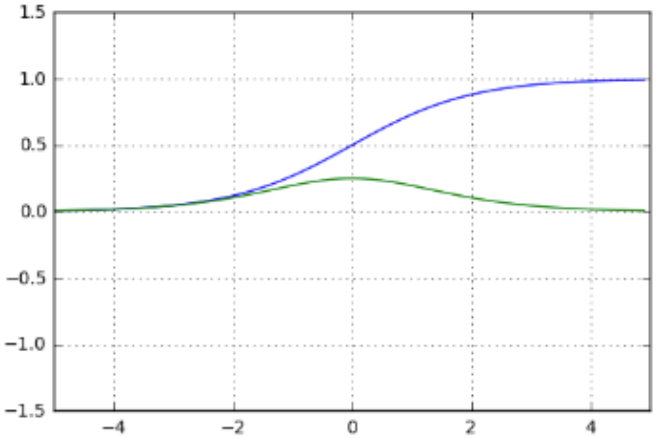


the sigmoid function



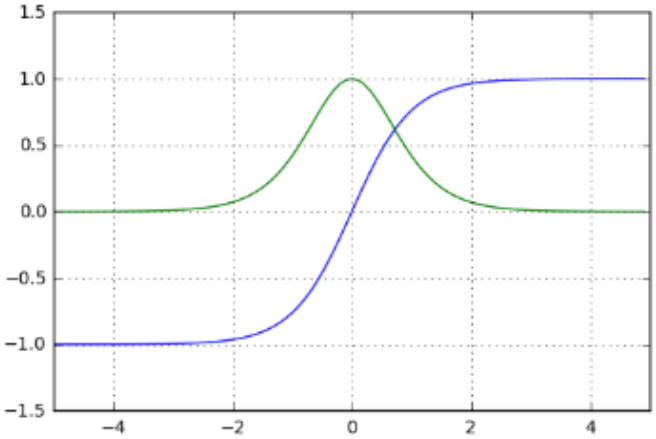
ADD NON LINEARITIES TO THE PROCESS

ACTIVATION FUNCTIONS



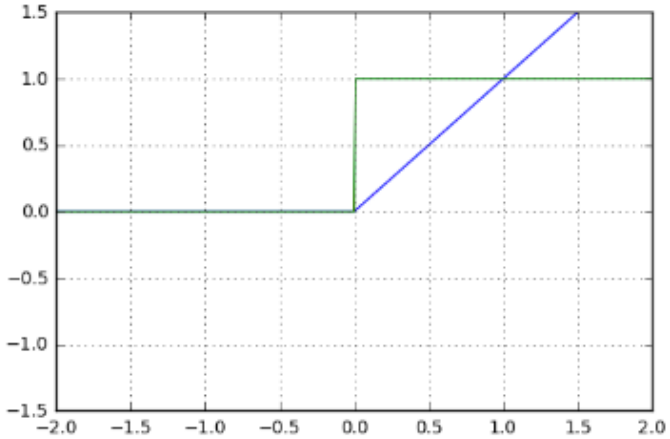
$$\text{sigm}(x) = \frac{1}{1+e^{-x}}$$

$$\text{sigm}'(x) = \text{sigm}(x)(1-\text{sigm}(x))$$



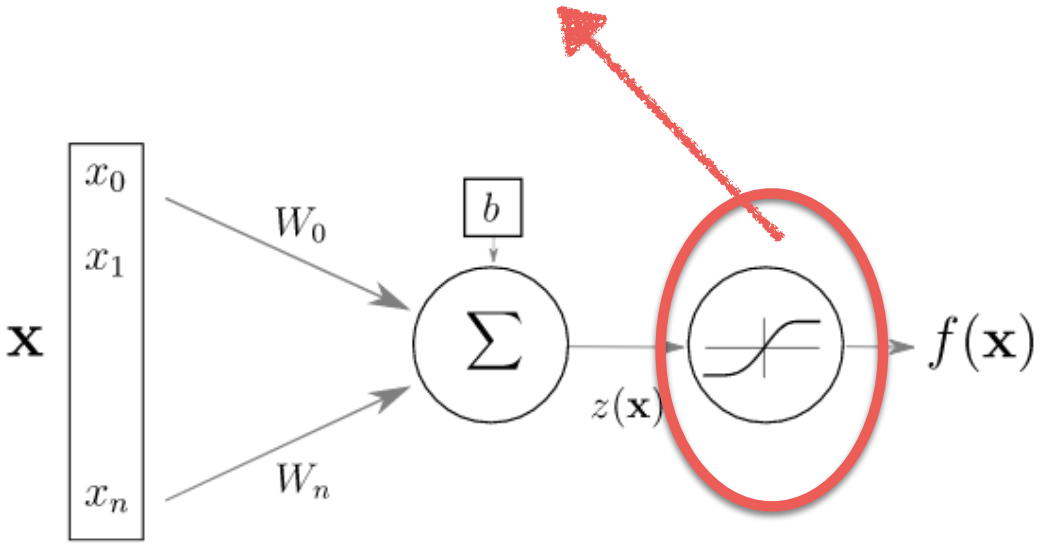
$$\tanh(x) = \frac{e^{2x}-1}{e^{2x}+1}$$

$$\tanh'(x) = 1-\tanh(x)^2$$



$$\text{relu}(x) = \max(0,x)$$

$$\text{relu}'(x) = 1_{x>0}$$



GO HERE:

https://github.com/mhuertascompany/Saas-Fee/blob/main/hands-on/session1/hello_ANN.ipynb

REMEMBER WE NEED A LOSS FUNCTION …

REMEMBER WE NEED A LOSS FUNCTION …

LET’S SART WITH A SIMPLE CLASSIFICATION PROI

BINARY CLASSIFICATION LOSS

WE TYPICALLY USE THE BINARY CROSS-ENTROPY LOSS:

$$H_p(q) = -\frac{1}{N}\sum_{i=1}^{N} y_i.log(p(y_i)) + (1-y_i).log(1-p(y_i))$$

NUMBER
F TRAINING EXAMPLES

GROUND TRUTH

NETWORK OUTPUT
(SIGMOID)

GROUND TRUTH

NETWORK OUTPUT
(SIGMOID)

BINARY CLASSIFICATION LOSS

WE MINIMIZE THE CROSS ENTROPY BETWEEN THE TRUE [q(y)] AND PREDICTED [p(y)] DISTRIBUTIONS

$$H_p(q) = -\frac{1}{N}\sum_{i=1}^{N} y_i.log(p(y_i)) + (1-y_i).log(1-p(y_i))$$

NUMBER
F TRAINING EXAMPLES

GROUND TRUTH

NETWORK OUTPUT (SIGMOID)

GROUND TRUTH

NETWORK OUTPUT (SIGMOID)

NEURAL NETWORKS AS STATISTICAL MODELS

Let's have a look at the "binary cross-entropy loss". Where does it come from?

$$H_p(q) = -\frac{1}{N}\sum_{i=1}^{N} y_i.log(p(y_i)) + (1-y_i).log(1-p(y_i))$$

GROUND TRUTH

NETWORK OUTPUT (SOFTMAX)

GROUND TRUTH

NETWORK OUTPUT (SOFTMAX)

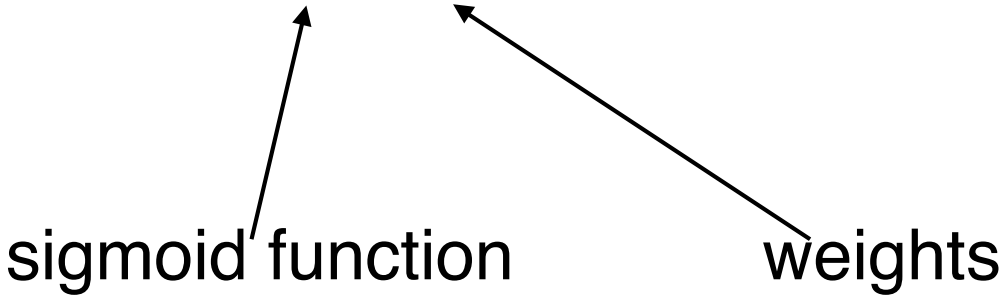
we have a set of independent realizations:

$$(x_i, y_i); i = 1, ..., N$$

and want to find the underlying probability distribution of y given x:

Since y can only take 0 / 1 values, we assume it can be parametrized with a Bernouilli distribution:

$$P(y_i = 0|x_i) = 1 - sigm(f_w(x_i)) \qquad P(y_i = 1|x_i) = sigm(f_w(x_i))$$



So the goal is to find the values of w (weights) that generate a Bernouilli distribution for y given a set of N independent observations

This can be achieved via Maximum Likelihood estimation:

The likelihood of a given observation under the Bernouilli assumption can be written as:

$$L(w; x_i, y_i) = [sigm(f_w(x_i))]^{y_i} [1 - sigm(f_w(x_i))]^{1-y_i}$$

which is equal to $[sigm(f_w(x_i))]$ if y=1 and $[1 - sigm(f_w(x_i))]$ if y=0

And the likelihood of the entire sample is the product of the likelihoods:

$$L(w; x_i, y_i) = \prod_{i=1}^{N} [sigm(f_w(x_i))]^{y_i} [1 - sigm(f_w(x_i))]^{1-y_i}$$

So, the log-likelihood:

$$l(w; x_i, y_i) = \sum_{i=1}^{N} y_i \times \log[sigm(f_w(x_i))] + (1 - y_i) \times \log[1 - sigm(f_w(x_i))]$$

EREFORE EQUIVALENT TO THE CROSS-ENTROPY LOSS:

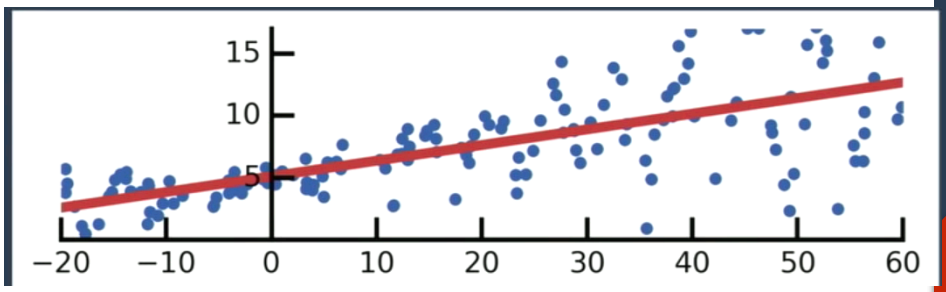
$$l(w; x_i, y_i) = \sum_{i=1}^{N} y_i \times \log[sigm(f_w(x_i))] + (1 - y_i) \times \log[1 - sigm(f_w(x_i))]$$

$$H_p(q) = -\frac{1}{N} \sum_{i=1}^{N} y_i.log(p(y_i)) + (1 - y_i).log(1 - p(y_i))$$

WHEN YOU DO A BINARY CLASSIFICATION WITH NEURAL NETWORKS YOU ARE SIMPLY FINDING THE WEIGHTS OF YOUR MODEL THAT MAXIMIZE THE LIKELIHOOD OF A BERNOUILLI DISTRIBUTION

NOTE THAT SINCE fw IS FIXED (THE ARCHITECTURE), WE FIND A SOLUTION AMONG A POSSIBLE SET OF SOLUTIONS

ıAT ABOUT REGRESSIONS?




```
model = tf.keras.Sequential([
  tf.keras.layers.Dense(hidden_units, ...),
  tf.keras.layers.Dense(1),
])
model.compile(loss=tf.keras.mean_squared_error)
```

WHEN USING THE MEAN SQUARED ERROR, WE ARE ASSUMING THAT THE OUTPUT POINTS FOLLOW A NORMAL DISTRIBUTION. OUR ESTIMATOR IS THEREFORE THE MEAN OF THE NORMAL PDF THAT MAXIMIZES THE LIKELIHOOD.

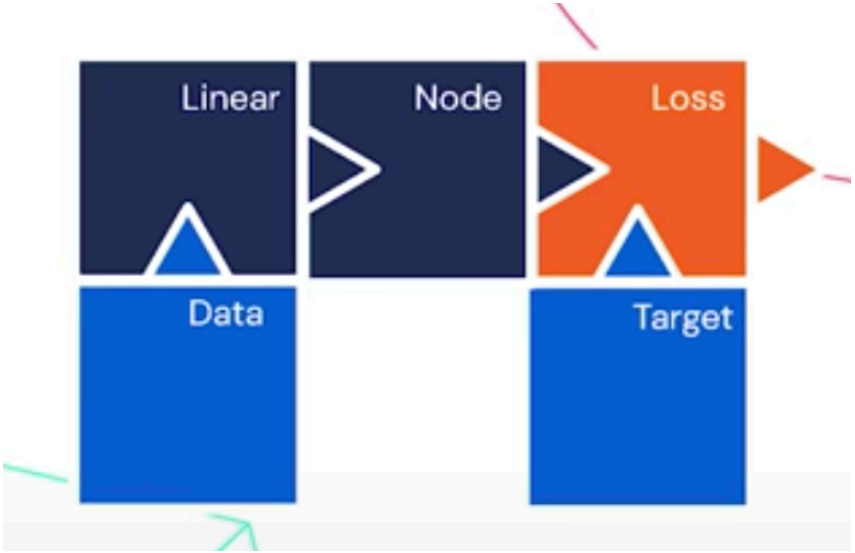
$$L(w, \sigma^2; y, X) = (2\pi\sigma^2)^{-N/2} \exp(-\frac{1}{2\sigma^2} \sum_{i=1}^{N} (y_i - f_w(x_i))^2)$$

weights

neural network

OK, SO NOW WE HAVE THE 3 MAIN INGREDIENTS THAT COMPOSE AN ANN:

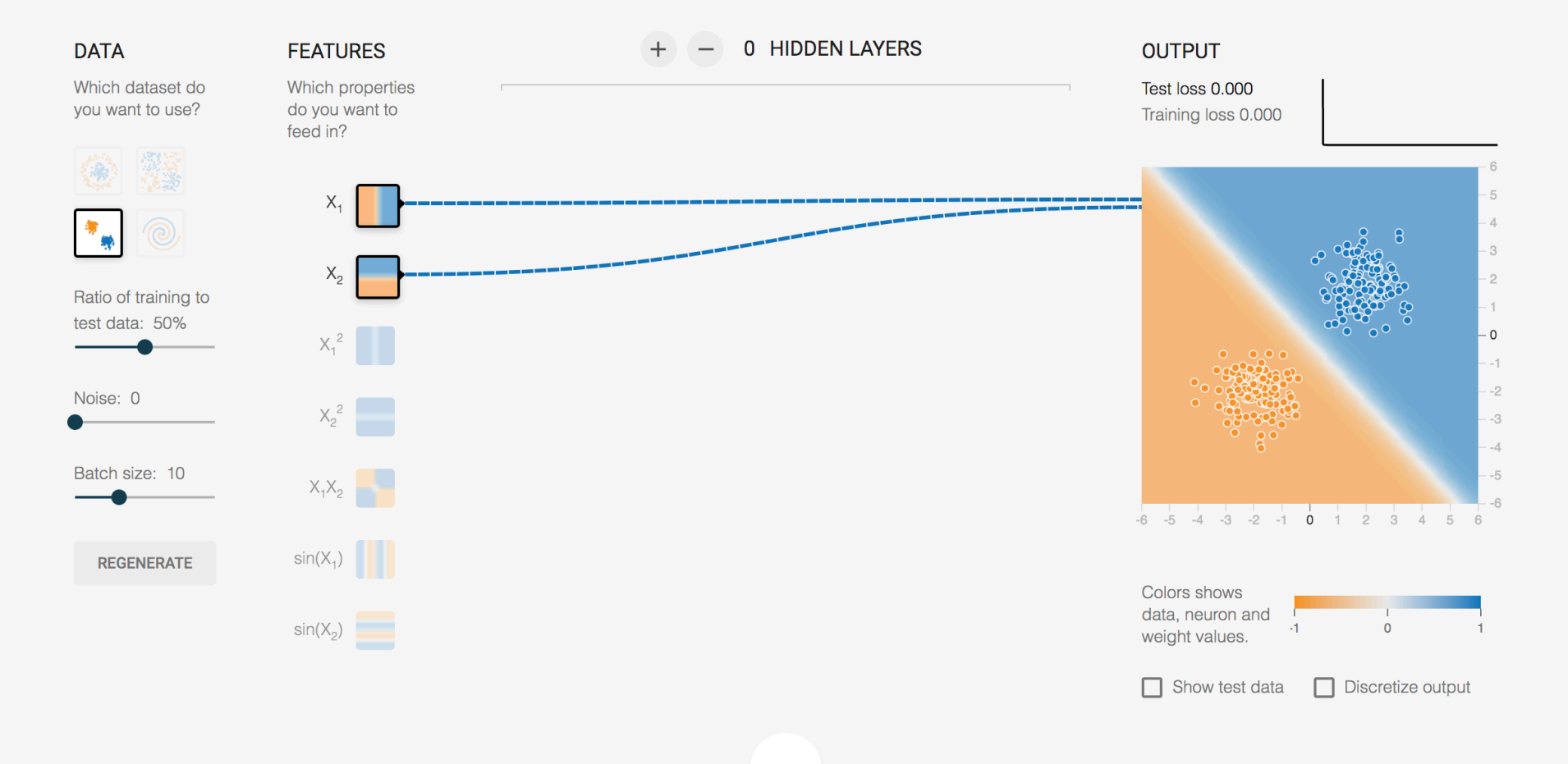
1. LINEAR NEURON OR UNIT
2. NON LINEARITIES (ACTIVATION FUNCTION)
3. LOSS FUNCTION



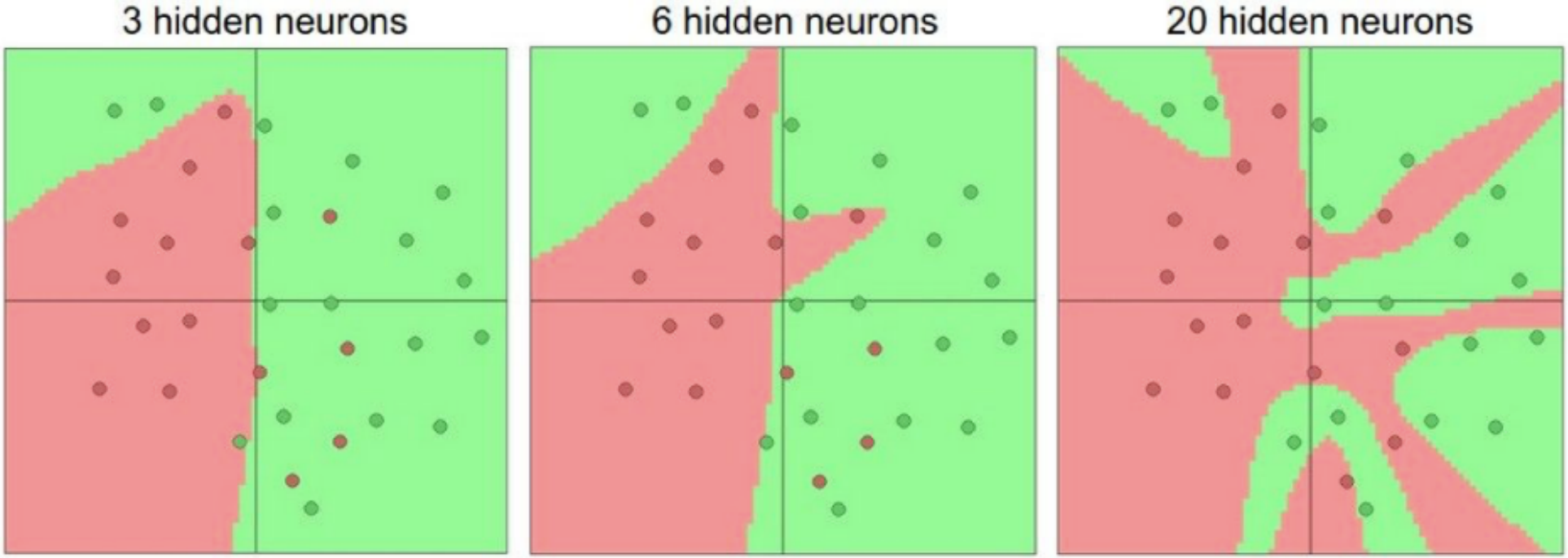
(deepmind @Czarnecki)

LET'S SEE WHAT WE CAN DO WITH THIS SIMPLE MODEL!

https://
playground.tensorflow.org/



HIDDEN LAYERS ALLOW INCREASING COMPLEXITY



More complex functions allow increasing complexity

Credit: Karpathy

UNIVERSAL APPROXIMATION THEOREM

FOR ANY CONTINUOS FUNCTION FOR A HYPERCUBE [0,1]d TO REAL NUMBERS, AND EVERY POSITIVE EPSILON, THERE EXISTS A SIGMOID BASED 1-HIDDEN LAYER NEURAL NETWORK THAT OBTAINS AT MOST EPSILON ERROR IN FUNCTIONAL SPACE

Cybenko+89

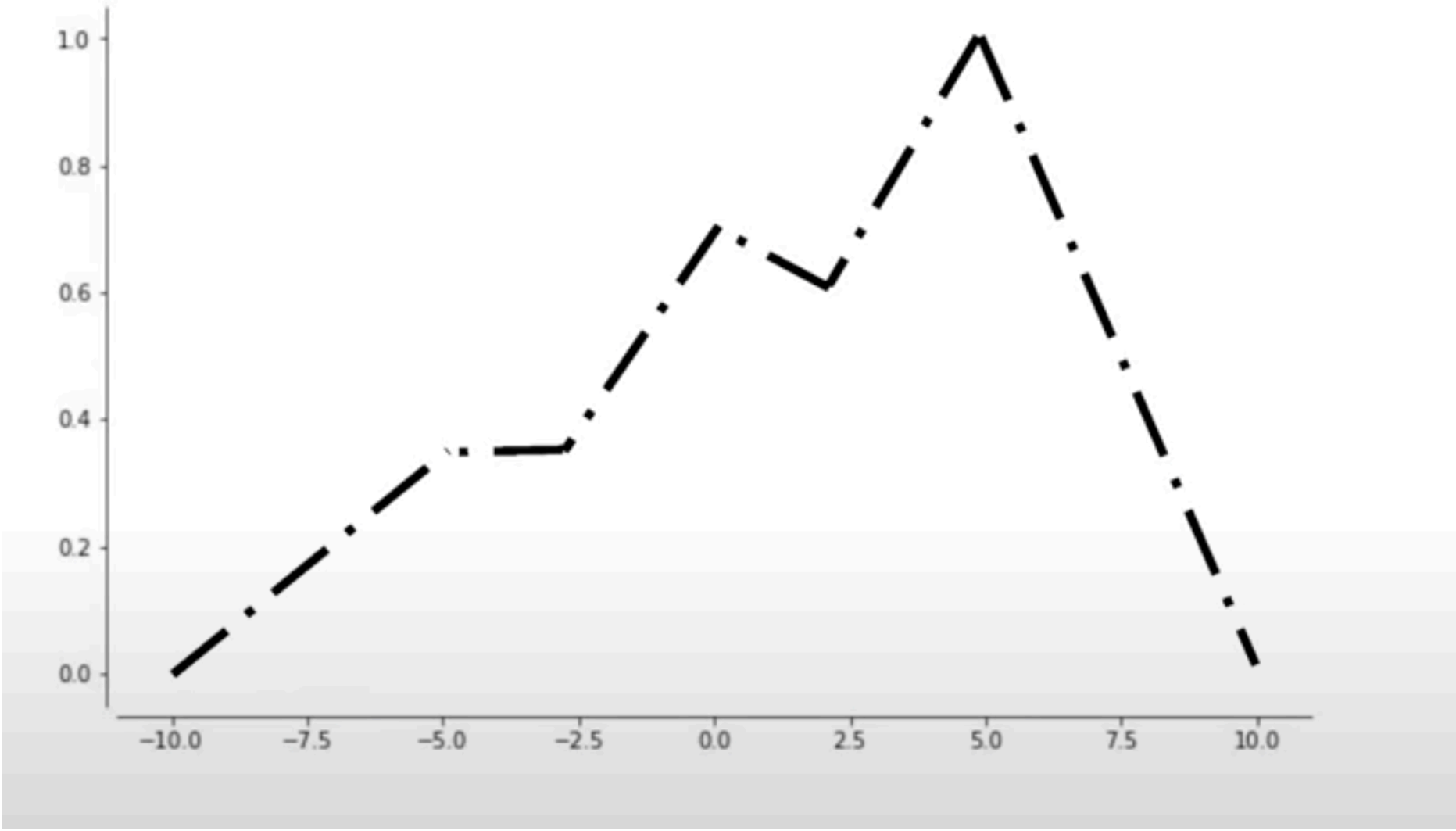
"BIG ENOUGH NETWORK CAN APPROXIMATE, BUT NOT REPRESENT ANY SMOOTH FUNCTION. THE MATH DEMONSTRATION IMPLIES SHOWING THAT NETWORS ARE DENSE IN THE SPACE OF TARGET FUNCTIONS"

UNIVERSAL APPROXIMATION THEOREM

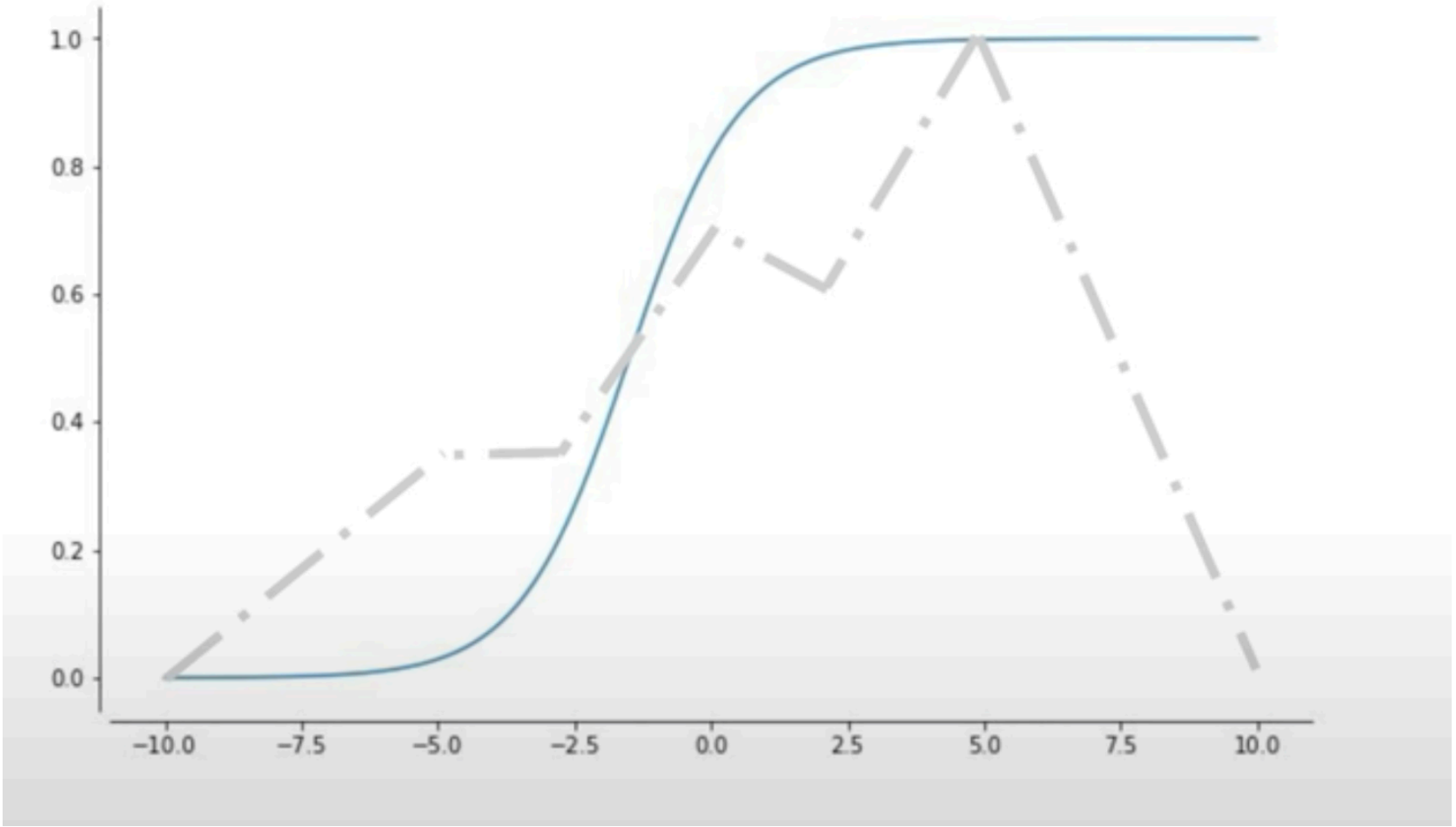
FOR ANY CONTINUOS FUNCTION FOR A HYPERCUBE [0,1]d TO REAL NUMBERS, NON-CONSTANT, BOUNDED AND CONTINUOUS ACTIVATION FUNCTION f, AND EVERY POSITIVE EPSILON, THERE EXISTS A1-HIDDEN LAYER NEURAL NETWORK USING f THAT OBTAINS AT MOST EPSILON ERROR IN FUNCTIONAL SPACE

Horvik+91

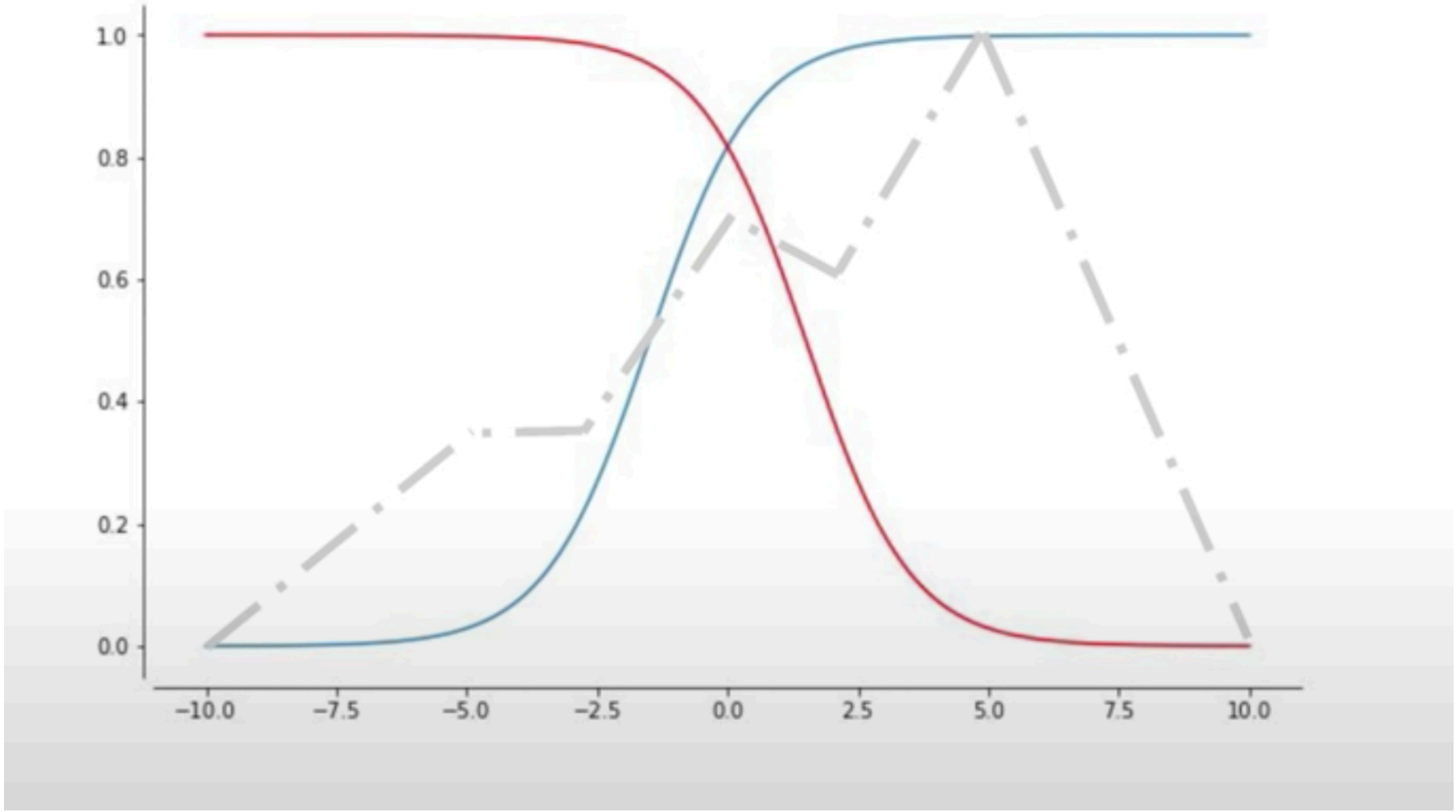
"BIG ENOUGH NETWORK CAN APPROXIMATE, BUT NOT REPRESENT ANY SMOOTH FUNCTION. THE MATH DEMONSTRATION IMPLIES SHOWING THAT NETWORS ARE DENSE IN THE SPACE OF TARGET FUNCTIONS"



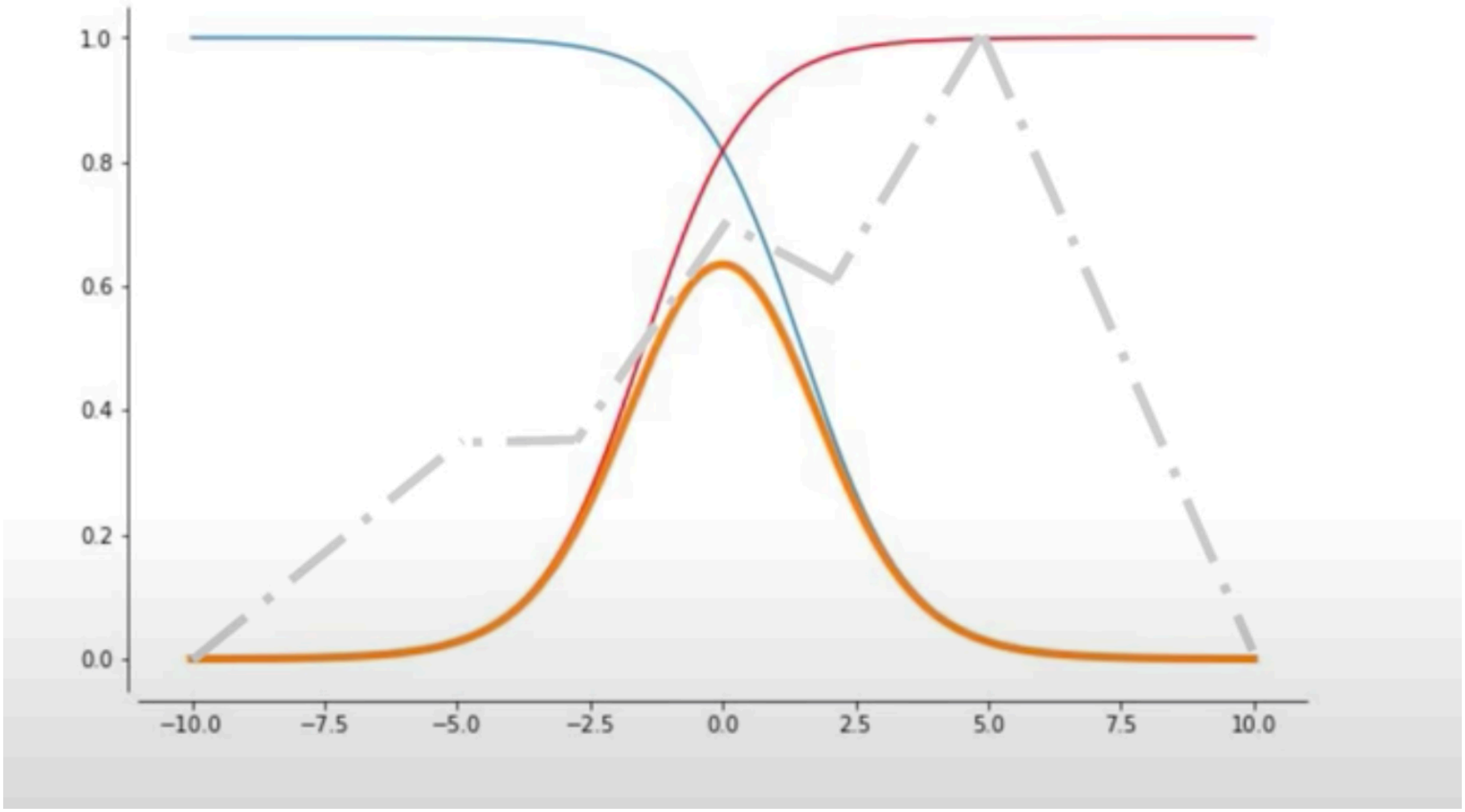
(deepmind @Czarnecki)



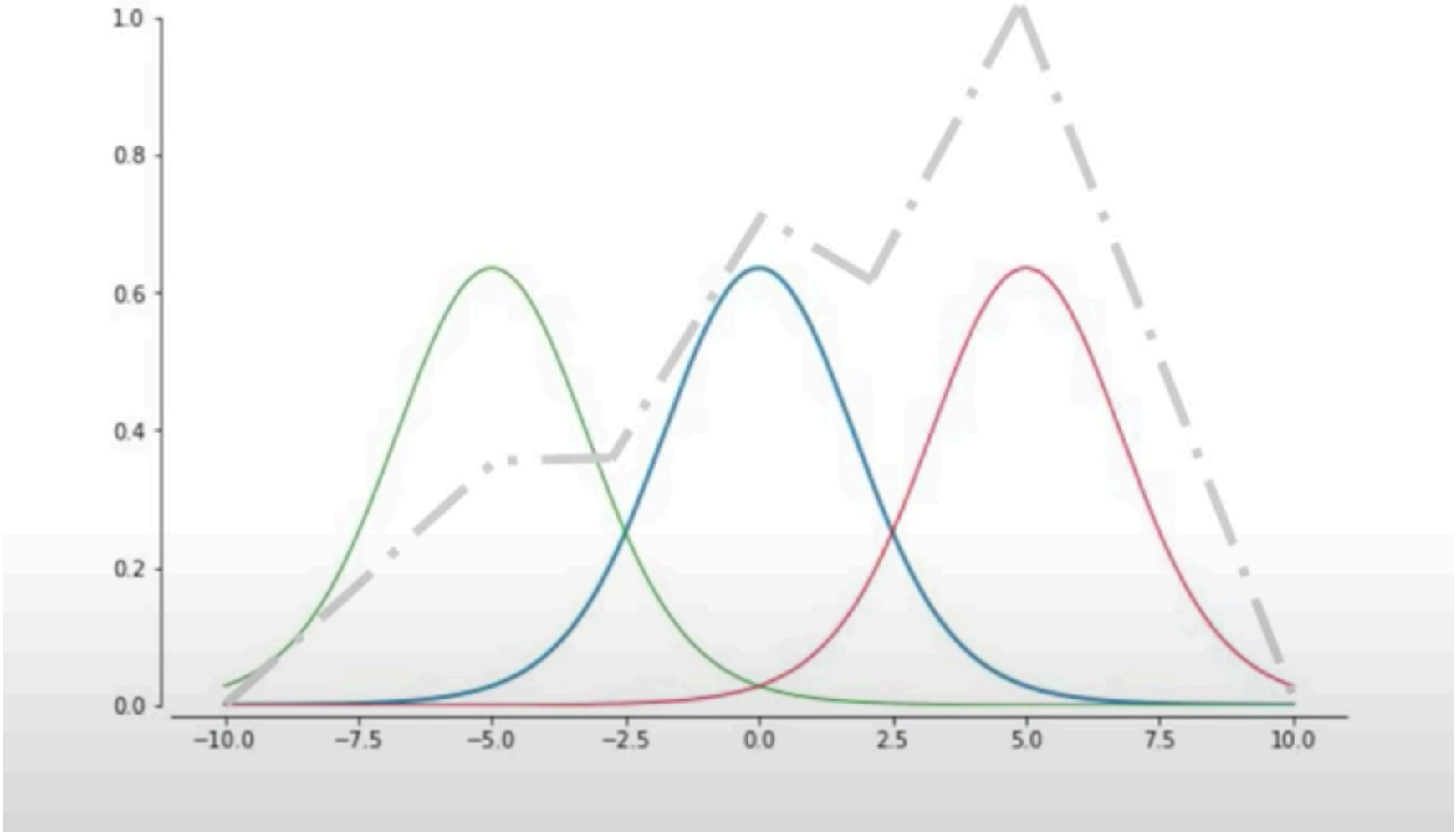
(deepmind
@Czarnecki)



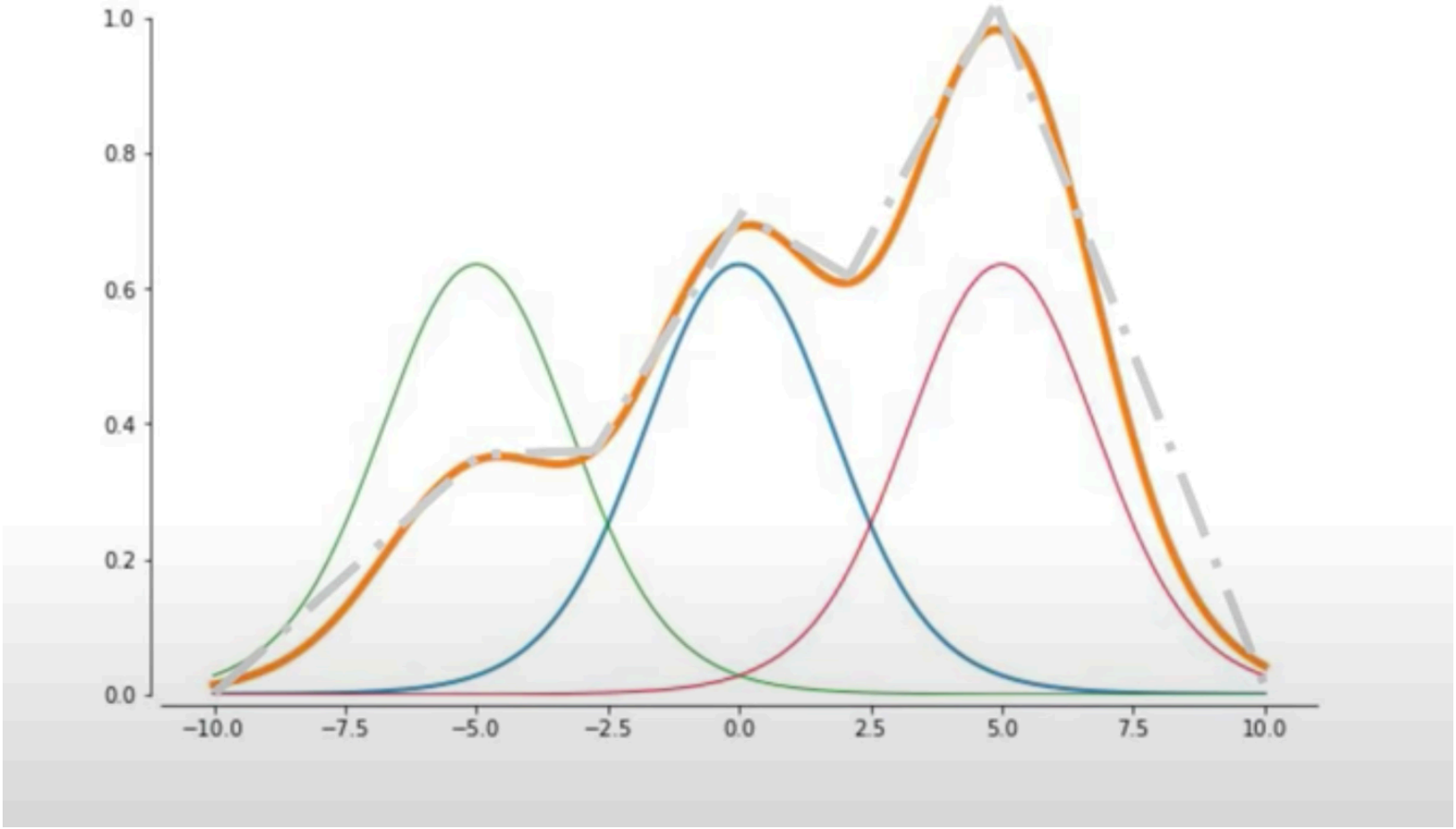
(deepmind
@Czarnecki)



(deepmind
@Czarnecki)

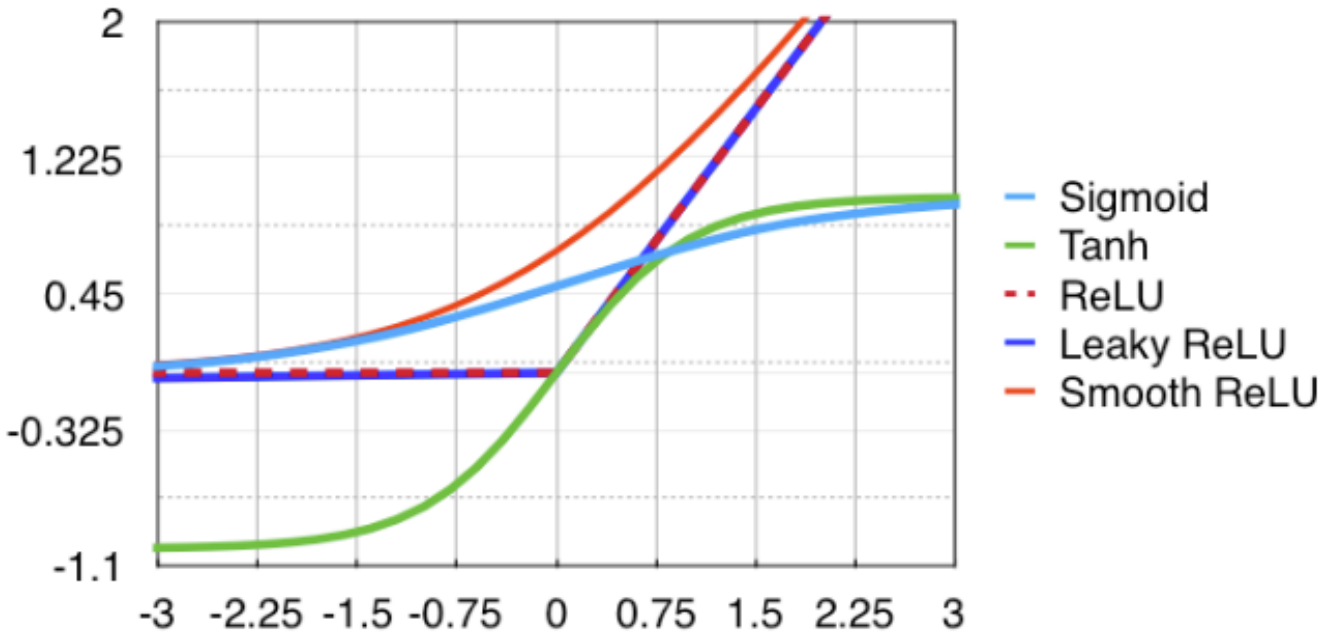


(deepmind
@Czarnecki)



(deepmind
@Czarnecki)

ACTIVATION FUNCTIONS



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

Tanh: $f(x) = tanh(x)$

ReLu: $f(x) = max(0, x)$

Soft ReLu: $f(x) = log(1+e^{x})$

Leaky ReLu: $f(x) = \epsilon x + (1-\epsilon)max(0, x)$

SOFTMAX

A generalization of the SIGMOID ACTIVATION

$$softmax(\mathbf{x}) = \frac{e^{\mathbf{x}}}{\sum_{i=1}^{n} e^{x_i}}$$

THE OUTPUT IS NORMALIZED BETWEEN 0 AND 1

THE COMPONENTS ADD TO 1

CAN BE INTERPRETED AS A PROBABILITY

$$p(Y = c|X = \mathbf{x}) = softmax(z(\mathbf{x}))_c$$

SO LET’S GO DEEPER AND DEEPER!

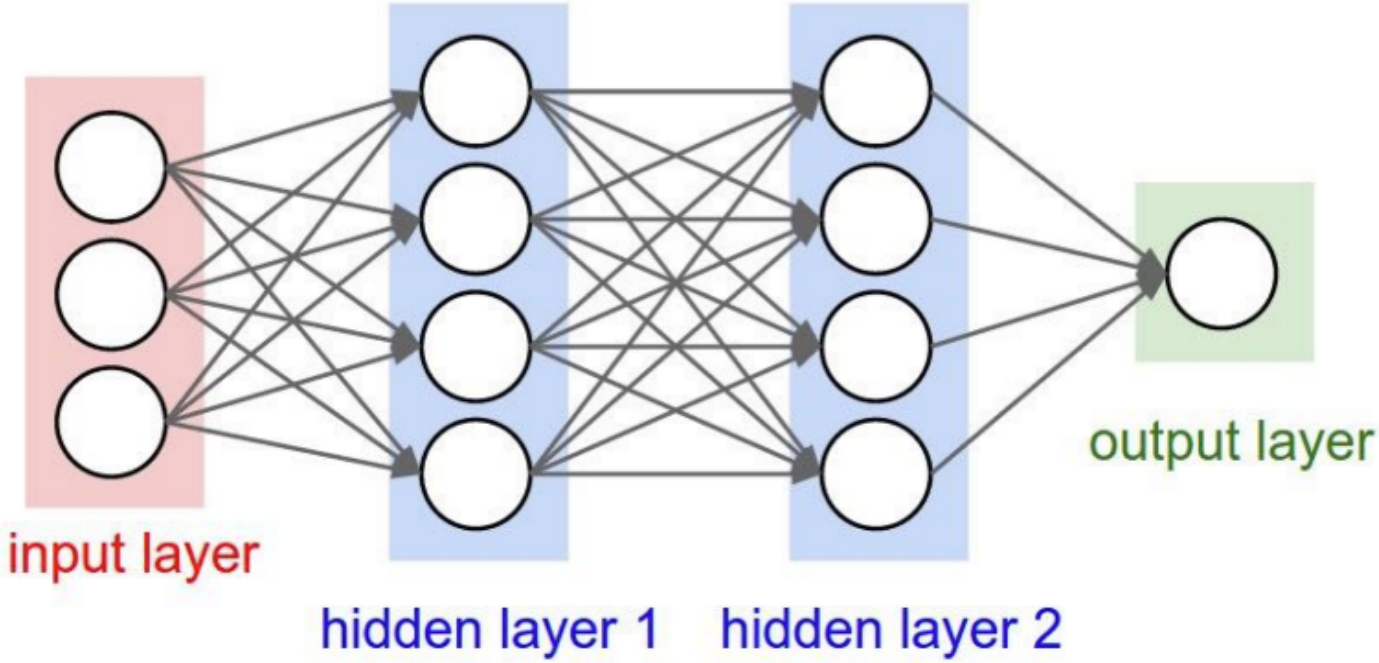
YES BUT…

NOT SO STRAIGHTFORWARD, DEEPER MEANS MORE WEIGHTS, MORE DIFFICULT OPTIMIZATION, RISK OF OVERFITTING…

OK, SO NOW LET’S FIND THE WEIGHTS

OPTIMIZATION

[OR HOW TO FIND THE WEIGHTS?]

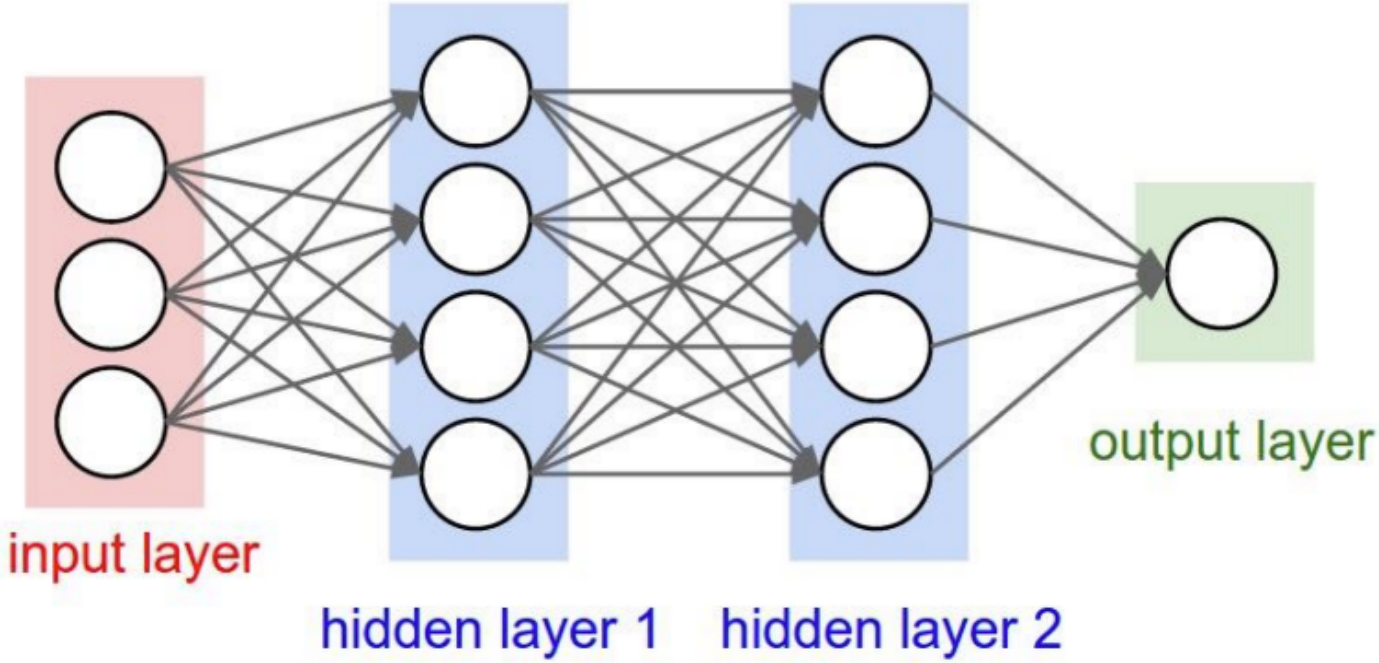


$$p = g_3(W_3 g_2(W_2 g_1(W_1 \vec{x_0})))$$

NETWORK FUNCTION

OPTIMIZATION

[OR HOW TO FIND THE WEIGHTS?]



$$p = g_3(W_3 g_2(W_2 g_1(W_1 \vec{x_0})))$$

$$\frac{1}{N}\sum_{i=1}^{N}(y_i - p_i)^2$$

LOSS FUNCTION

WE SIMPLY WANT TO MINIMIZE THE LOSS FUNCTION WITH RESPECT TO THE WEIGHTS, i.e. FIND THE WEIGHTS THAT GENERATE THE MINIMUM LOSS

WE SIMPLY WANT TO MINIMIZE THE LOSS FUNCTION WITH RESPECT TO THE WEIGHTS, i.e. FIND THE WEIGHTS THAT GENERATE THE MINIMUM LOSS

WE THEN USE STANDARD MINIMIZATION ALGORITHMS THAT YOU ALL KNOW…

FOR EXAMPLE….

Gradient Descent

$$W_{t+1} = W_t - \lambda_t \nabla f(W_t)$$

[gradient]

Newton

$$W_{t+1} = W_t - \lambda [Hf(W_t)]^{-1} \nabla f(W_t)$$

[hessian]

NEWTON CONVERGES FASTER…

FOR EXAMPLE….

Gradient Descent

$$W_{t+1} = W_t - \lambda_t \nabla f(W_t)$$

[gradient]

Newton

$$W_{t+1} = W_t - \lambda [Hf(W_t)]^{-1} \nabla f(W_t)$$

[hessian]

NEWTON CONVERGES FASTER…

BUT NEEDS THE HESSIAN

$$\mathbf{H} = \begin{bmatrix} \frac{\partial^2 f}{\partial W_1^2} & \frac{\partial^2 f}{\partial W_1 \, \partial W_2} & \cdots & \frac{\partial^2 f}{\partial W_1 \, \partial W_n} \\ \frac{\partial^2 f}{\partial W_2 \, \partial W_1} & \frac{\partial^2 f}{\partial W_2^2} & \cdots & \frac{\partial^2 f}{\partial W_2 \, \partial W_n} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial^2 f}{\partial W_n \, \partial W_1} & \frac{\partial^2 f}{\partial W_n \, \partial W_2} & \cdots & \frac{\partial^2 f}{\partial W_n^2} \end{bmatrix}$$

FOR EXAMPLE….

Gradient Descent

$$W_{t+1} = W_t - \lambda_t \nabla f(W_t)$$

[gradient]

Newton

$$W_{t+1} = W_t - \lambda [Hf(W_t)]^{-1} \nabla f(W_t)$$

[hessian]

NEWTON CONVERGES FASTER…

BUT NEEDS THE HESSIAN

MOST USED BY FAR….

$$\mathbf{H} = \begin{bmatrix} \frac{\partial^2 f}{\partial W_1^2} & \frac{\partial^2 f}{\partial W_1 \partial W_2} & \cdots & \frac{\partial^2 f}{\partial W_1 \partial W_n} \\ \frac{\partial^2 f}{\partial W_2 \partial W_1} & \frac{\partial^2 f}{\partial W_2^2} & \cdots & \frac{\partial^2 f}{\partial W_2 \partial W_n} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial^2 f}{\partial W_n \partial W_1} & \frac{\partial^2 f}{\partial W_n \partial W_2} & \cdots & \frac{\partial^2 f}{\partial W_n^2} \end{bmatrix}$$

FOR EXAMPLE….

Gradient Descent

$$W_{t+1} = W_t - \lambda_t \nabla f(W_t)$$

[gradient]

EVERYTHING RELIES
ON COMPUTING THE GRADIENT

MOST USED BY FAR….

Newton

$$W_{t+1} = W_t - \lambda [Hf(W_t)]^{-1} \nabla f(W_t)$$

[hessian]

NEWTON CONVERGES FASTER…

BUT NEEDS THE HESSIAN

$$\mathbf{H} = \begin{bmatrix} \frac{\partial^2 f}{\partial W_1^2} & \frac{\partial^2 f}{\partial W_1 \partial W_2} & \cdots & \frac{\partial^2 f}{\partial W_1 \partial W_n} \\ \frac{\partial^2 f}{\partial W_2 \partial W_1} & \frac{\partial^2 f}{\partial W_2^2} & \cdots & \frac{\partial^2 f}{\partial W_2 \partial W_n} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial^2 f}{\partial W_n \partial W_1} & \frac{\partial^2 f}{\partial W_n \partial W_2} & \cdots & \frac{\partial^2 f}{\partial W_n^2} \end{bmatrix}$$

NICE, BUT I NEED TO COMPUTE TE GRADIENT AT EVERY ITERATION OF AN ARBITRARY COMPLEX FUNCTION!