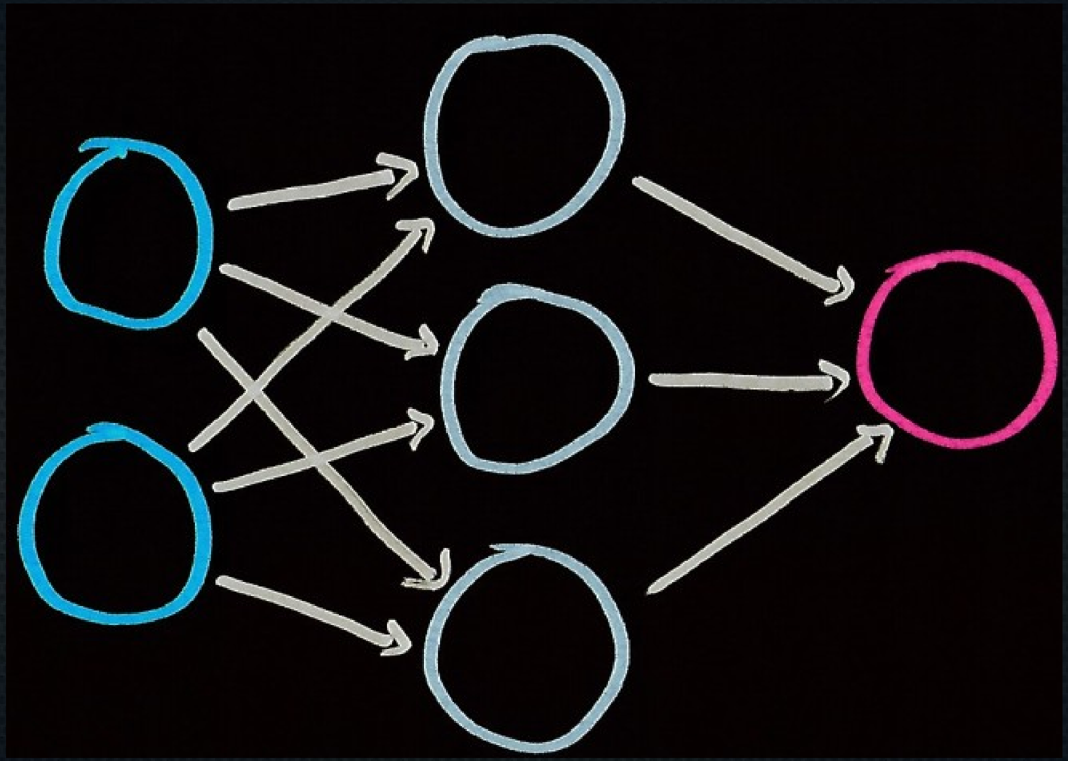
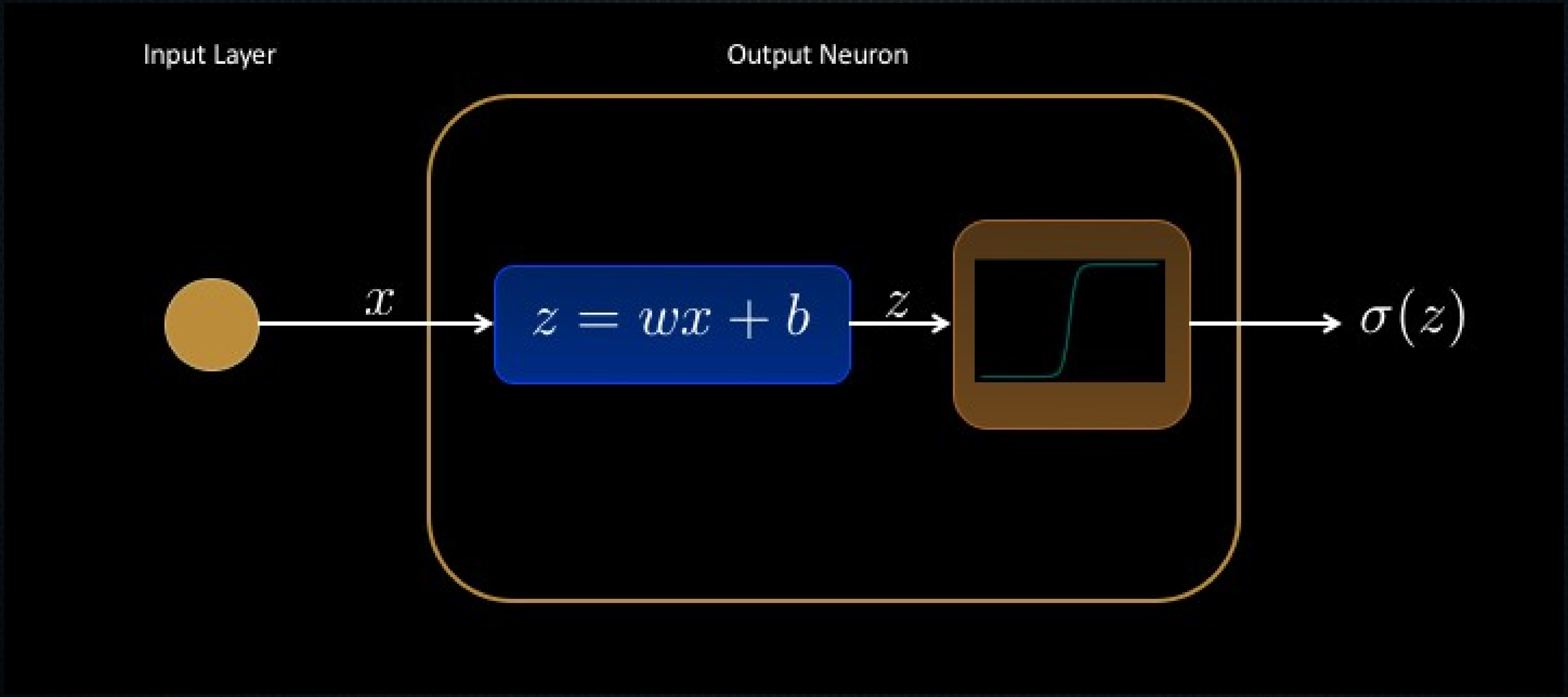
Switching gears: neural networks



Source: https://thesharperdev.com/build-your-first-neural-network-part-2/

What do neural nets have to do with logistic regression?

- A single neuron is a logistic regressor!*



Source: https://thedatafrog.com/en/articles/logistic-regression/

*Given sigmoid activation function (which is not current standard practice anymore, but was at first)

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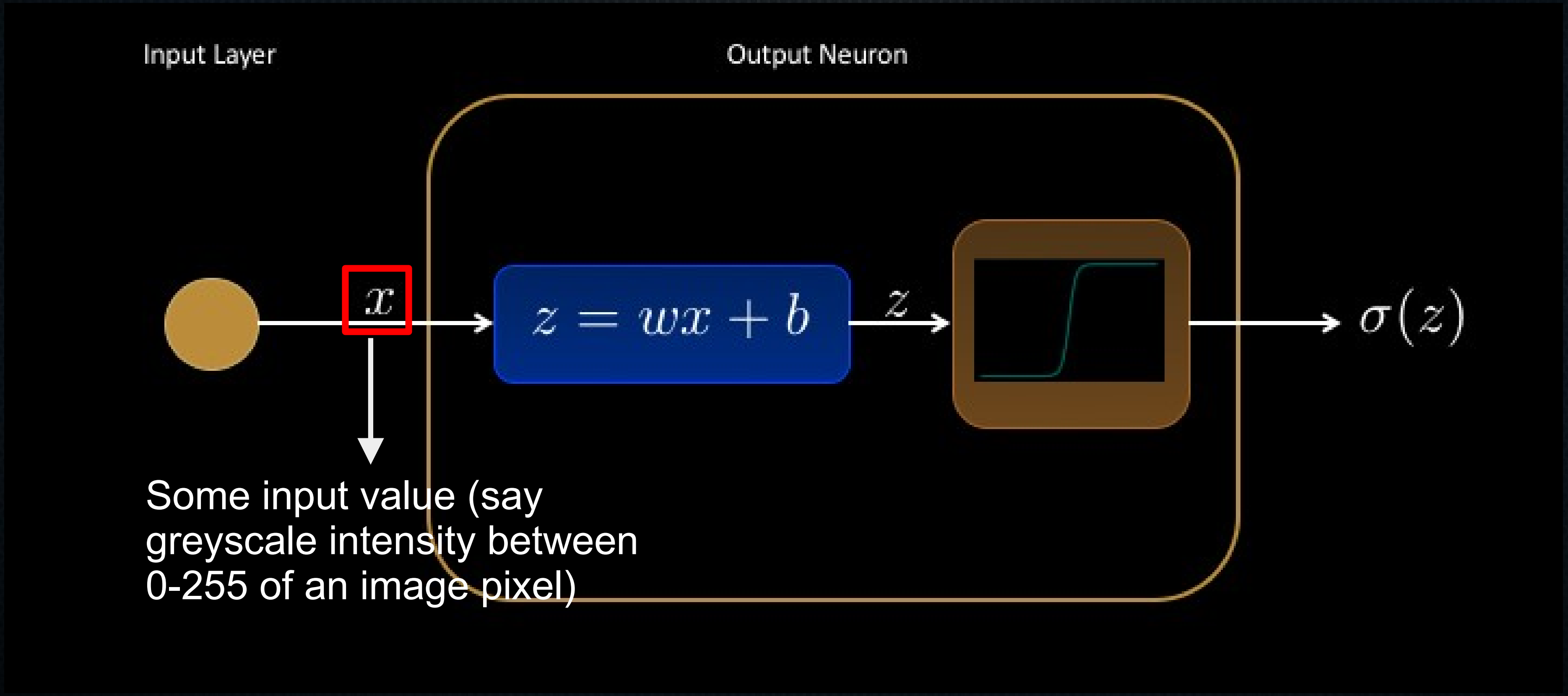

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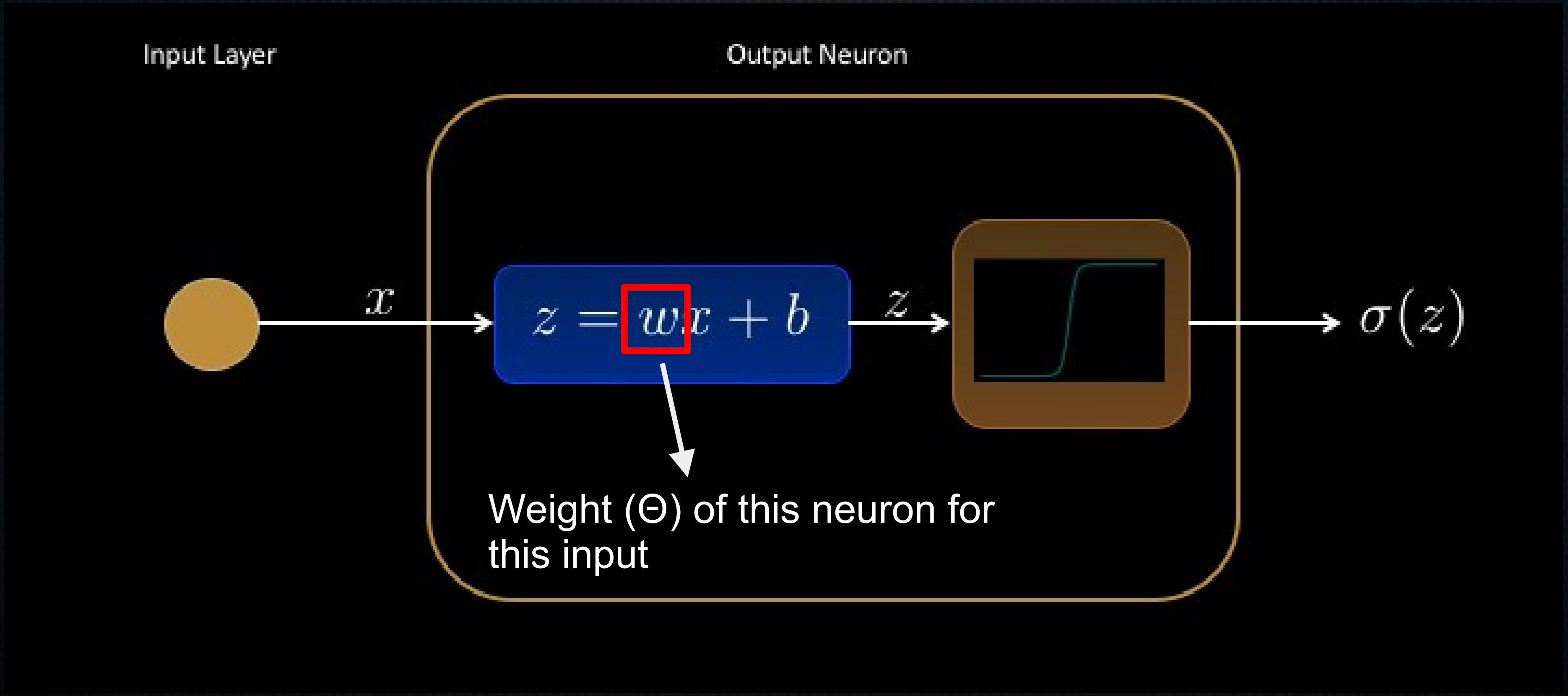

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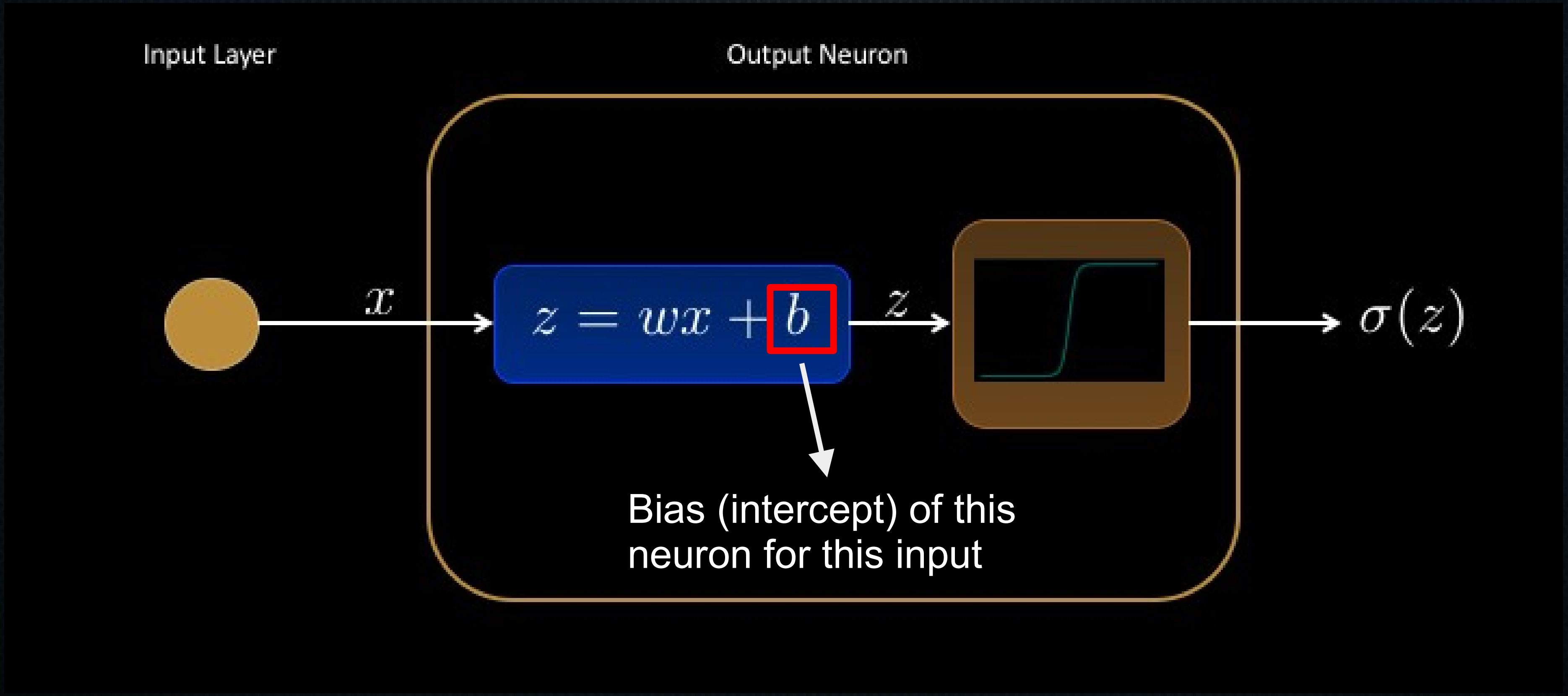

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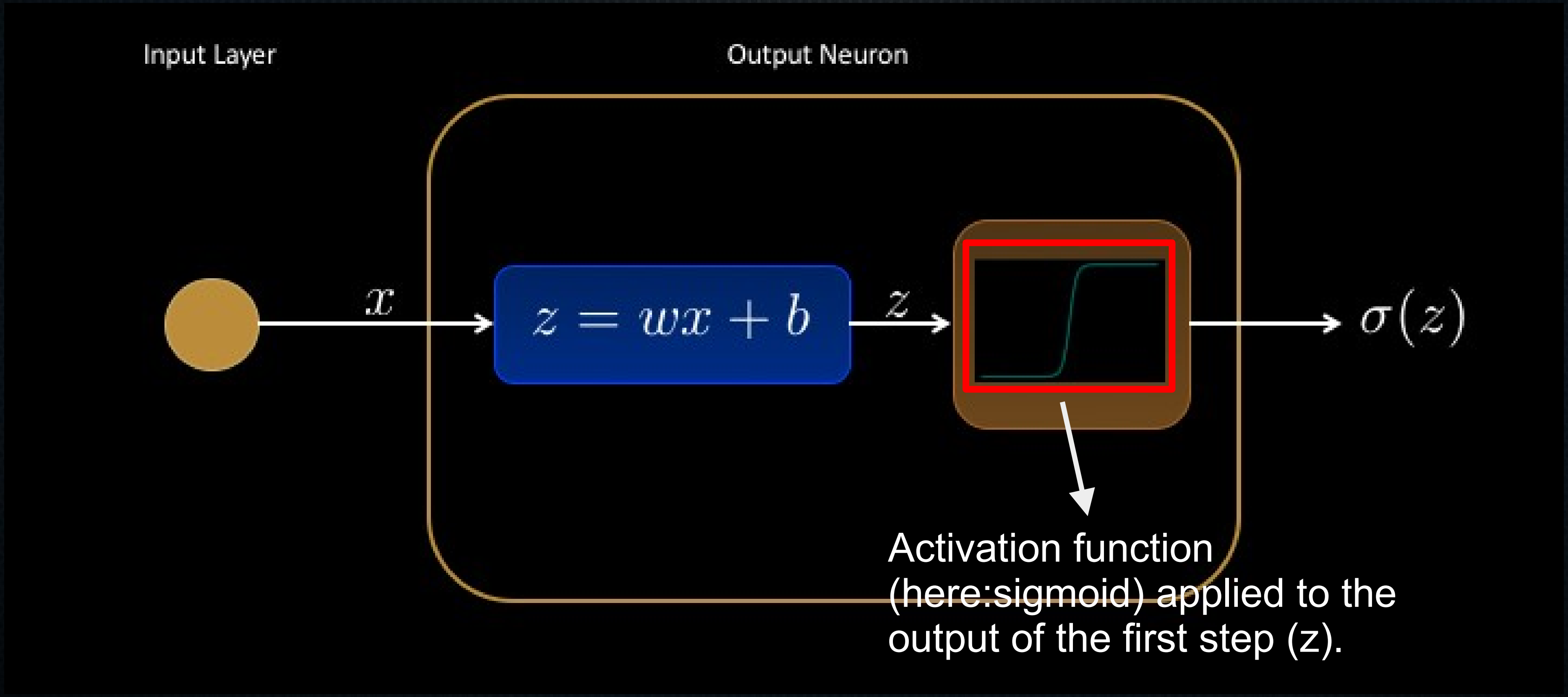

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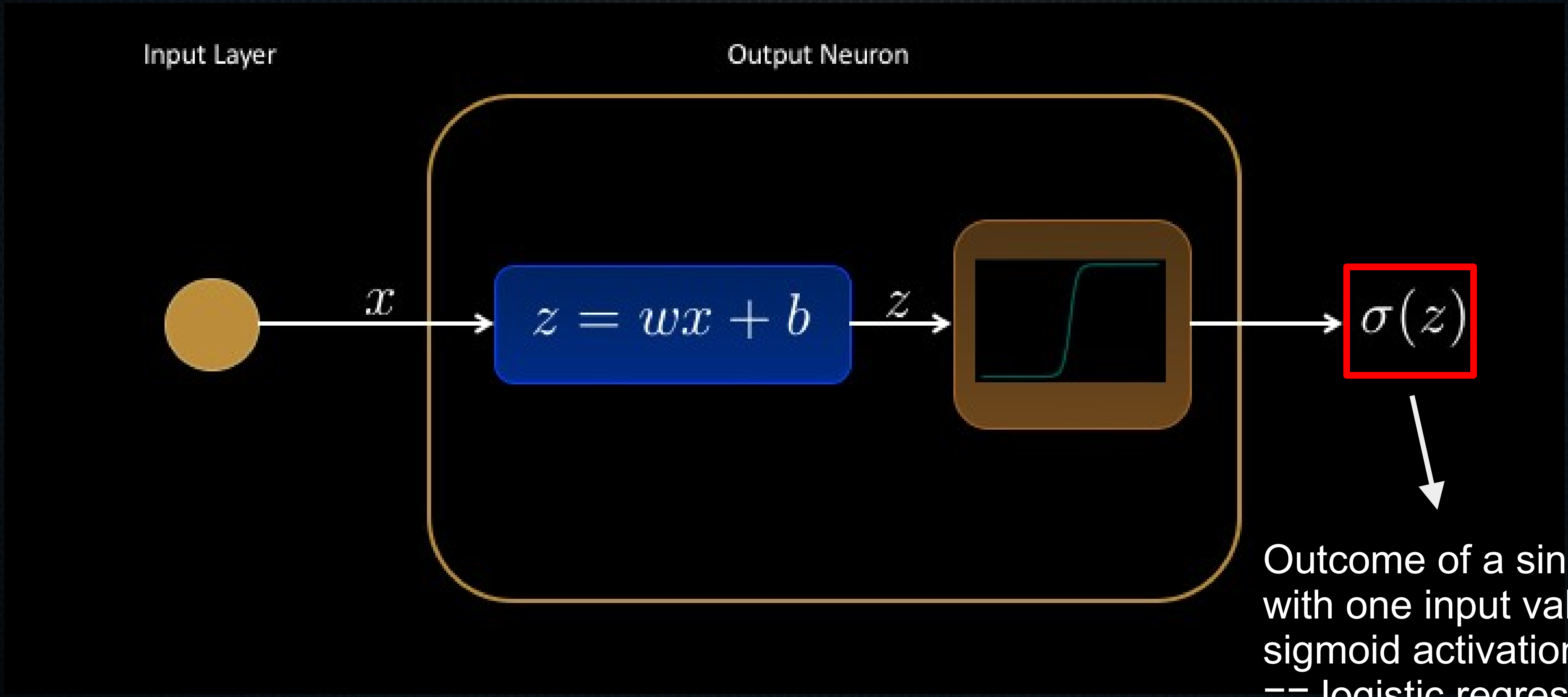

Outcome of a single neuron with one input value and sigmoid activation function == logistic regressor with 1 parameter (and bias)

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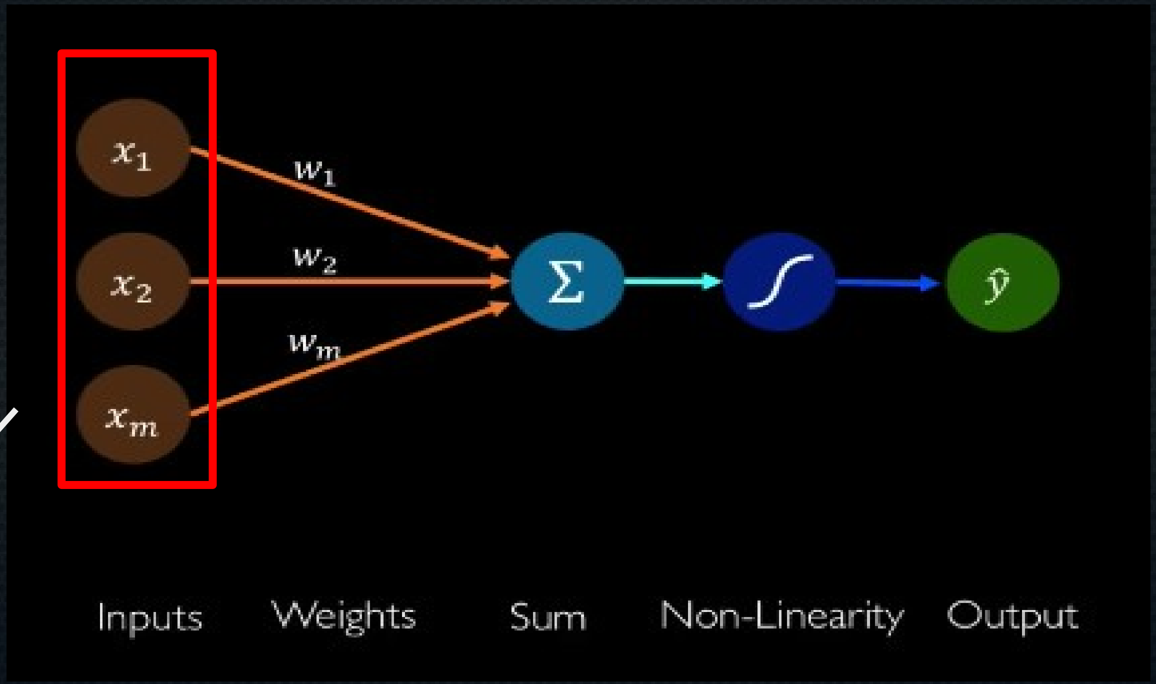

Multiple inputs: summation of those inputs' weights and the neuron's bias

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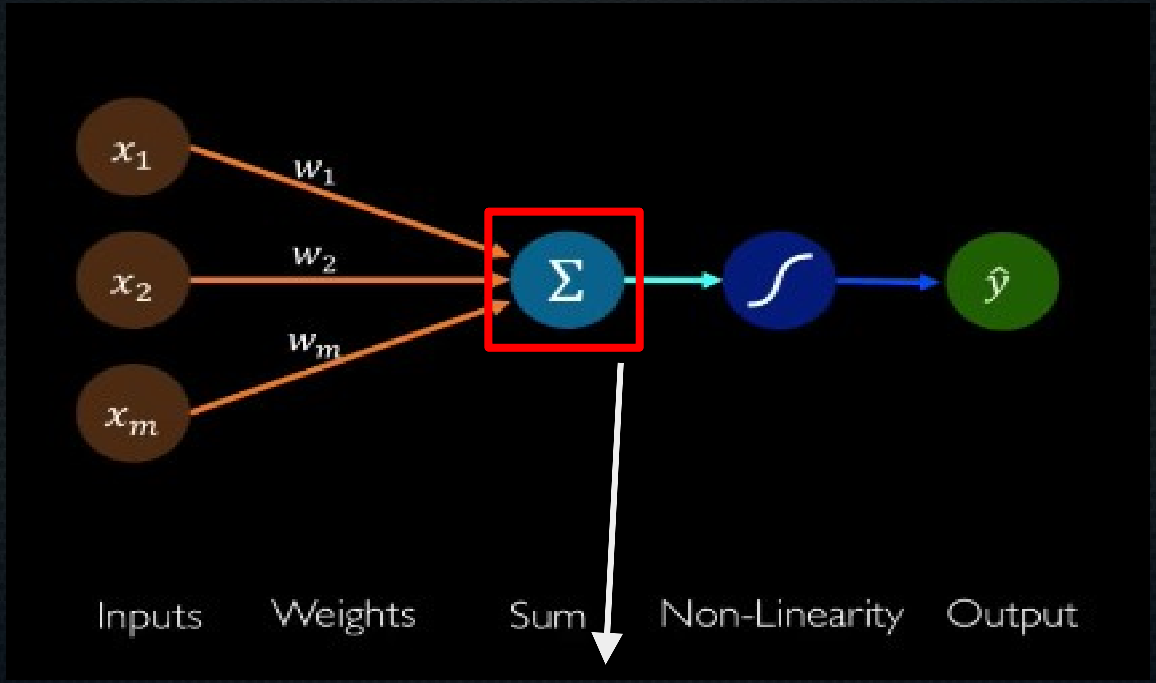

$$b+\sum_{i=1}^{m} w_i \cdot x_i$$

What do neural nets have to do with logistic regression?

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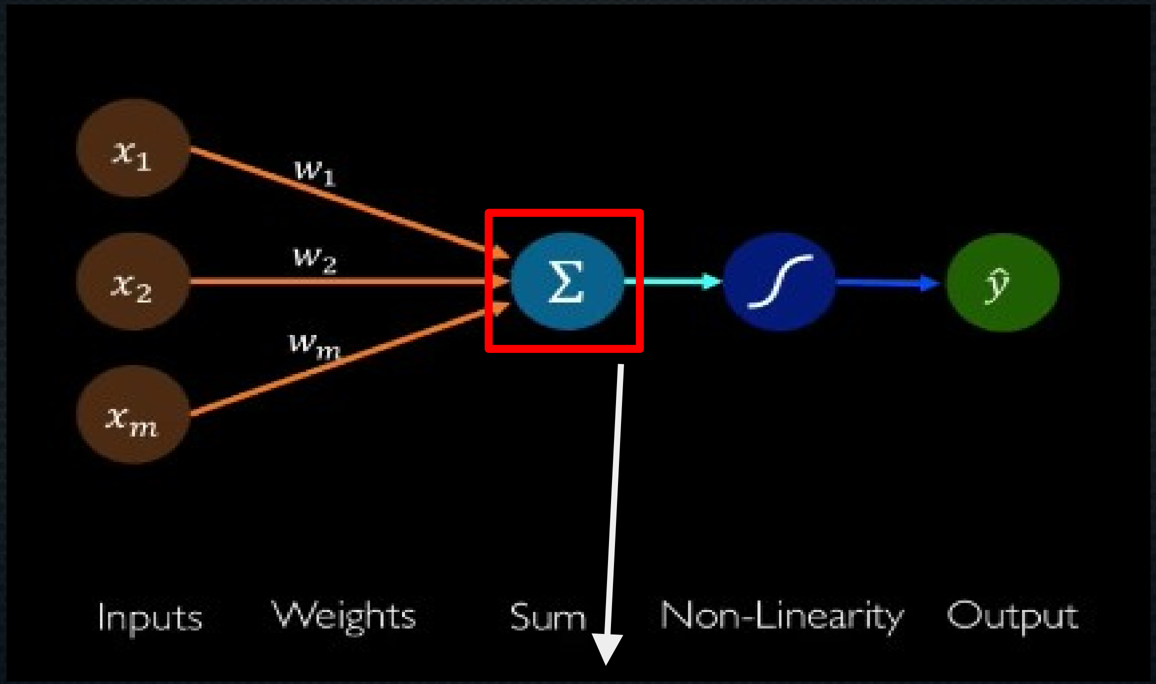

Or, in linear algebra notation: $\begin{bmatrix} 1 & x_1 & x_2 & x_m \end{bmatrix} \begin{bmatrix} b \\ w_1 \\ w_2 \\ w_m \end{bmatrix}$

What do neural nets have to do with logistic regression?

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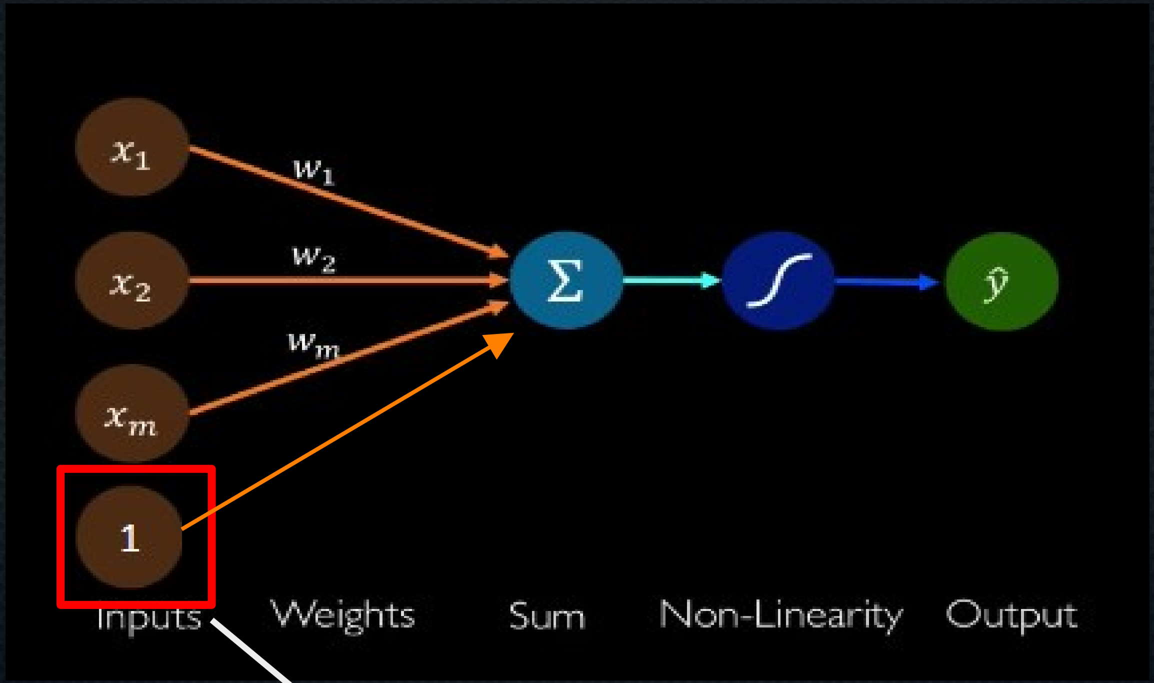

$$\begin{bmatrix} \boxed{1} & x_1 & x_2 & x_m \end{bmatrix} \begin{bmatrix} b \\ w_1 \\ w_2 \\ w_m \end{bmatrix}$$

Bias unit (always 1, same for every neuron, most often not shown)

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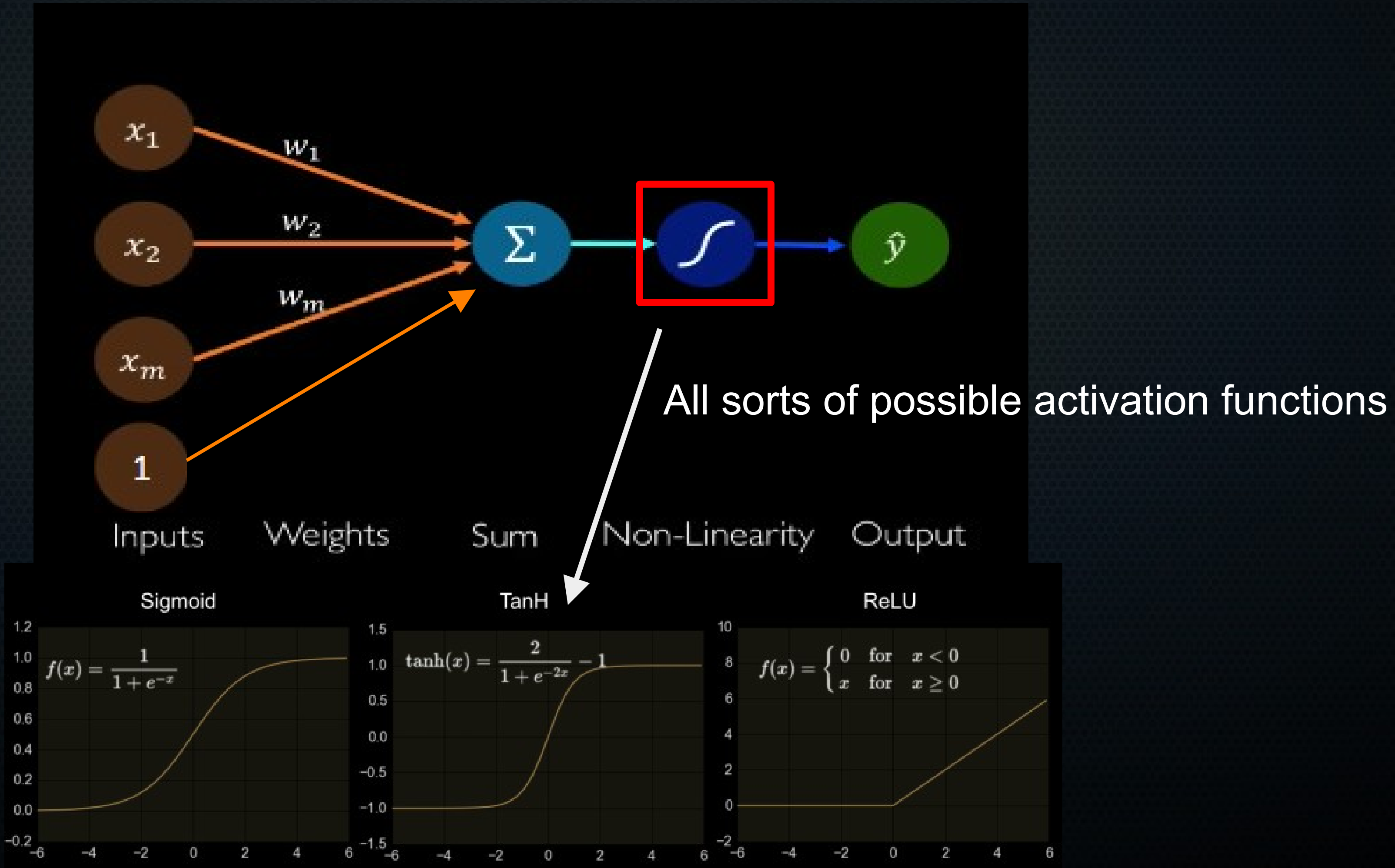

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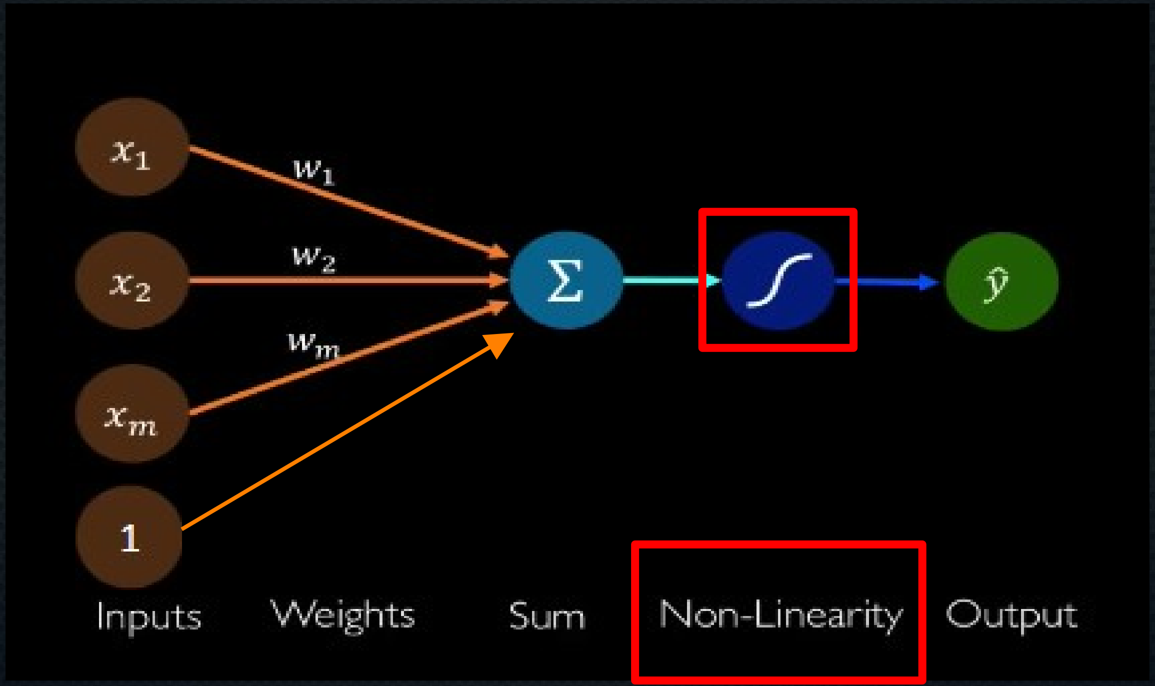

- Why non-linearity?

What do neural nets have to do with logistic regression?

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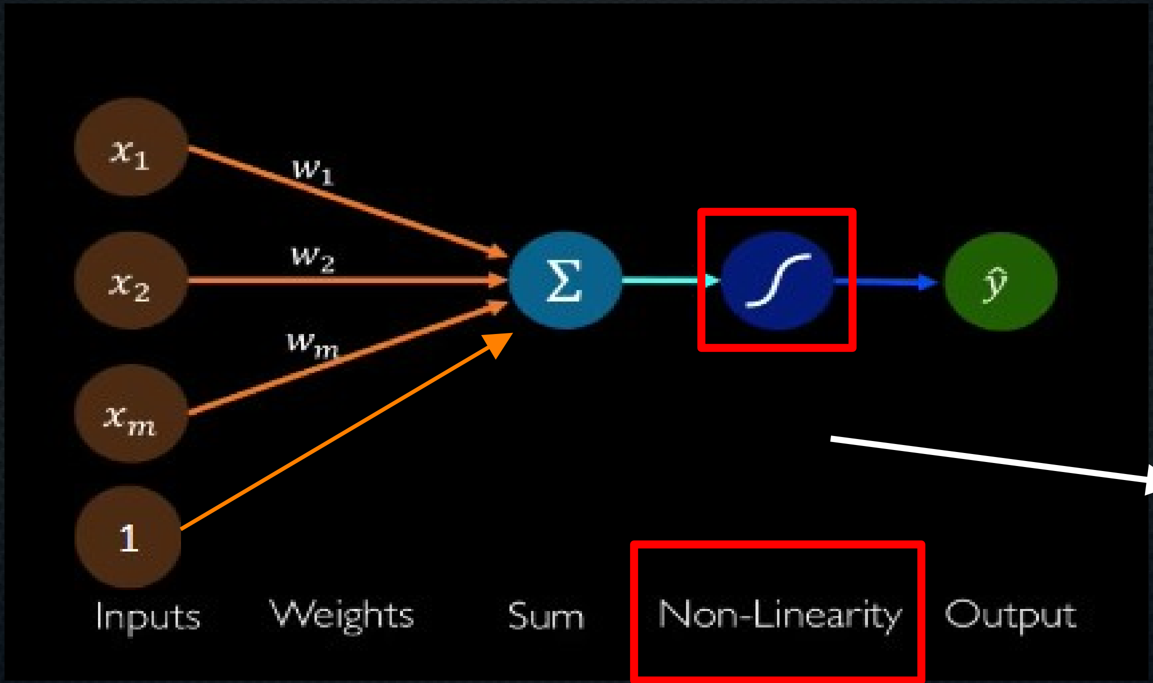
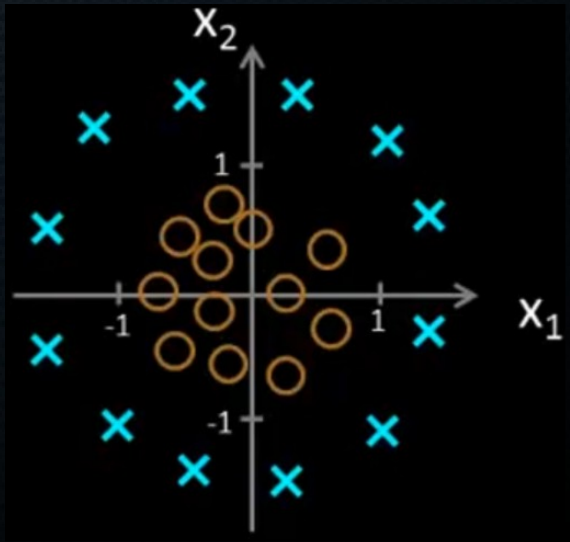
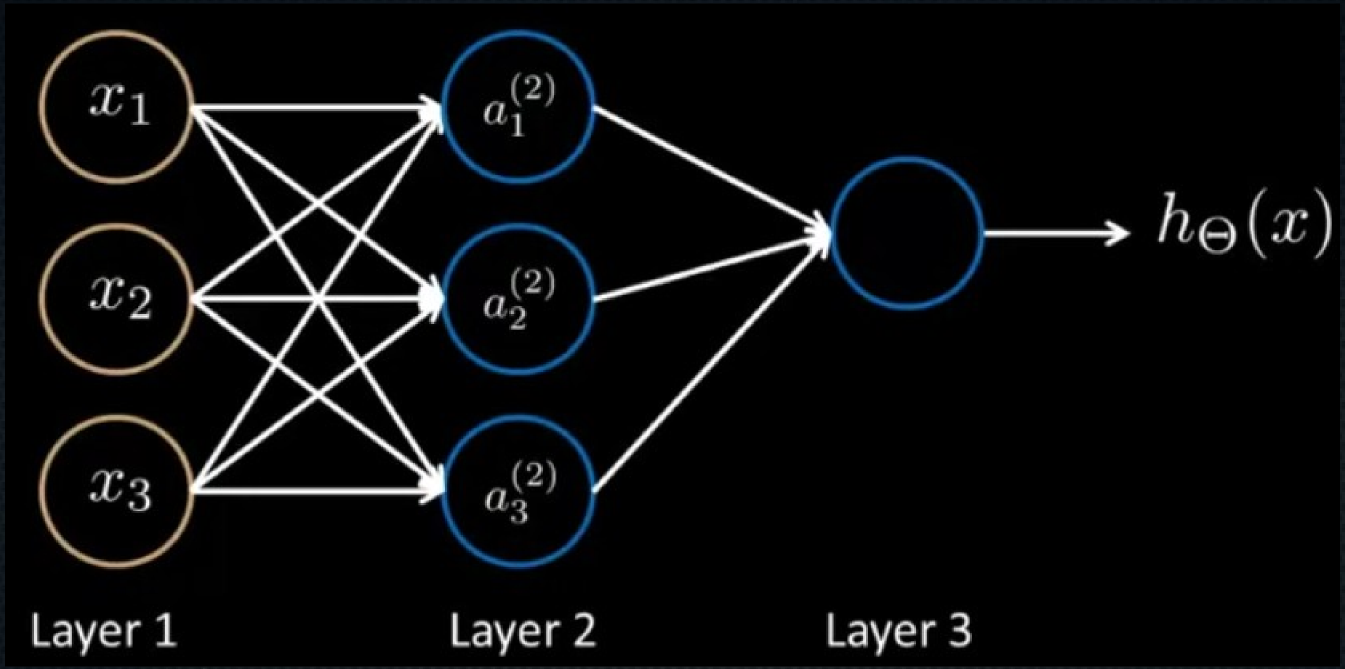




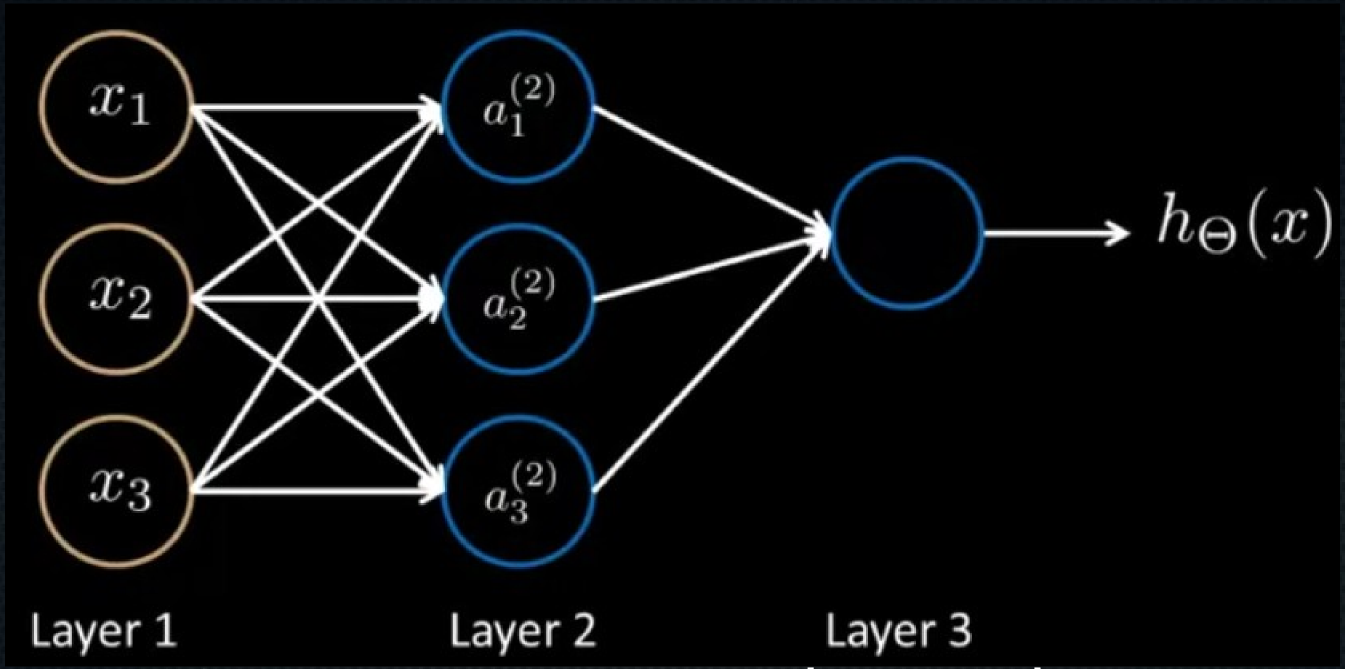
- Why non-linearity? → without them, a NN (no matter how deep) could only approximate linear functions

Workings of a simple neural network



Input layer: shown as neurons, are just features

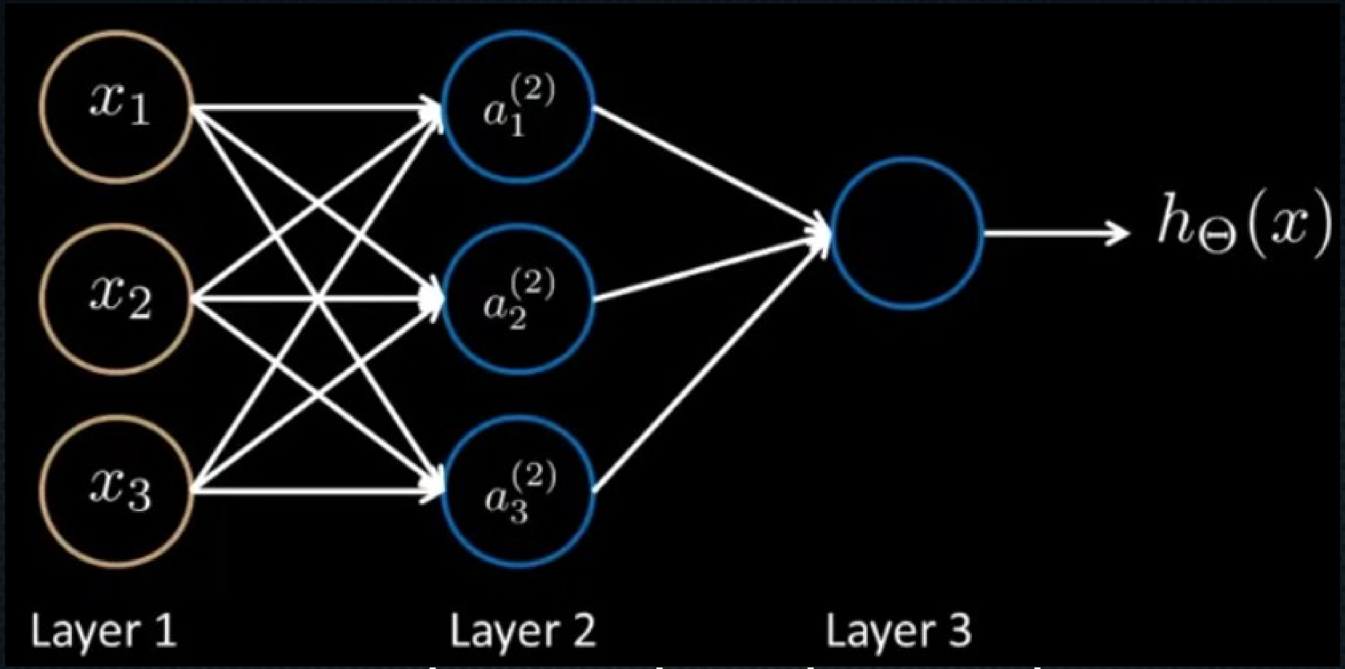
Workings of a simple neural network



Input layer: shown as neurons, are just features

Output layer: final result of the neural net

Workings of a simple neural network

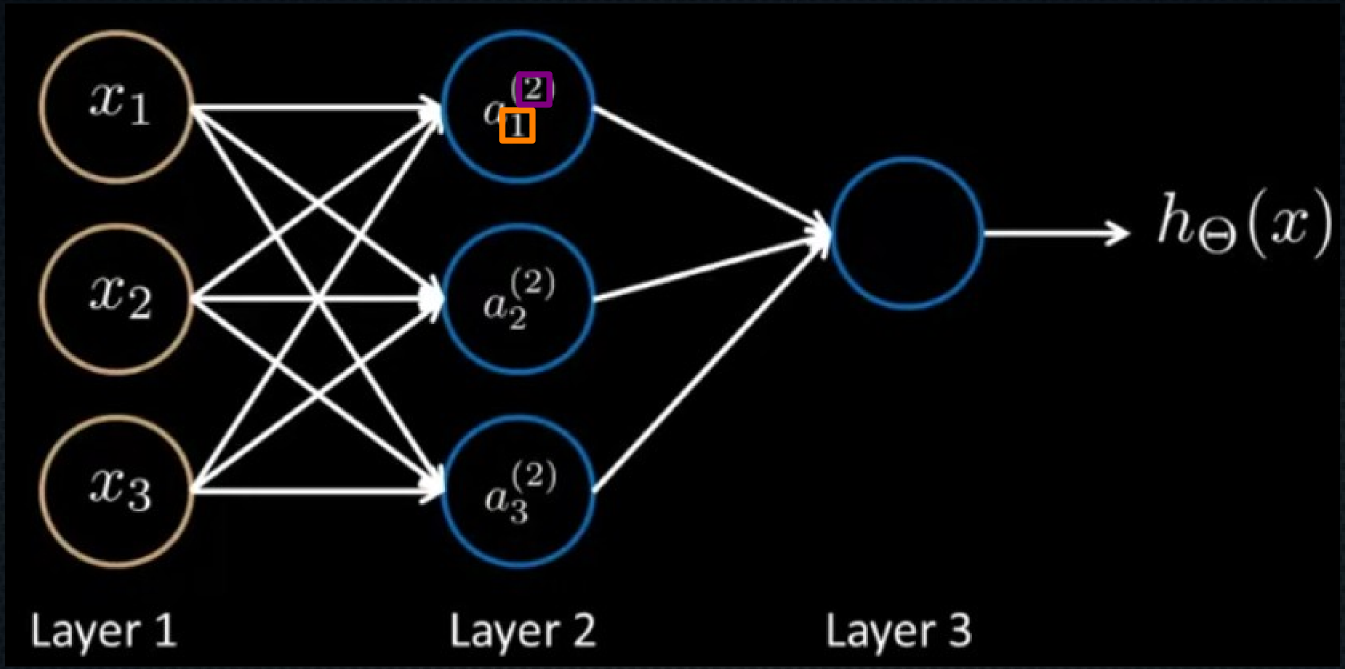


Input layer: shown as neurons, are just features

Output layer: final result of the neural net

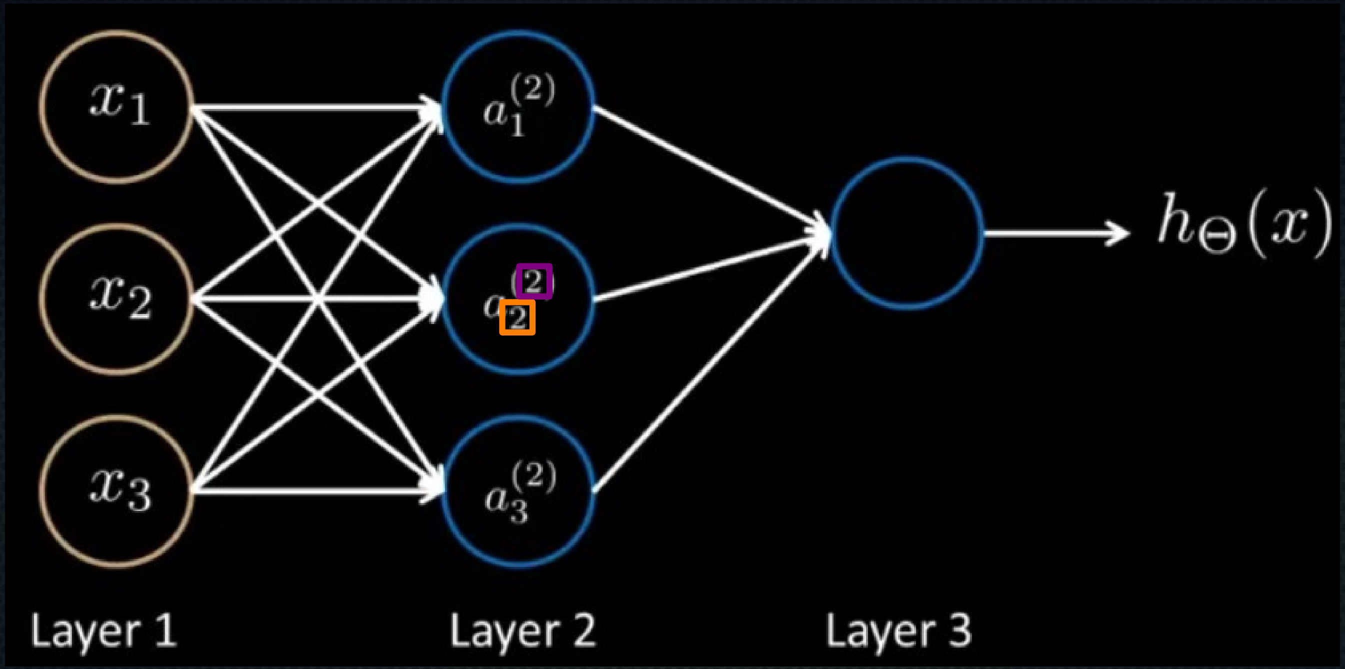
Hidden layer(s): intermediate layers whose outputs are not directly observed (hence hidden). Here: 1 HL. Facebook's DenseNet family of NNs had 121-264 HLs in 2016 (0.8-15.3 million parameters).

Workings of a simple neural network



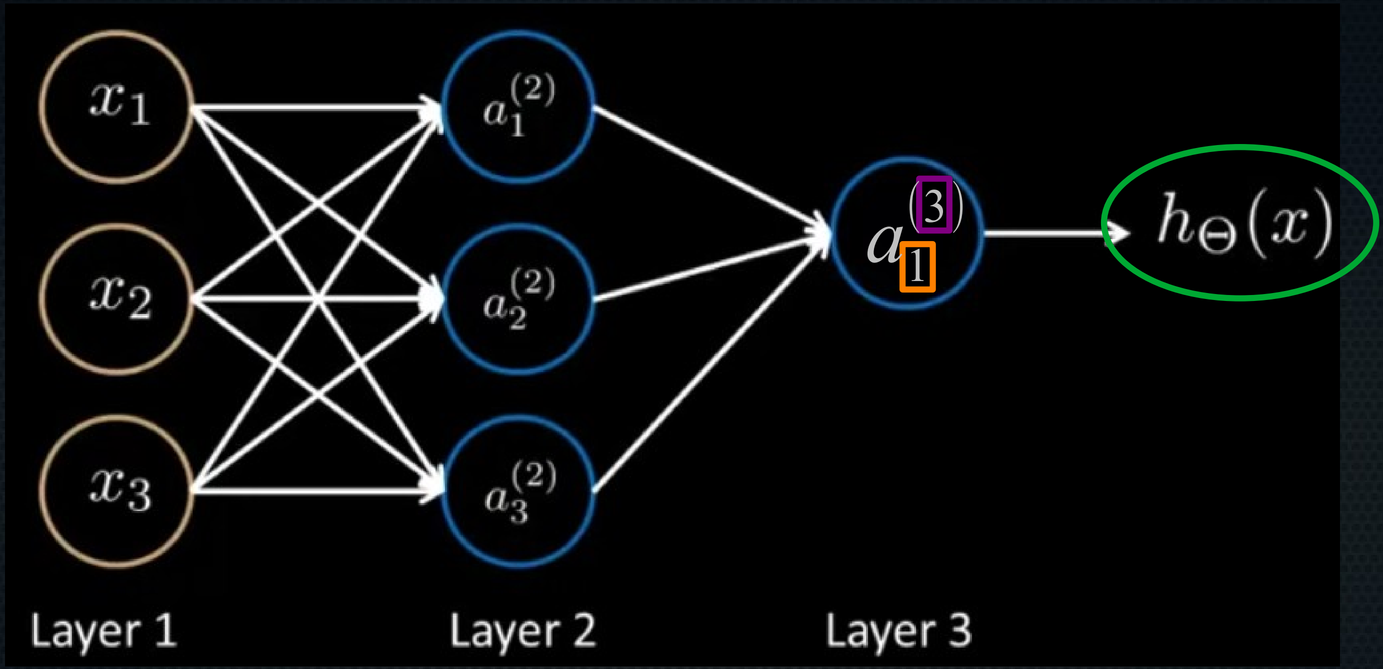
Activation of neuron **1** in the **2**nd layer of the network.

Workings of a simple neural network



Activation of neuron **2** in the **2**nd layer of the network.

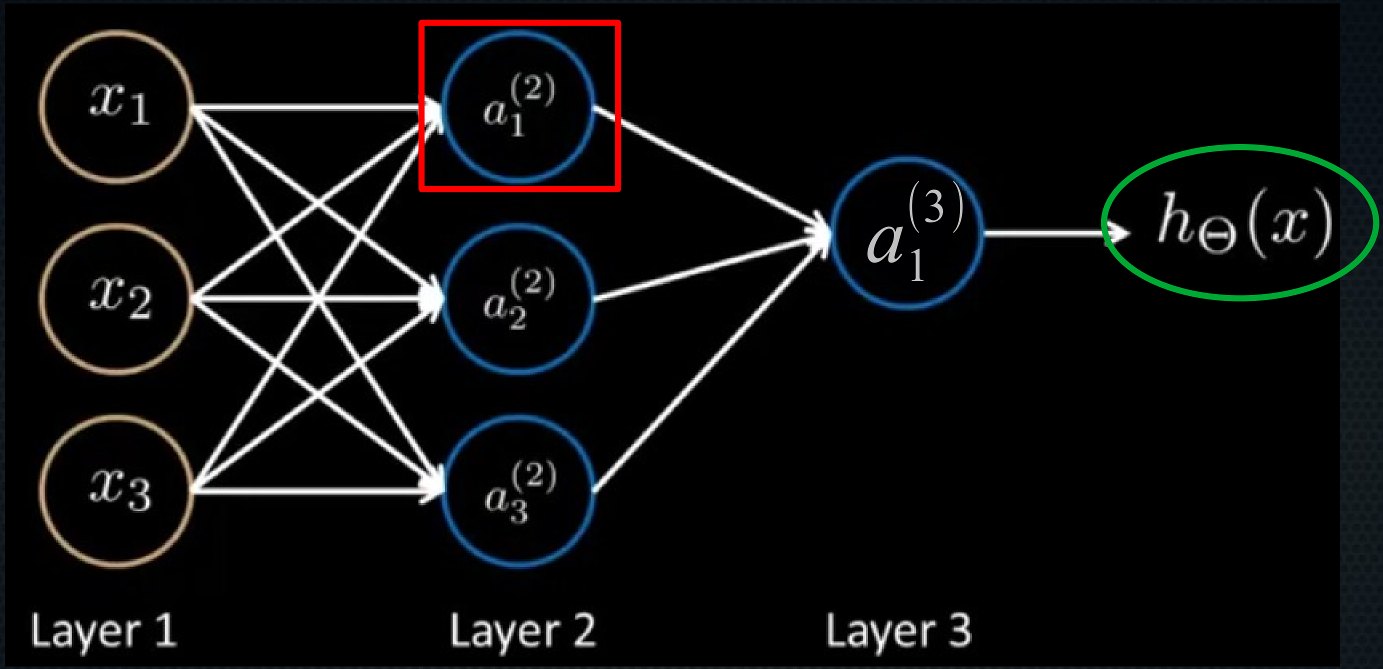
Workings of a simple neural network



https://www.louisbouchard.ai/densenet-explained/

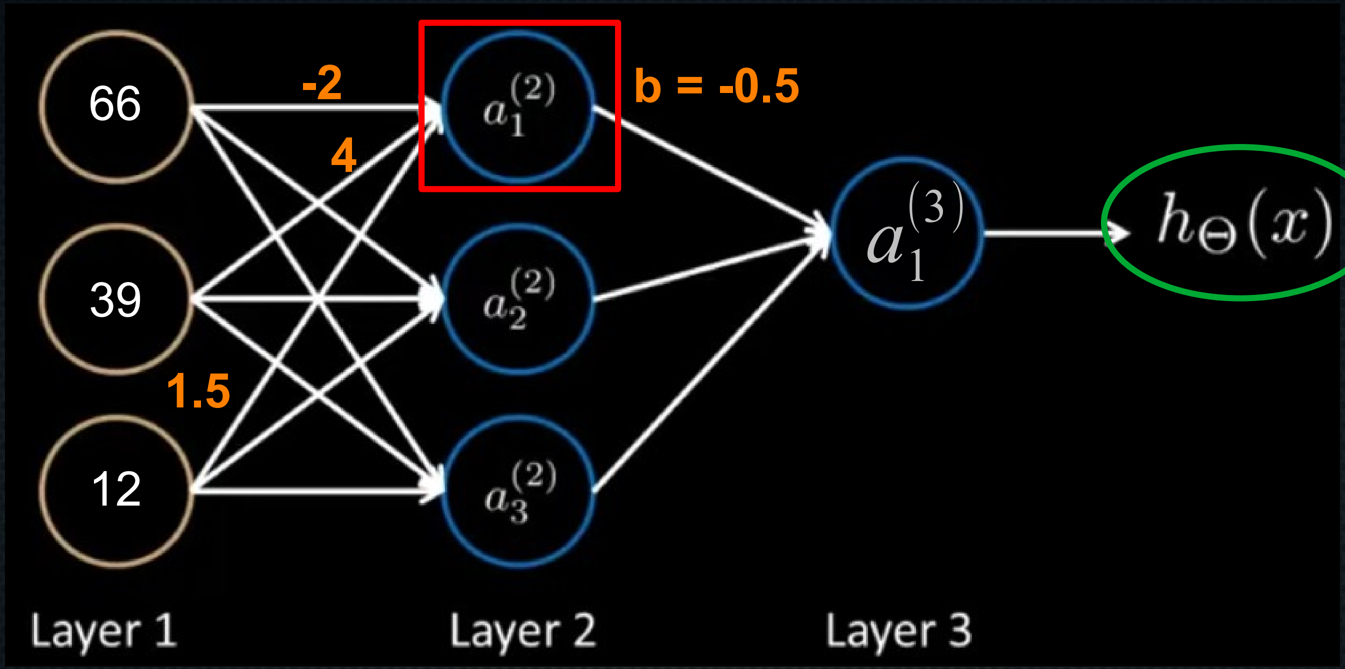
Activation of neuron **1** in the **3**rd layer of the network.

What is this network calculating?



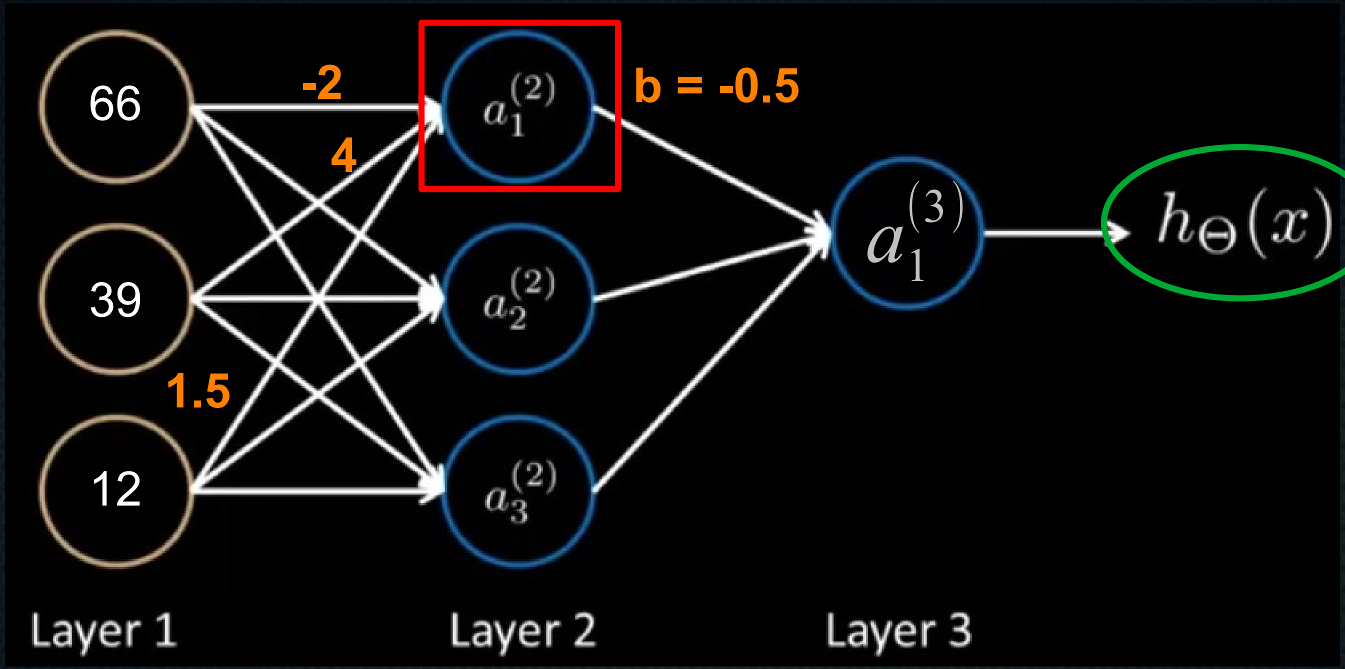
$$\sigma\left(\begin{bmatrix}1 & x_1 & x_2 & x_3\end{bmatrix}\begin{bmatrix}b \\ w_1 \\ w_2 \\ w_3\end{bmatrix}\right)$$

What is this network calculating?



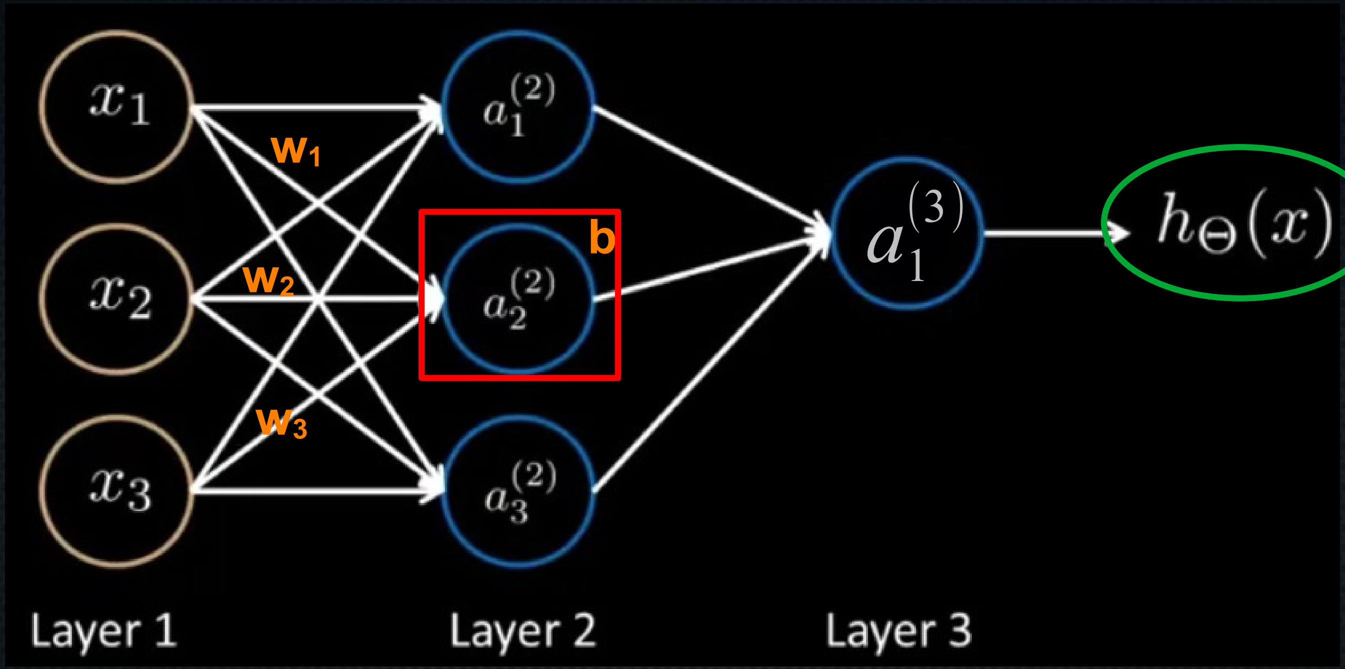
$$\sigma\left(\begin{bmatrix}1 & x_1 & x_2 & x_3\end{bmatrix}\begin{bmatrix}b \\ w_1 \\ w_2 \\ w_3\end{bmatrix}\right) \rightarrow \sigma\left(\begin{bmatrix}1 & 66 & 39 & 12\end{bmatrix}\begin{bmatrix}-0.5 \\ -2 \\ 4 \\ 1.5\end{bmatrix}\right)$$

What is this network calculating?



$$\sigma\left(\begin{bmatrix}1 & 66 & 39 & 12\end{bmatrix}\begin{bmatrix}-0.5\\-2\\4\\1.5\end{bmatrix}\right) \rightarrow \sigma(41.5) \rightarrow 0.999\ldots$$

What is this network calculating?



$$\sigma\left(\begin{bmatrix} 1 & x_1 & x_2 & x_3 \end{bmatrix} \begin{bmatrix} b \\ w_1 \\ w_2 \\ w_3 \end{bmatrix}\right)$$

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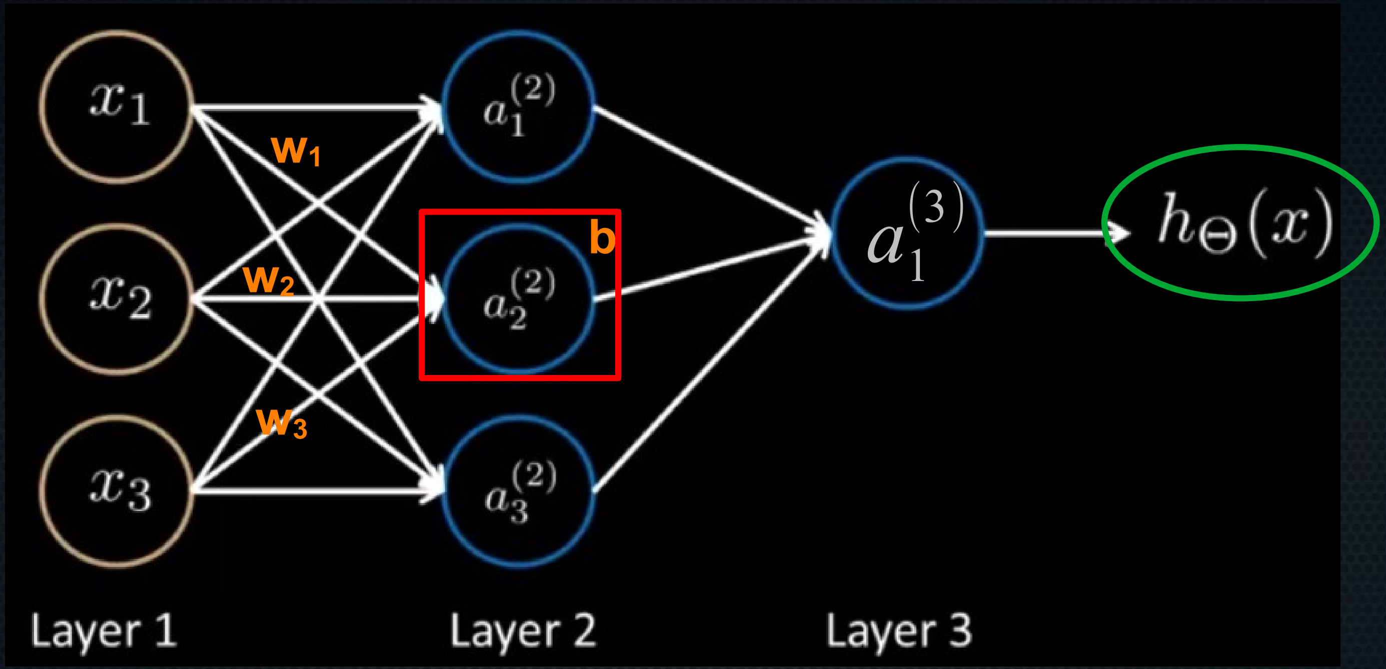
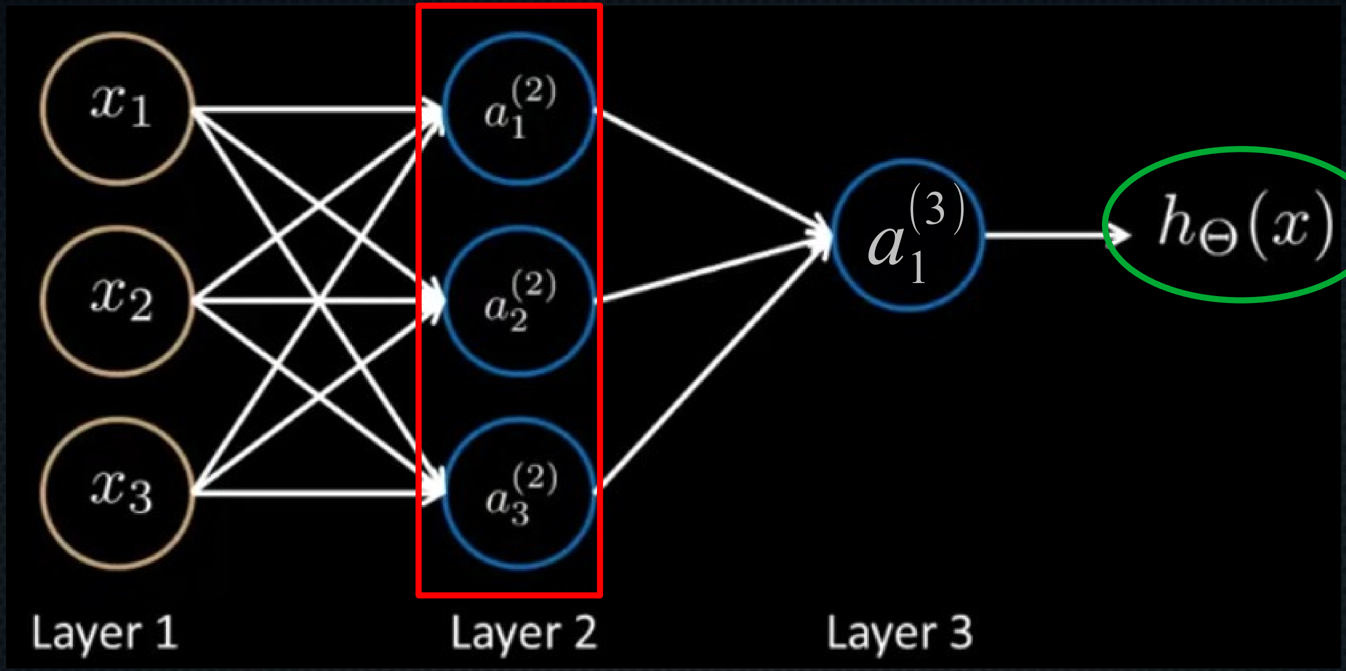


$$\sigma\left(\begin{bmatrix}1 & x_1 & x_2 & x_3\end{bmatrix}\begin{bmatrix}b \\ w_1 \\ w_2 \\ w_3\end{bmatrix}\right) \longrightarrow$$

Calculate for all units at the same time with a theta matrix $\Theta^{(j)}$

What is this network calculating?

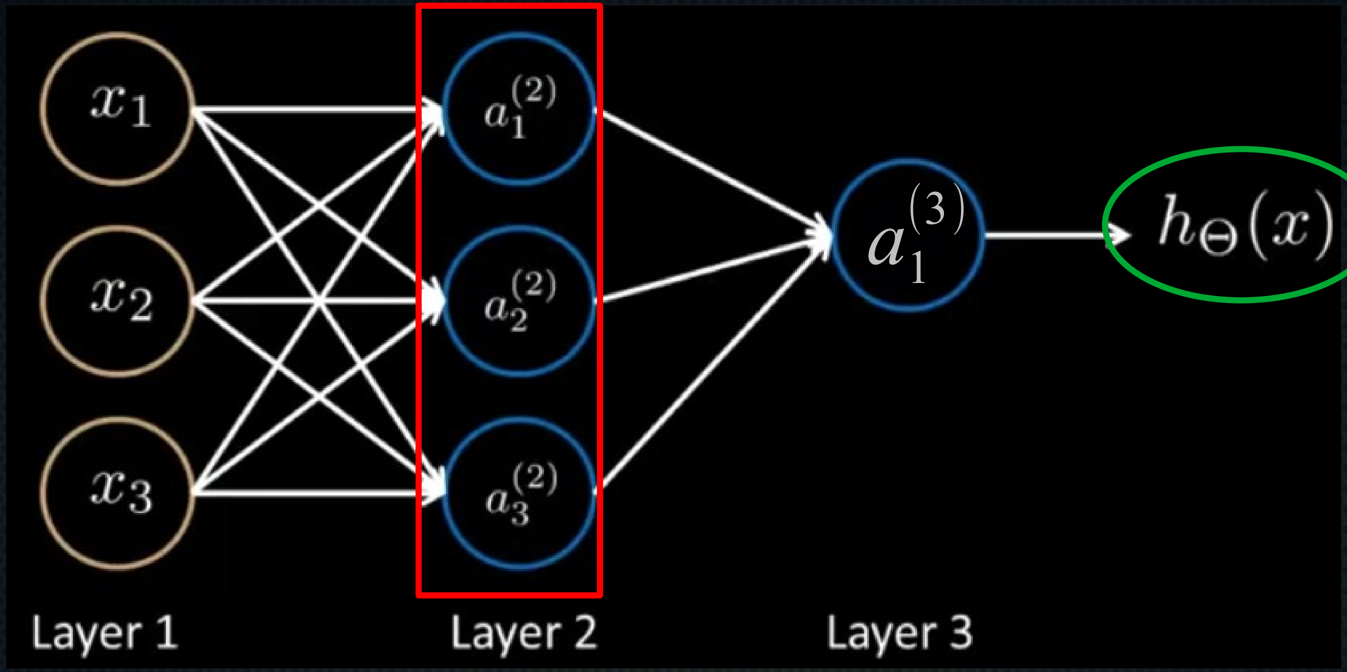


$$\sigma\left(\begin{bmatrix}1 & x_1 & x_2 & x_3\end{bmatrix}\begin{bmatrix} b_1 & b_2 & b_3 \\ w_{11} & w_{21} & w_{31} \\ w_{12} & w_{22} & w_{32} \\ w_{13} & w_{23} & w_{33} \end{bmatrix}\right) \longrightarrow \sigma(\begin{bmatrix}1 & 2 & 3\end{bmatrix})$$

$$\downarrow$$

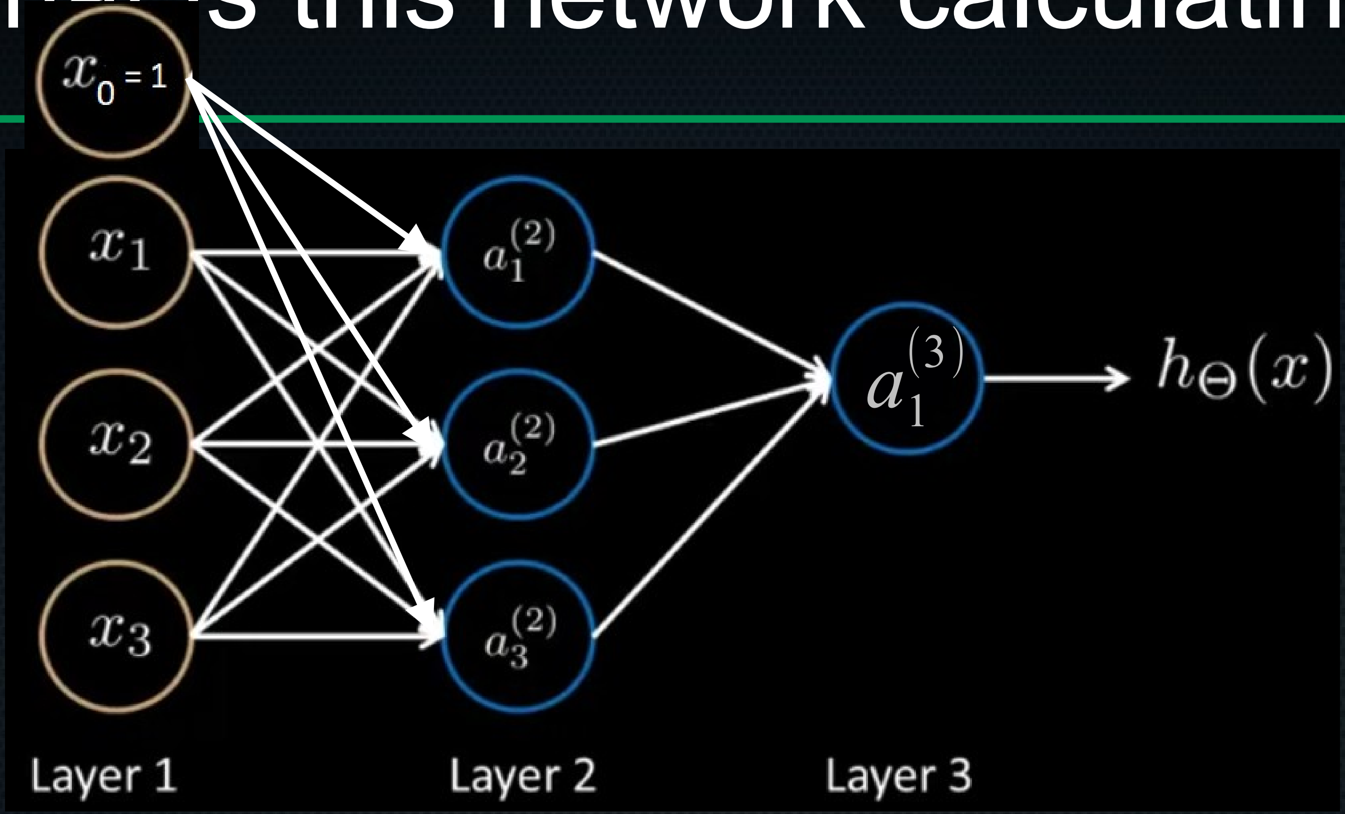
$$\boxed{\begin{bmatrix}\sigma(1) & \sigma(2) & \sigma(3)\end{bmatrix}}$$

What is this network calculating?



$$\sigma\left(\begin{bmatrix} b_1 & w_{11} & w_{12} & w_{13} \\ b_2 & w_{21} & w_{22} & w_{23} \\ b_3 & w_{31} & w_{32} & w_{33} \end{bmatrix}\begin{bmatrix} 1 \\ x_1 \\ x_2 \\ x_3 \end{bmatrix}\right) \longrightarrow \sigma\left(\begin{bmatrix} 1 \\ 2 \\ 3 \end{bmatrix}\right) \longrightarrow \boxed{\begin{bmatrix} \sigma(1) \\ \sigma(2) \\ \sigma(3) \end{bmatrix}}$$

What is this network calculating?

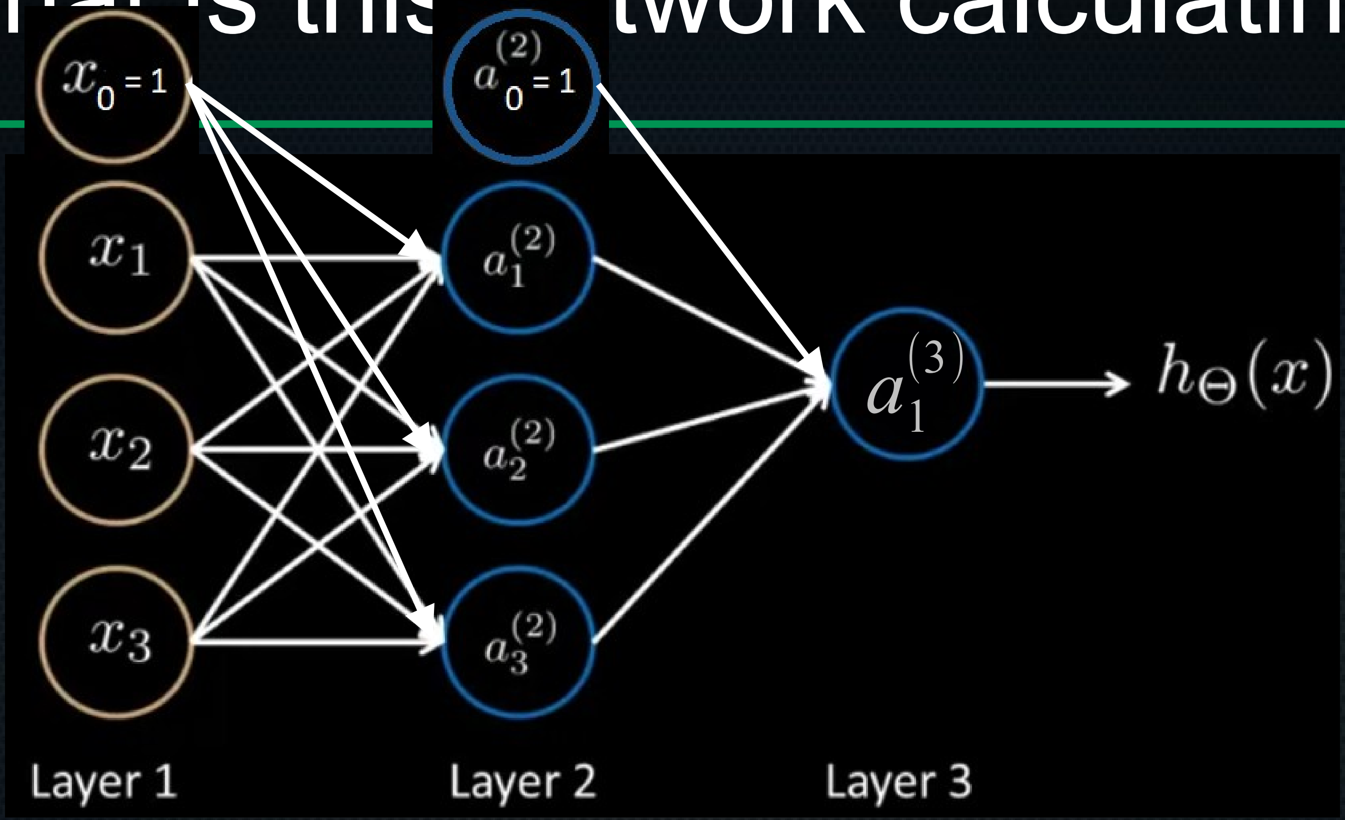


$$a_1^{(2)} = g(\Theta_{10}^{(1)}x_0 + \Theta_{11}^{(1)}x_1 + \Theta_{12}^{(1)}x_2 + \Theta_{13}^{(1)}x_3)$$
$$a_2^{(2)} = g(\Theta_{20}^{(1)}x_0 + \Theta_{21}^{(1)}x_1 + \Theta_{22}^{(1)}x_2 + \Theta_{23}^{(1)}x_3)$$
$$a_3^{(2)} = g(\Theta_{30}^{(1)}x_0 + \Theta_{31}^{(1)}x_1 + \Theta_{32}^{(1)}x_2 + \Theta_{33}^{(1)}x_3)$$

$\Theta^{(1)}$ (layer 1 to layer 2)

$$\begin{bmatrix} b_1 & w_{11} & w_{12} & w_{13} \\ b_2 & w_{21} & w_{22} & w_{23} \\ b_3 & w_{31} & w_{32} & w_{33} \end{bmatrix}$$

What is this network calculating?

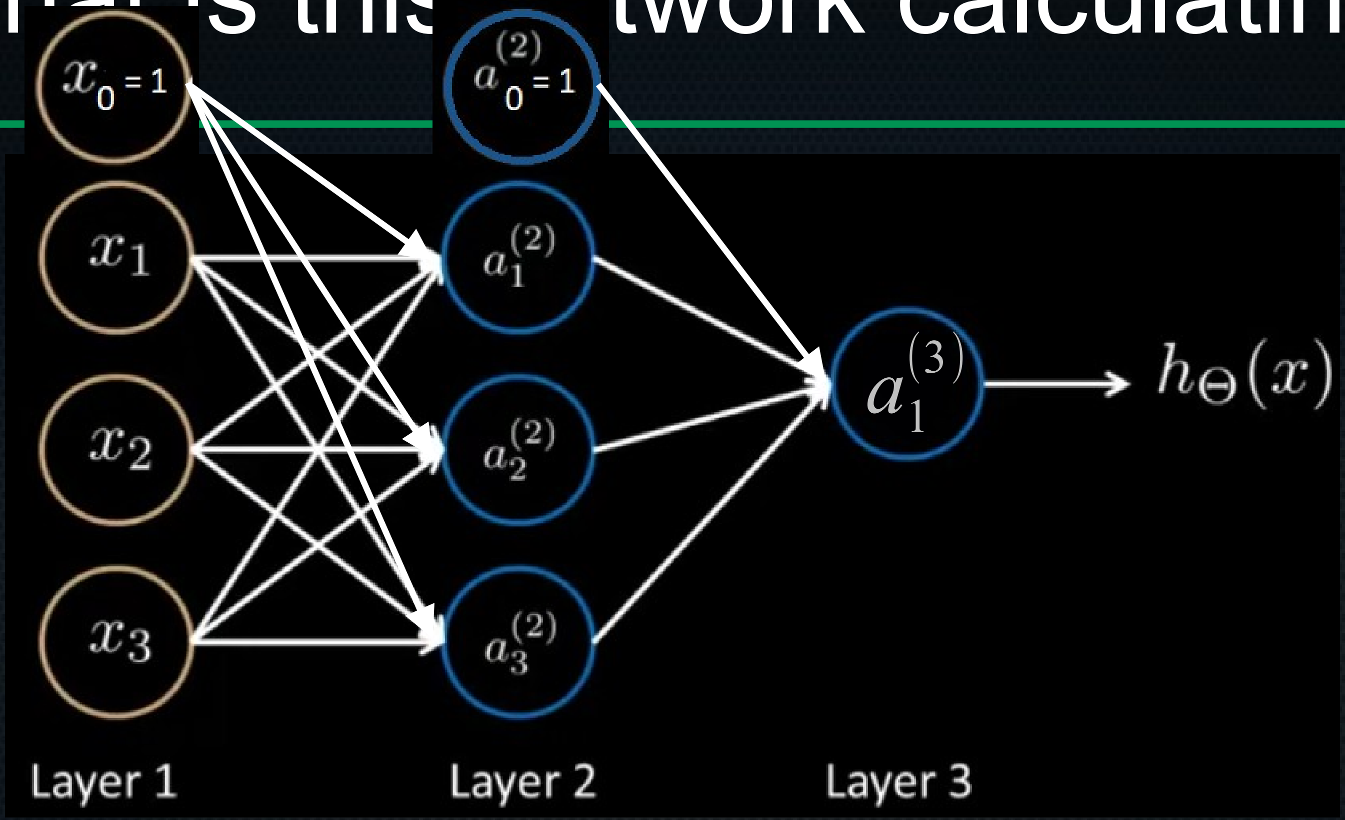


$\Theta^{(2)}$ (layer 2 to layer 3)

$$h_\Theta(x) = a_1^{(3)} = g(\Theta_{10}^{(2)} a_0^{(2)} + \Theta_{11}^{(2)} a_1^{(2)} + \Theta_{12}^{(2)} a_2^{(2)} + \Theta_{13}^{(2)} a_3^{(2)})$$

$$\begin{bmatrix} b_1 & w_{11} & w_{12} & w_{13} \end{bmatrix}$$

What is this network calculating?



- This calculation of the output of the network is called forward propagation

How do we perform?

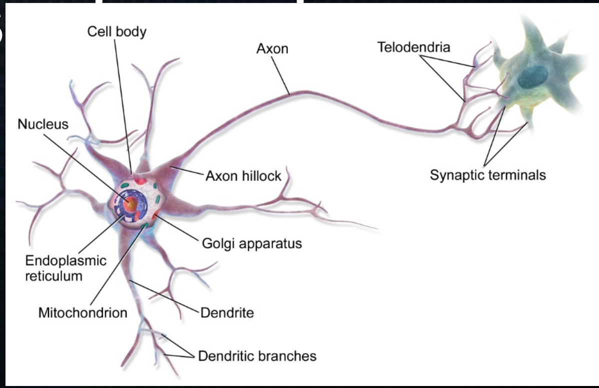
- Just like before, there is a cost function.
- But we will talk about that and its implementation tomorrow!

How do we get parameters?

- Just like before, there is a cost function and a way to minimise this. But it’s a bit more involved.
- To get parameters, we will use the principle of backpropagation. We’ll get to that tomorrow.
- First, we need to discuss *why* we want to use neural networks at all!

Why neural networks?

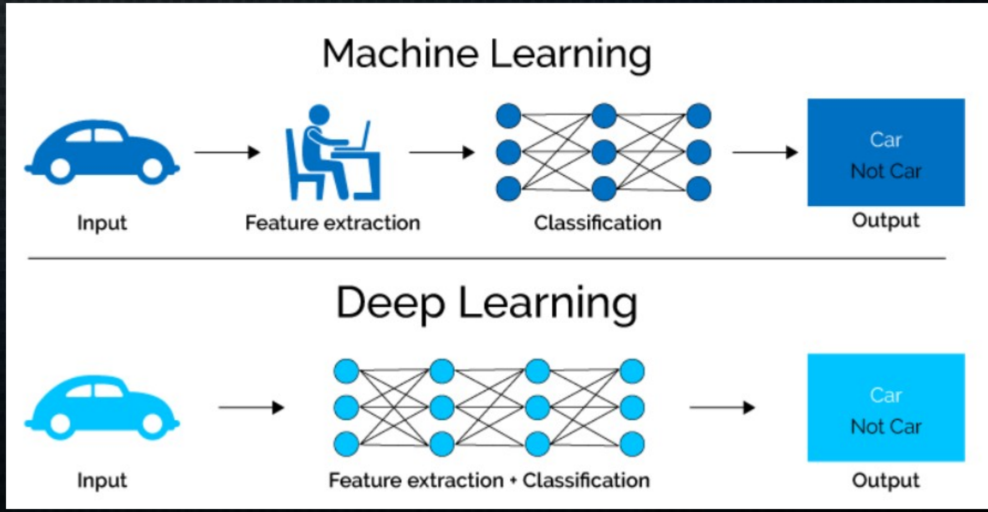
- Best performing algorithms for complex tasks, bar none.
- Known potential of hierarchical organisation of simple units because of biological examples (though neural networks are not good models of actual neurons)
- Observation in frogs and cat visual cortex: there are specific layers of neurons, where earlier layers detect basic shapes (lines, edges) with later layers incorporating this information into more complex features about what is seen.



Source: https://en.wikipedia.org/wiki/Axon#/media/File:Blausen_0657_MultipolarNeuron.png

Why neural networks?

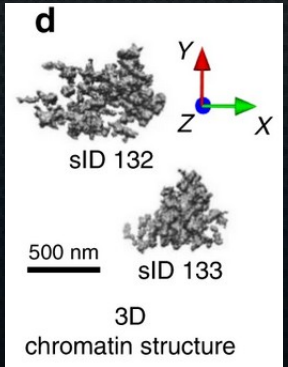
- Until now, we decided on the features to give to our algorithms: think tumour size, biopsy test scores, etc.
- With neural networks and images, the situation changes: we don't arduously describe what is in each image, but rather let the network learn to extract and combine features *so that* it can classify training examples correctly.

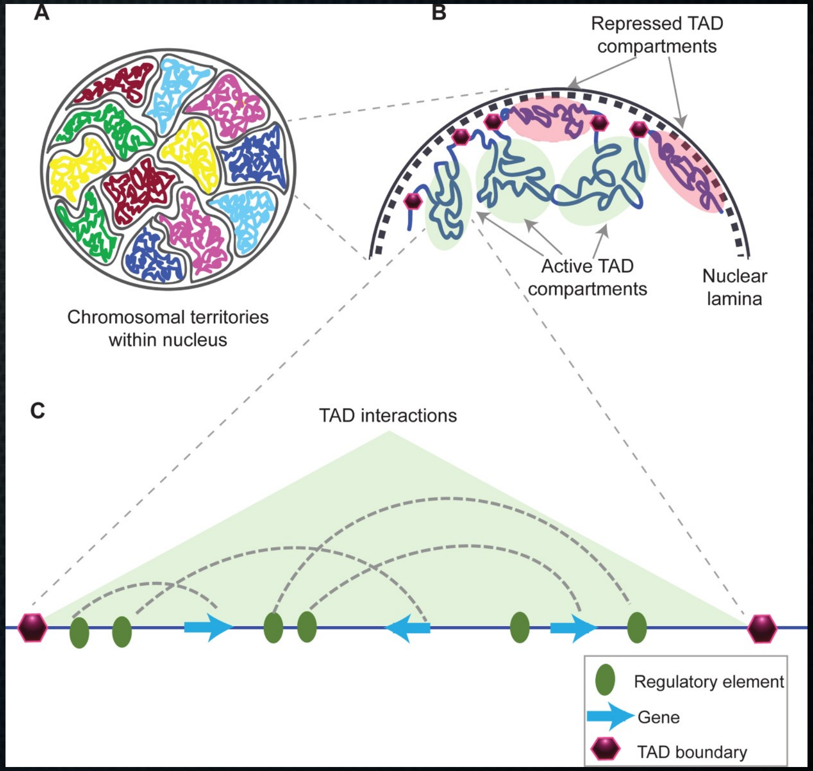


Source: https://towardsdatascience.com/cnn-application-on-structured-data-automated-feature-extraction-8f2cd28d9a7e

Why neural networks?

- Caveat for biology: it can be quite difficult to translate biological problems into a framework fit for deep learning, for reasons that will become clear later.
- Example: in images, nearby pixels probably hold similar information, i.e. are involved in the same thing. Due to (long-range) 3D-folding of DNA, linearly far DNA can be close together functionally. You need to encode network or input to accomodate this!





Source: https://en.wikipedia.org/wiki/Topologically_associating_domain#/media/File:Structural_organization_of_chromatin.png

Source: Trzaskoma, P., Ruszczycki, B., Lee, B., Pels, K. K., Krawczyk, K., Bokota, G., ... & Wilczyński, G. M. (2020). Ultrastructural visualization of 3D chromatin folding using volume electron microscopy and DNA in situ hybridization. Nature communications, 11(1), 1-9.

Why neural networks?

- The mythical property of *universal approximation*. This says that neural networks can approximate any function with arbitrary accuracy, even with only **1** hidden layer (given enough neurons in it).

Why neural networks?

- The mythical property of *universal approximation*. This says that neural networks can approximate any function with arbitrary accuracy, even with only **1** hidden layer (given enough neurons in it).
- How can that be? You will find out in-depth in the next practical.
- Of course, that doesn't necessarily mean we would have the data to *train* such a neural network efficiently. Just that it is provable that for *any continuous function* a neural network can exist that approximates it as well as you like.

Recap so far

- Neural networks can be thought of as hiërarchical sets of logistic regressors
- We essentially make earlier layers learn useful features for distinction on their own, and can use these best possible learned features for the classification by the final unit(s)
- Parsing an example through the network and getting the output is called forward propagation
- *Universal approximation* holds that, in principle, neural networks can learn any continuous function arbitrarily well.

Making simple functions ourselves

- Networks with a single hidden layer can approximate any function. Let‘s get some more intuition by building our own logic circuit.

Making simple functions ourselves

- Networks with a single hidden layer can approximate any function. Let‘s get some more intuition by building our own logic circuit.
- Boolean operators:

NOT

x	x'
0	1
1	0

AND

x	y	xy
0	0	0
0	1	0
1	0	0
1	1	1

OR

x	y	$x+y$
0	0	0
0	1	1
1	0	1
1	1	1

XOR

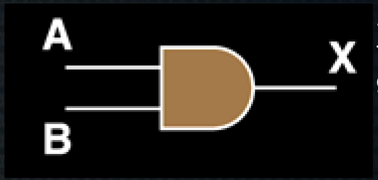
x	y	$x \oplus y$
0	0	0
0	1	1
1	0	1
1	1	0

Source: https://introcs.cs.princeton.edu/java/71boolean/

Making simple functions ourselves

- Networks with a single hidden layer can approximate any function. Let‘s get some more intuition by building our own logic circuit.
- Boolean operators:

Only if two incoming connections are on, the output is on



Source: https://www.electronics-tutorial.net/digital-logic-gates/and-gate/

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$\boxed{\text{AND}}$

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0	1	1
1	0	1
1	1	1

XOR

x	y	$x \oplus y$
0	0	0
0	1	1
1	0	1
1	1	0

Source: https://introcs.cs.princeton.edu/java/71boolean/

Making simple functions ourselves

- Networks with a single hidden layer can approximate any function. Let‘s get some more intuition by building our own logic circuit.
- Boolean operators:

Only if either incoming connection is on, the output is on

Source: https://projectiot123.com/2019/05/26/introduction-to-xor-gate/

NOT

x	x'
0	1
1	0

AND

x	y	xy
0	0	0
0	1	0
1	0	0
1	1	1

OR

x	y	$x+y$
0	0	0
0	1	1
1	0	1
1	1	1

$\boxed{\textit{XOR}}$

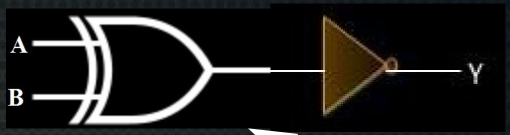
x	y	$x \oplus y$
0	0	0
0	1	1
1	0	1
1	1	0

Source: https://introcs.cs.princeton.edu/java/71boolean/

Making simple functions ourselves

- Networks with a single hidden layer can approximate any function. Let‘s get some more intuition by building our own logic circuit.
- Boolean operators:

Combine: XNOR



Source: https://www.tutorialspoint.com/computer_logical_organization/logic_gates.htm

NOT

x	x'
0	1
1	0

XNOR

Inputs		Output
A	B	A ⊙ B
0	0	1
0	1	0
1	0	0
1	1	1

XOR

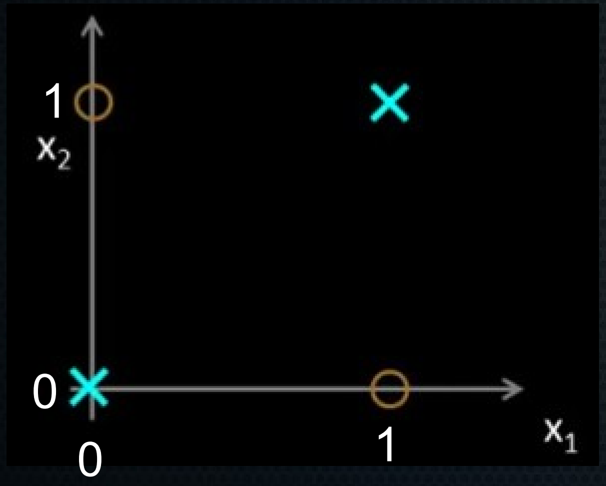
x	y	$x \oplus y$
0	0	0
0	1	1
1	0	1
1	1	0

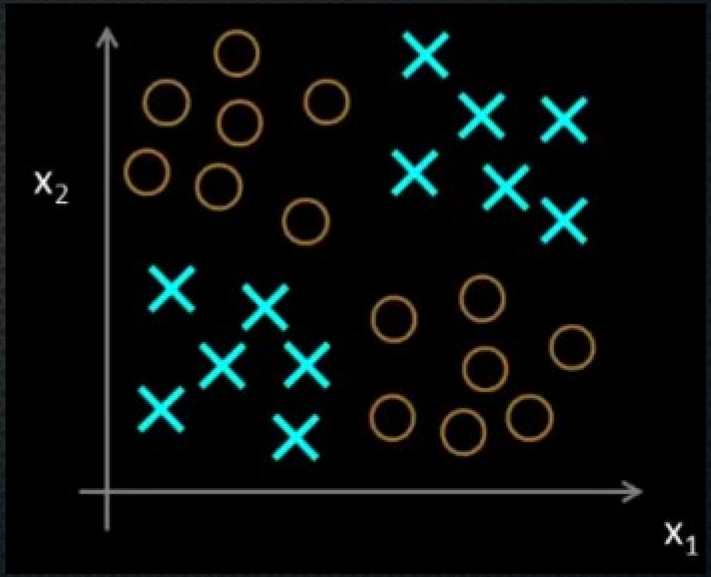
Source: https://introcs.cs.princeton.edu/java/71boolean/

See for more info: https://www.tutorialspoint.com/computer_logical_organization/logic_gates.htm

Making simple functions ourselves

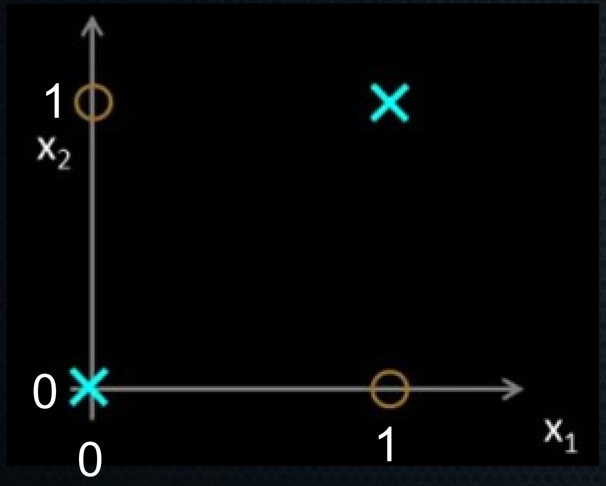
- Motivating example:

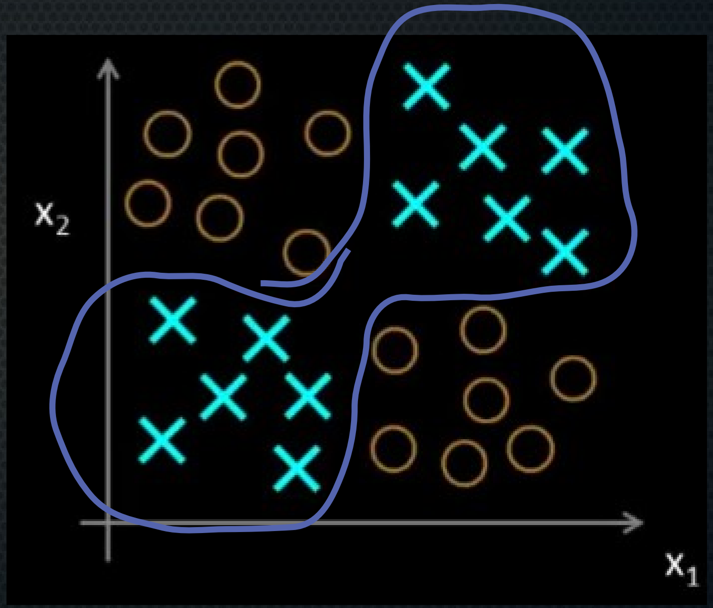




Making simple functions ourselves

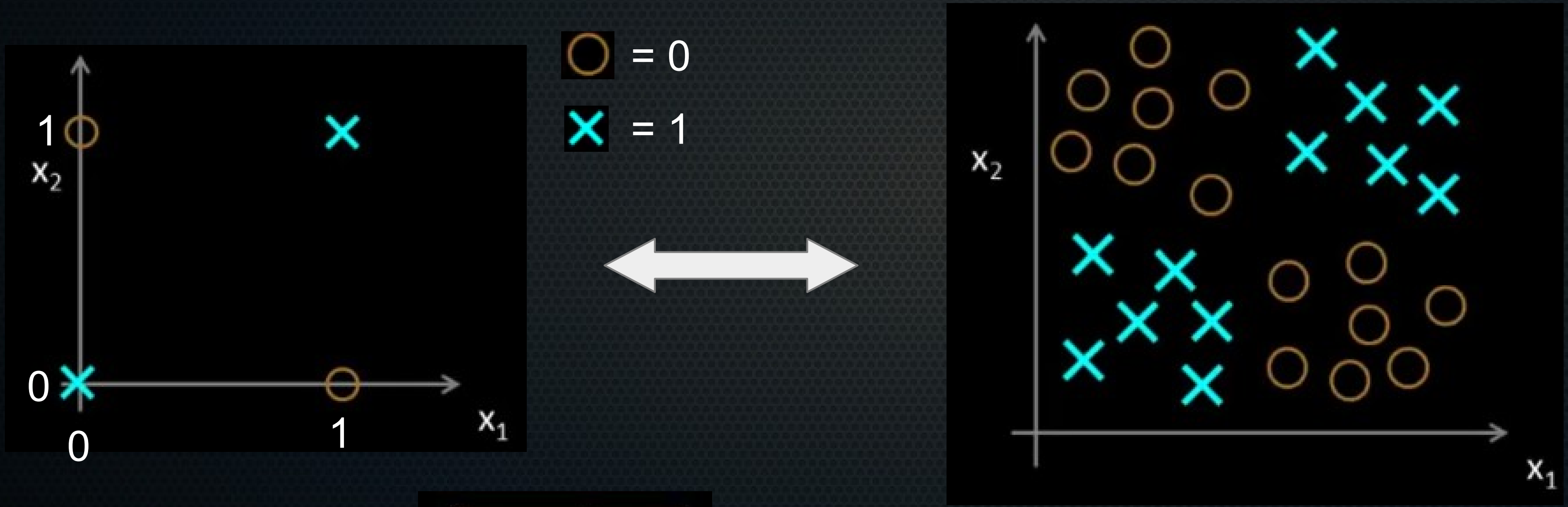
- Motivating example:





Making simple functions ourselves

- Motivating example:

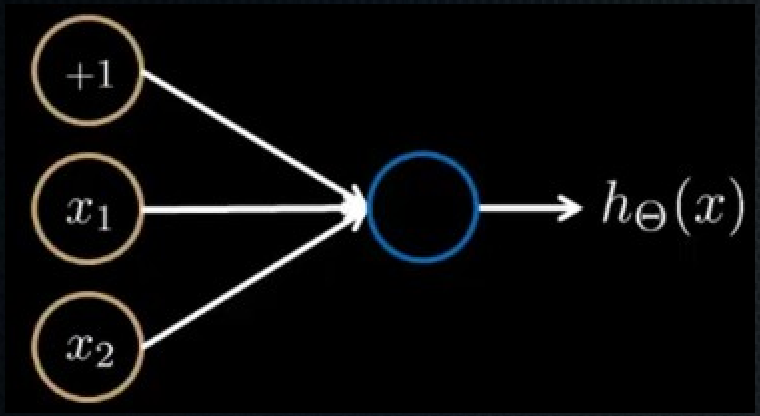


x_1 XNOR x_2

Inputs		Output
x_1	x_2	x_1 XNOR x_2
0	0	1
0	1	0
1	0	0
1	1	1

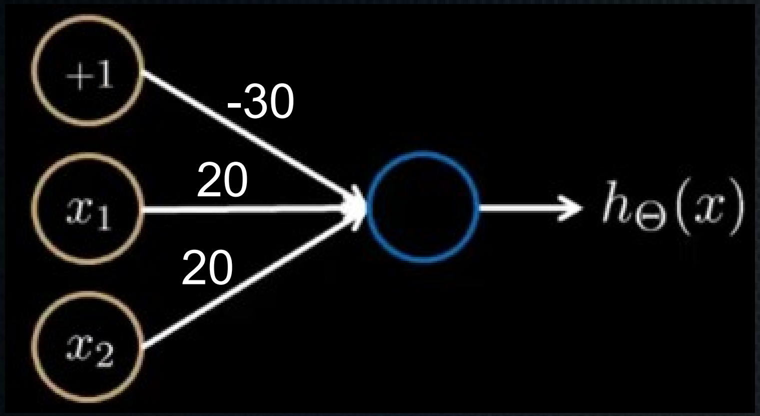
Making simple functions ourselves

- AND function → x_1 and x_2 can be either 0 or 1



Making simple functions ourselves

- AND function → x_1 and x_2 can be either 0 or 1

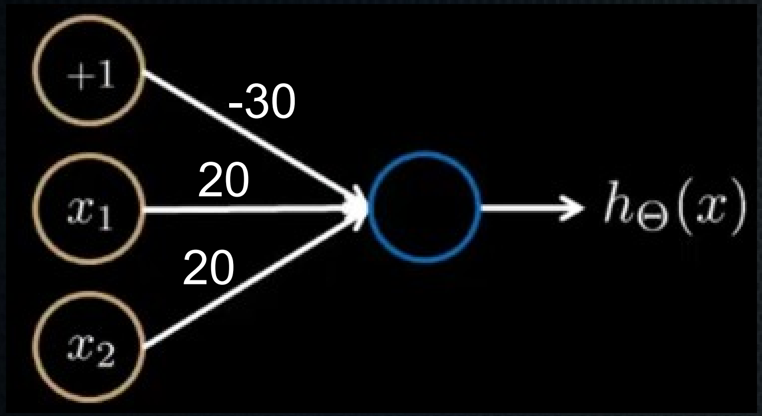


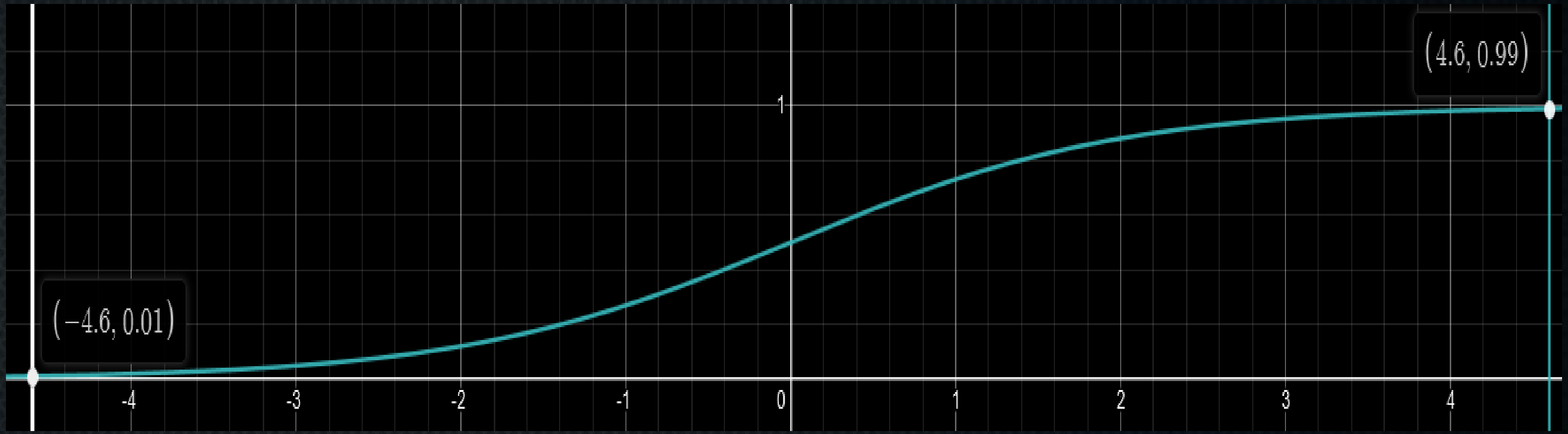
$$h_\theta(x) = sigmoid(-30 + 20 \cdot x_1 + 20 \cdot x_2)$$

$$h_\theta(x) = \sigma\left(\begin{bmatrix} -30 & 20 & 20 \end{bmatrix} \begin{bmatrix} 1 \\ x_1 \\ x_2 \end{bmatrix}\right)$$

Making simple functions ourselves

- AND function → x_1 and x_2 can be either 0 or 1

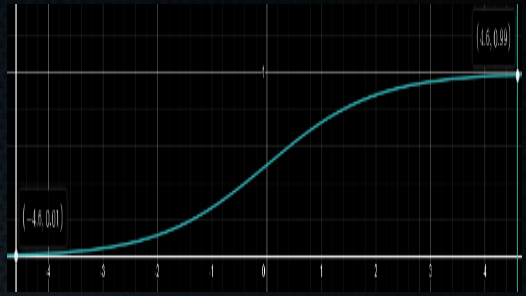


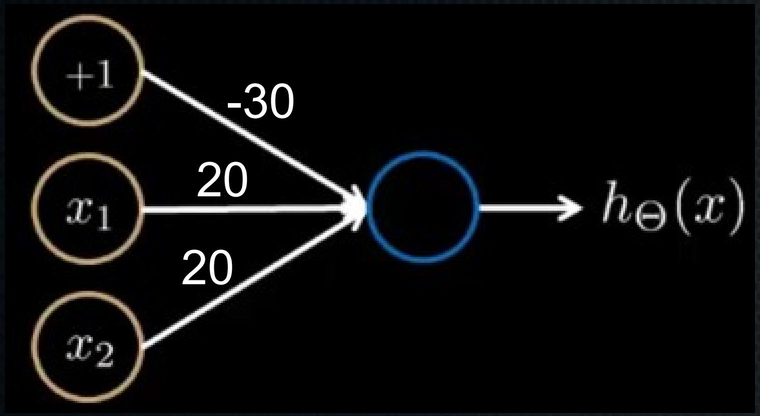


$$h_\theta(x) = sigmoid(-30 + 20 \cdot x_1 + 20 \cdot x_2)$$

Making simple functions ourselves: AND

- AND function → x_1 and x_2 can be either 0 or 1



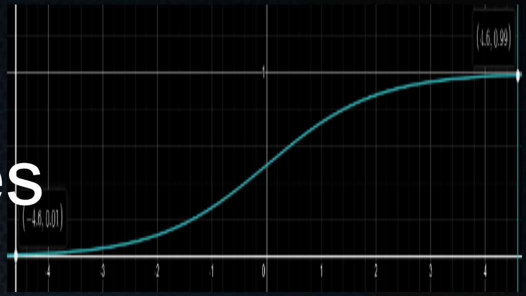


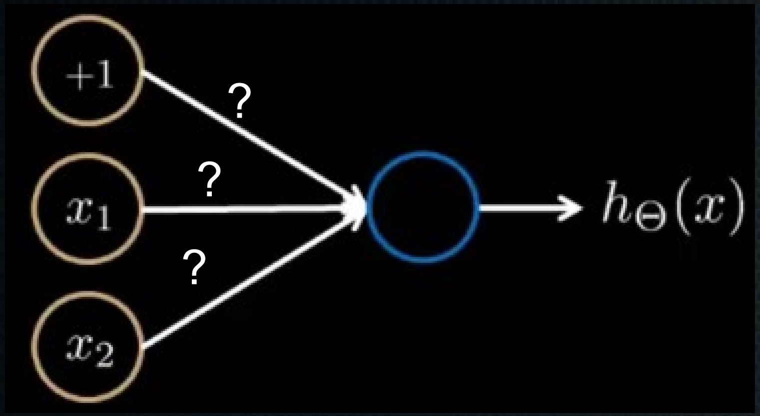
$$h_\theta(x) = sigmoid(-30 + 20 \cdot x_1 + 20 \cdot x_2)$$

x_1	x_2	$h_\Theta(x)$
0	0	$g(-30) \approx 0$
0	1	$g(-10) \approx 0$
1	0	$g(-10) \approx 0$
1	1	$g(10) \approx 1$

Making simple functions ourselves: OR

- Over to you: make an OR function → try
  it yourself and discuss with neighbours for 2 minutes





OR

x	y	x+y
0	0	0
0	1	1
1	0	1
1	1	1

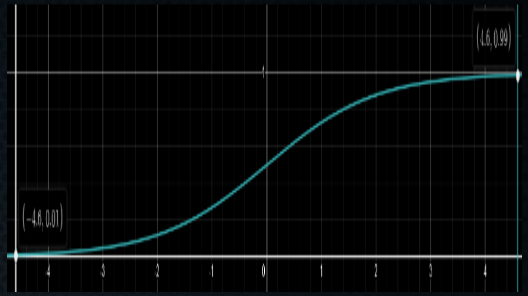
Zorg dat ik op de slide kan schrijven!

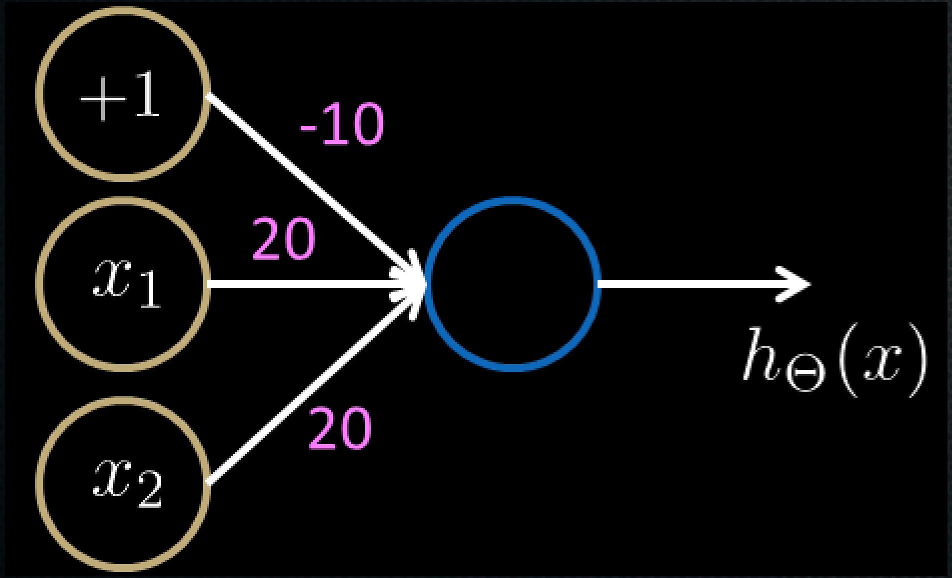
$$h_\theta(x) = sigmoid(? + ? \cdot x_1 + ? \cdot x_2)$$

Om hier truth table van studenten te maken

Making simple functions ourselves: OR

- Answer

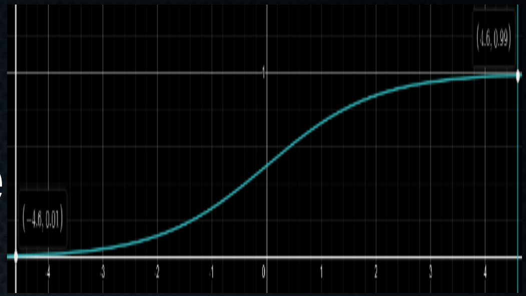


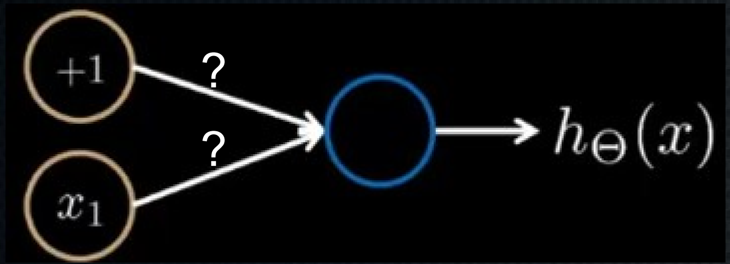


x_1	x_2	$h_\Theta(x)$
0	0	g(-10) ~= 0
0	1	g(-10+20) ~= 1
1	0	g(-10+20) ~= 1
1	1	g(-10 + 20 + 20) ~= 1

Making simple functions ourselves: NOT

- Over to you: make a NOT function → try
  it yourself and discuss with neighbours for 2 minute





NOT

x	x'
0	1
1	0

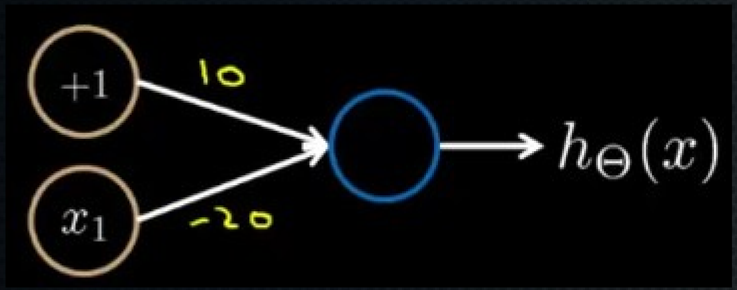
Zorg dat ik op de slide kan schrijven!

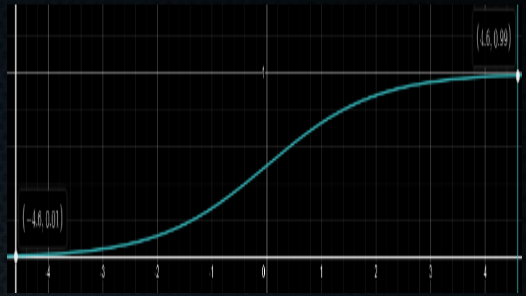
$$h_\theta(x) = sigmoid(? + ? \cdot x_1)$$

Om hier truth table van studenten te maken

Making simple functions ourselves: NOT

- Answer

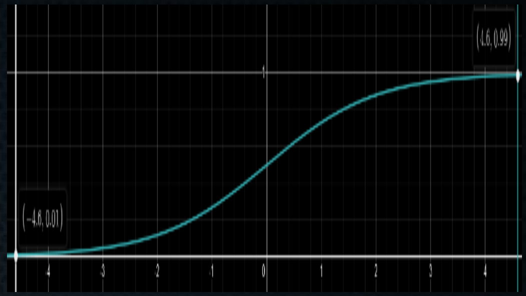


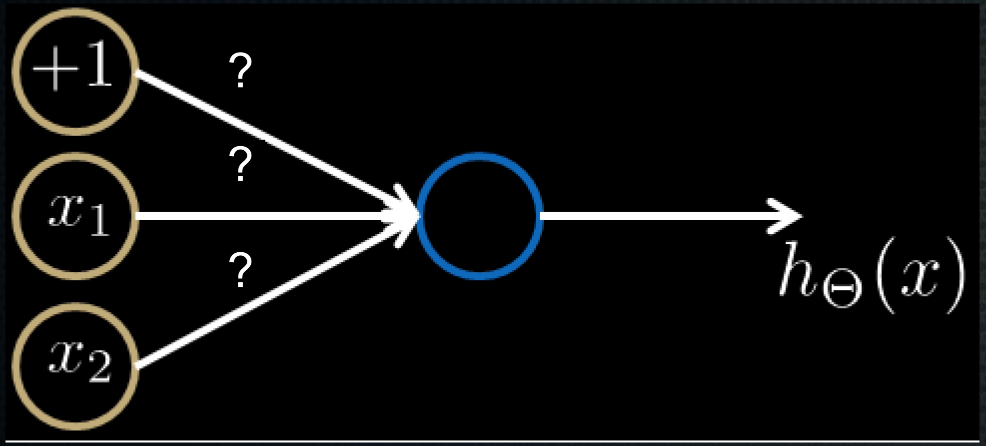


Just put a large negative weight in front of whatever you want to negate (enough to overcome the bias)

Making simple functions ourselves: (NOT x_1) AND (NOT x_2)

- Make NOT x_1 AND NOT x_2 → try it yourself and discuss with neighbours for 2 minutes





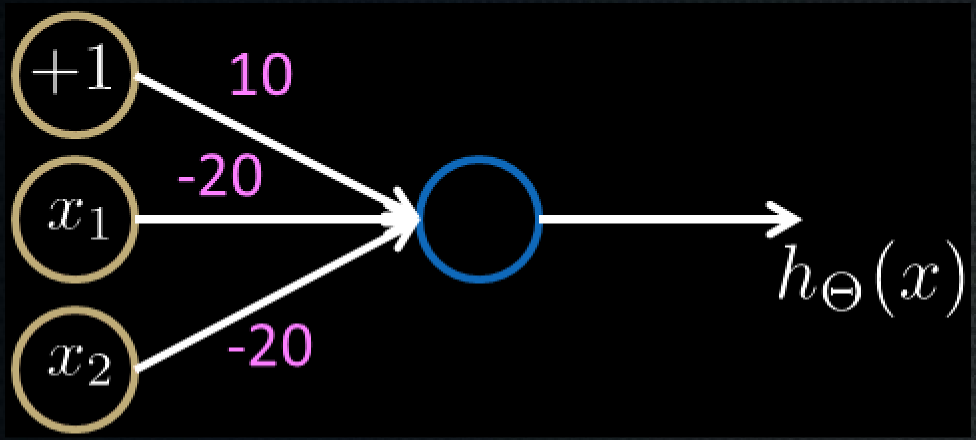
$$h_\theta(x) = sigmoid(? + ? \cdot x_1 + ? \cdot x_2)$$

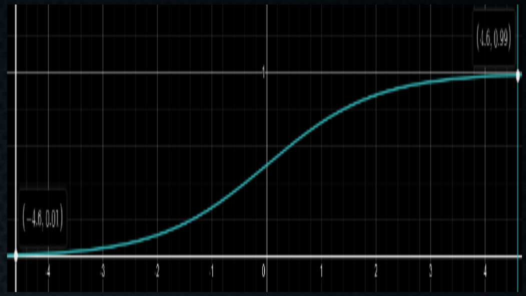
Zorg dat ik op de slide kan schrijven!

Om hier truth table van studenten te maken

Making simple functions ourselves: (NOT x_1) AND (NOT x_2)

- Answer

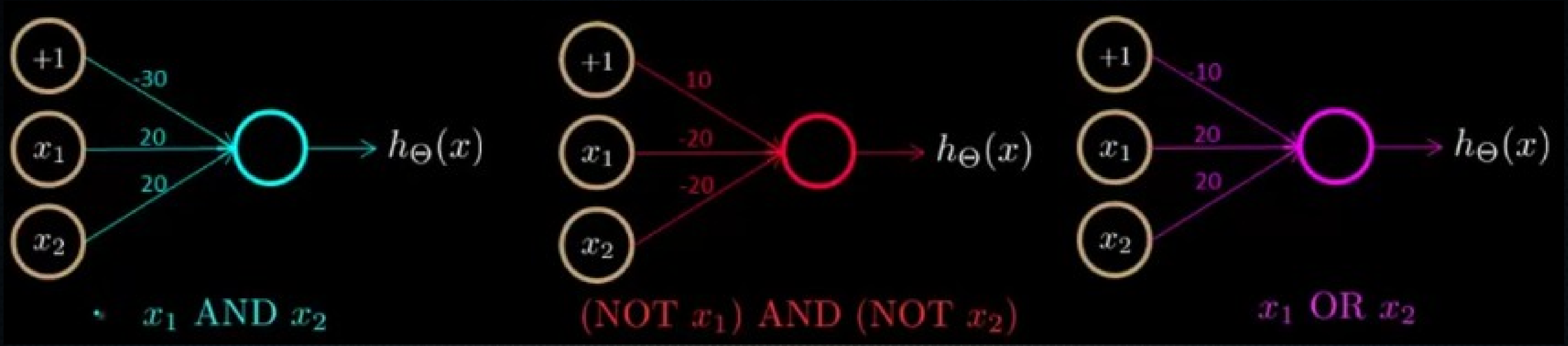


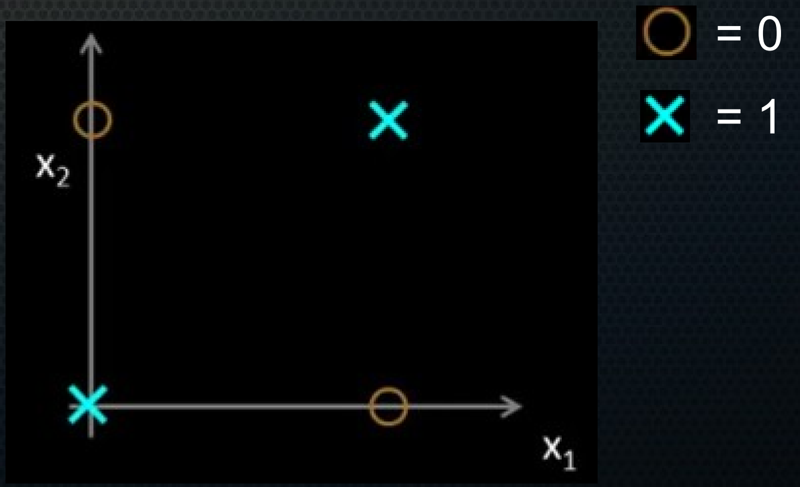


Just put a large negative weight in front of whatever you want to negate (enough to overcome the bias)

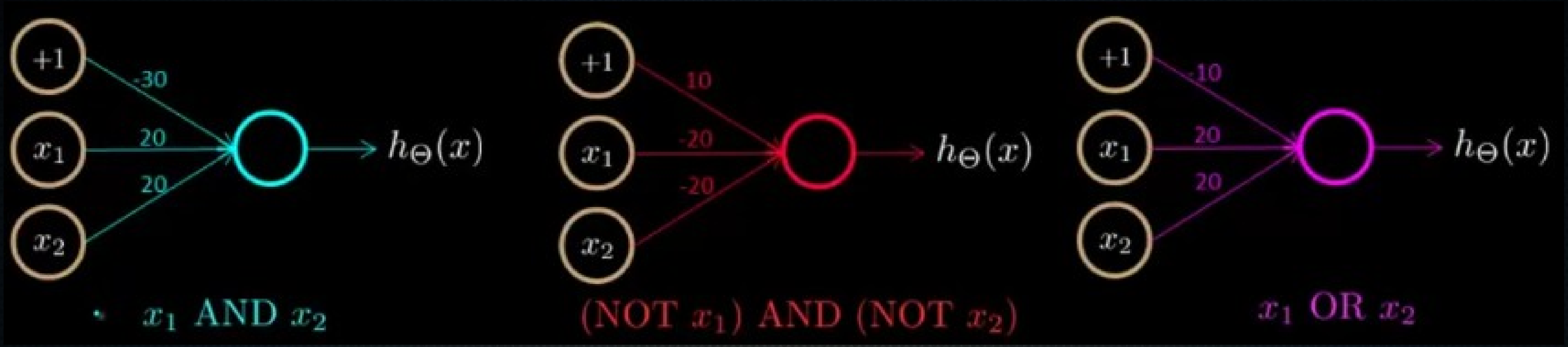
Only positive when $x_1 = x_2 = 0$

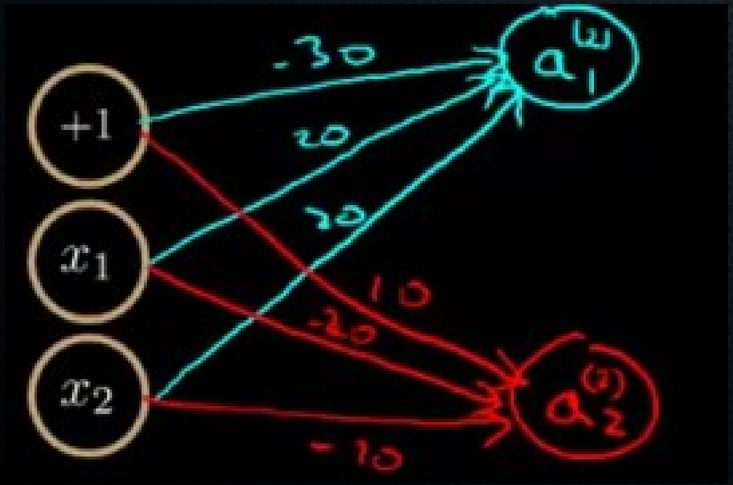
Finally: x_1 XNOR x_2



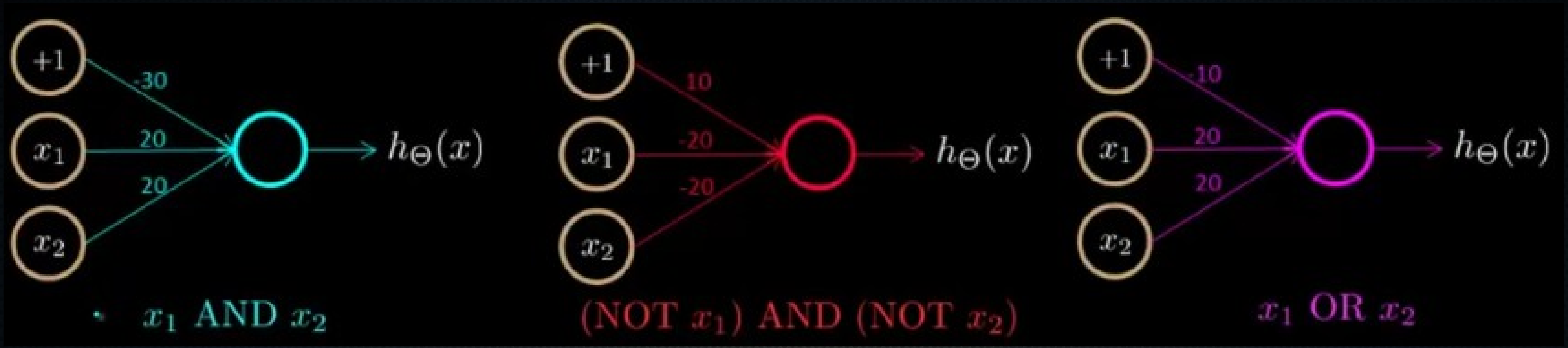


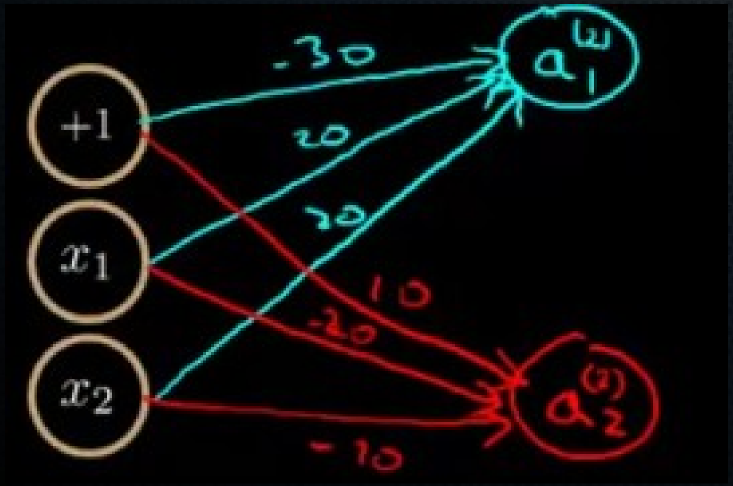
Finally: x_1 XNOR x_2





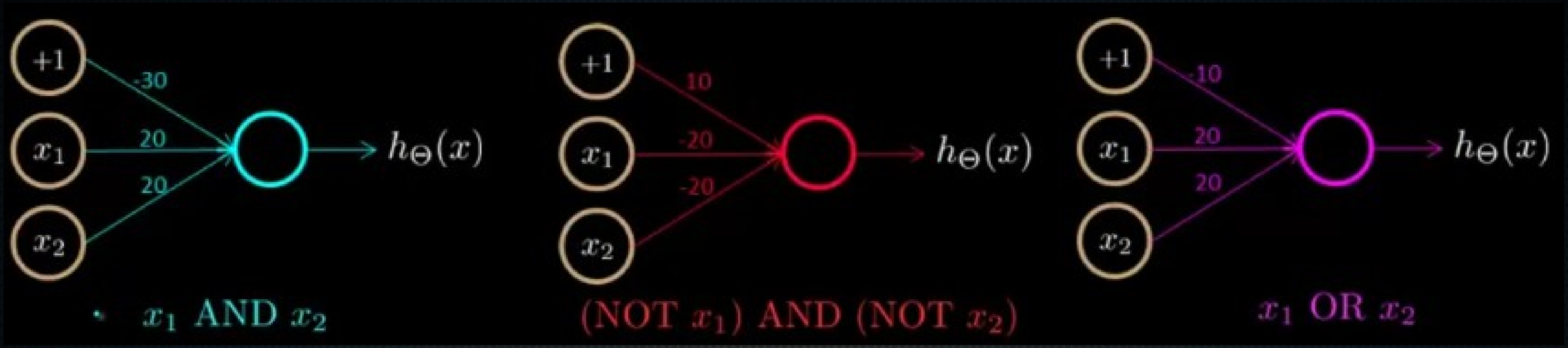
Finally: x_1 XNOR x_2





x_1	x_2	$a_1^{(2)}$	$a_2^{(2)}$
0	0	0	1
0	1	0	0
1	0	0	0
1	1	1	0

Finally: x_1 XNOR x_2

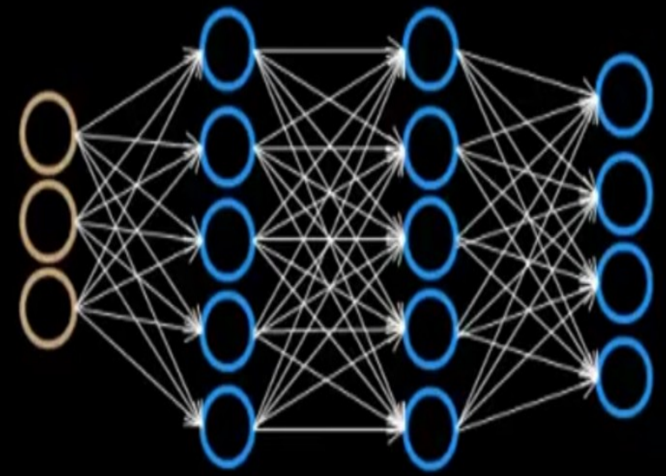


x_1	x_2	$a_1^{(2)}$	$a_2^{(2)}$	$h_\Theta(x)$
0	0	0	1	1
0	1	0	0	0
1	0	0	0	0
1	1	1	0	1

Computing complex functions

- This is an illustration of how neural networks work: earlier layers can compute simple functions like AND and OR. By combining those outputs, you can compute more complex functions.

Multiclass classification in neural nets

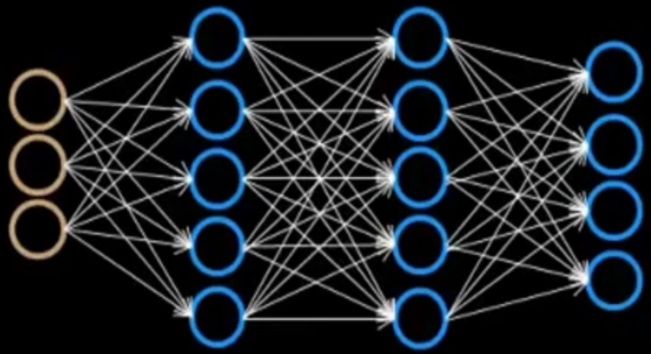


$h_\Theta(x) \in \mathbb{R}^4$

Want $h_\Theta(x) \approx \begin{bmatrix}1\\0\\0\\0\end{bmatrix}$, $h_\Theta(x) \approx \begin{bmatrix}0\\1\\0\\0\end{bmatrix}$, $h_\Theta(x) \approx \begin{bmatrix}0\\0\\1\\0\end{bmatrix}$, etc.

when pedestrian   when car   when motorcycle

Multiclass classification in neural nets



$h_\Theta(x) \in \mathbb{R}^4$

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when pedestrian when car when motorcycle

Training set: $(x^{(1)}, y^{(1)}), (x^{(2)}, y^{(2)}), \ldots, (x^{(m)}, y^{(m)})$

$y^{(i)}$ one of $\begin{bmatrix}1\\0\\0\\0\end{bmatrix}$, $\begin{bmatrix}0\\1\\0\\0\end{bmatrix}$, $\begin{bmatrix}0\\0\\1\\0\end{bmatrix}$, $\begin{bmatrix}0\\0\\0\\1\end{bmatrix}$

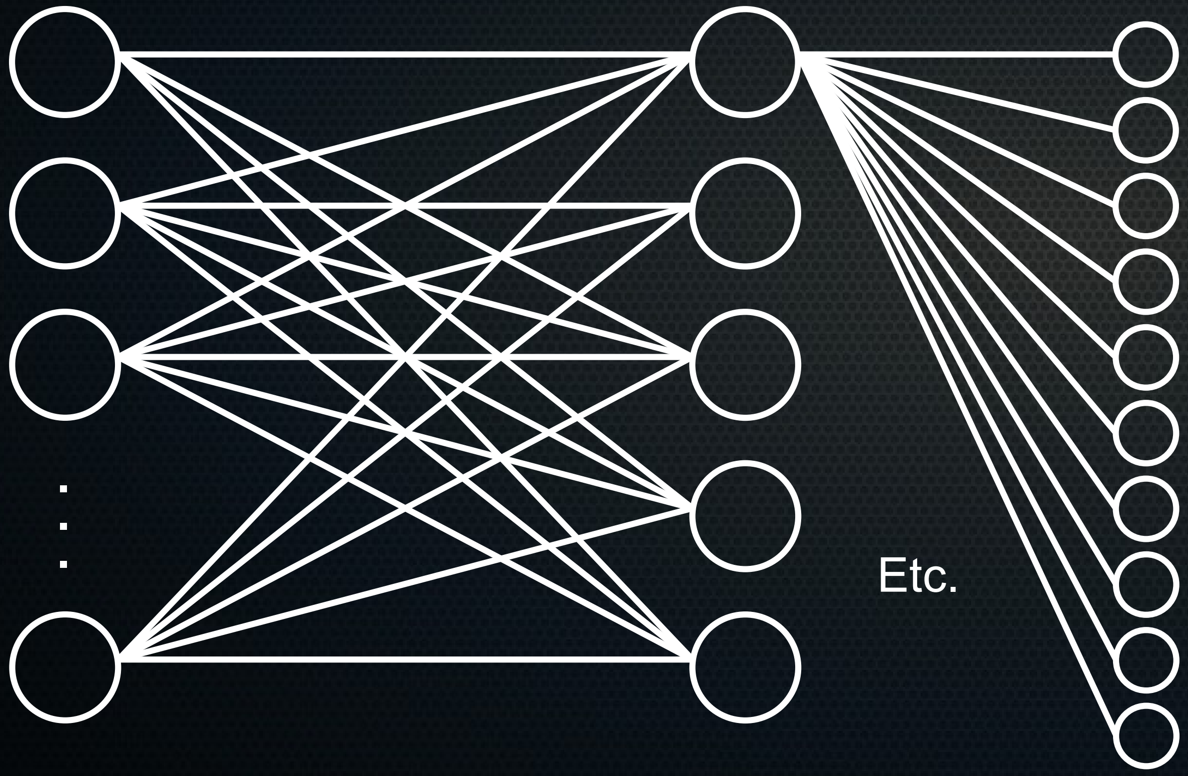
pedestrian car motorcycle truck

~~Previously~~

$\cancel{y \in \{1, 2, 3, 4\}}$

Question to you

- Say we have 10 classes and the following network, how many parameters in $\Theta^{(2)}$?



$\Theta^{(j)}$ = matrix of weights controlling function mapping from layer j to layer $j+1$

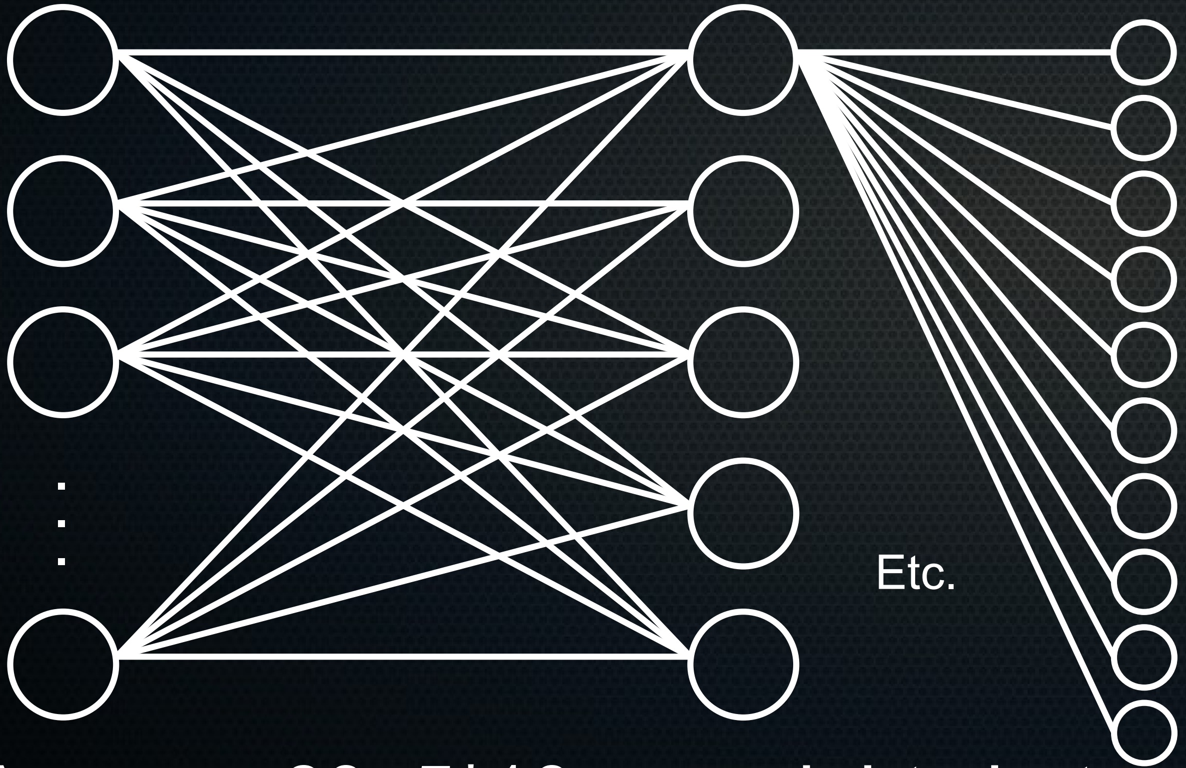
$$y^{(10)} = \begin{bmatrix} 0 \\ 0 \\ 1 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix}$$

Example:
10th training sample is class 3

Question to you

- Say we have 10 classes and the following network, how many parameters in $\Theta^{(2)}$?

$\Theta^{(j)} =$ matrix of weights controlling function mapping from layer j to layer $j+1$



$$y^{(10)} = \begin{bmatrix} 0 \\ 0 \\ 1 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix}$$

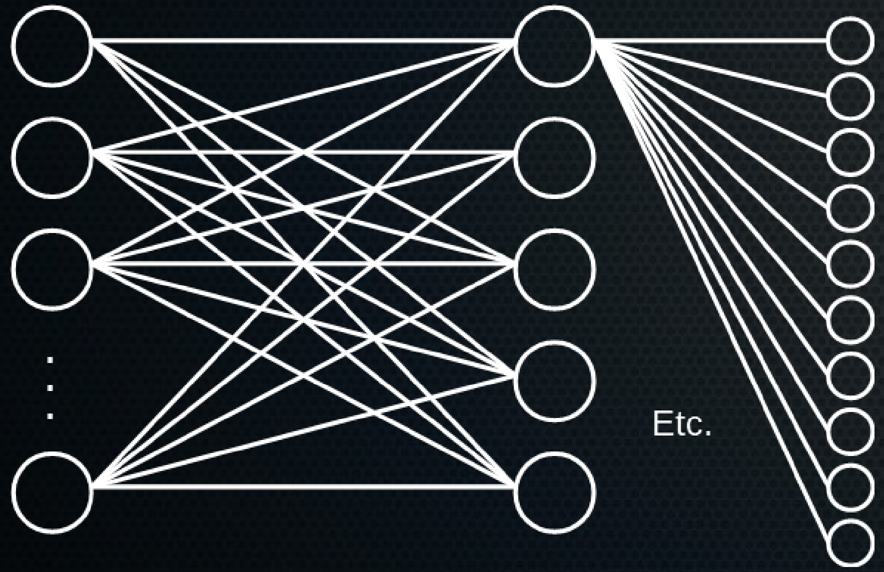
Example:
10th training sample is class 3

- Answer: 60. 5*10 → weights between units.
  + 10 → bias of each unit in output layer

Question to you

- Say we have 10 classes and the following network, how many parameters in $\Theta^{(2)}$?

$\Theta^{(j)} =$ matrix of weights controlling function mapping from layer j to layer $j+1$



$$\sigma\left(\overbrace{\begin{bmatrix} b_1 & w_{11} & w_{12} & w_{13} & w_{14} & w_{15} \\ b_2 & w_{21} & w_{22} & w_{23} & w_{24} & w_{25} \\ b_3 & w_{31} & w_{32} & w_{33} & w_{34} & w_{35} \\ b_4 & w_{41} & w_{42} & w_{43} & w_{44} & w_{45} \\ b_5 & w_{51} & w_{52} & w_{53} & w_{54} & w_{55} \end{bmatrix}}^{\Theta^{(2)}} \begin{bmatrix} 1 \\ a_1^{(2)} \\ a_2^{(2)} \\ a_3^{(2)} \\ a_4^{(2)} \\ a_5^{(2)} \end{bmatrix}\right)$$

- Answer: 60. 5*10 → weights between units.
  + 10 → bias of each unit in output layer

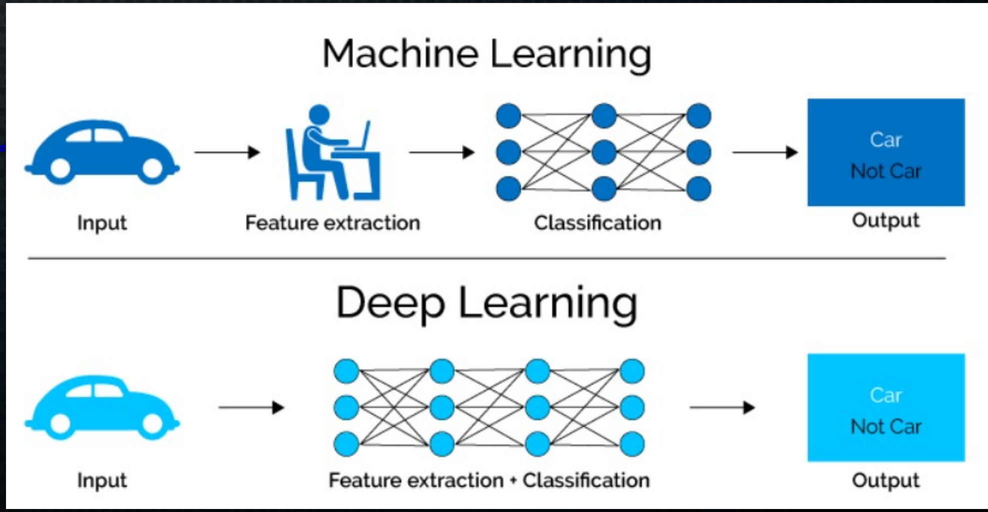
Summary

- We can use individual neurons to calculate simple logic functions
- We can combine the outputs of single neurons to calculate more complex (logic) functions
- For multiclass classification, we simply make class a vector, where we strive for the real class to be ~1, and all other classes 0.

Afternoon practical 1

- Laat de studenten kijken naar/lezen:
  https://www.youtube.com/watch?v=Ijqkc7OLenI en
  http://neuralnetworksanddeeplearning.com/chap4.html
  en :
  https://www.youtube.com/watch?v=aircAruvnKk&list=PLZHQObOWTQDNU6R1_67000Dx_ZCJB-3pi&index=1

  https://www.youtube.com/watch?v=I
  QObOWTQDNU6R1_67000Dx_ZCJ



Source: https://towardsdatascience.com/cnn-application-on-structured-data-automated-feature-extraction-8f2cd28d9a7e

Afternoon practical 2

- Multiclass logistic regression: geef bio dataset met, zeg, 6 kankerclasses en wat features.
  → laat splitsen in test en trainset
  → train 6 binaire classifiers (laat ook zelf data transformeren daartoe) met gradient descent
  →plot resultaat van elke classifier op train en testset gedurende training. (liefst in 6 aparte plotjes met decision boundary erop geprojecteerd)
- (optioneel) → laat zelfde kort doen op MNIST data
- Neural network:
  → start met vrijelijk 15 minuten klooien met https://playground.tensorflow.org/#activation=sigmoid&batchSize=10&dataset=circle&regDataset=reg-plane&learningRate=0.03&regularizationRate=0&noise=0&networkShape=4,2,2&seed=0.12635&showTestData=false&discretize=false&percTrainData=50&x=true&y=true&xTimesY=false&xSquared=false&ySquared=false&cosX=false&sinX=false&cosY=false&sinY=false&collectStats=false&problem=classification&initZero=false&hideText=false
  → geef netwerkarchitectuur + pretrained weights voor MNIST, laat:
  -MNIST-data visualiseren
  -zelf netwerkuitkomst bouwen middels correcte vermenigvuldigingen en toevoegen bias units
  -Afrondend: youtubefilmpje over GAN (https://www.youtube.com/watch?v=p5U4NgVGAwg) of jazzmuziek maken: https://www.youtube.com/watch?v=nA3YOFUCn4U of iets lezen over GANs als cool extra ding: https://medium.com/sigmoid/a-brief-introduction-to-gans-and-how-to-code-them-2620ee465c30
  Beste misschien: laat ze clip 1 en 2 kijken van 3blue1brown neural net (~halfuur)