Neural Networks

CISC 7026: Introduction to Deep Learning

University of Macau

Notation Change

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$$\boldsymbol{x} = \begin{bmatrix} x_1 \\ x_2 \\ \vdots \end{bmatrix}, \quad \boldsymbol{X} = \begin{bmatrix} x_{1,1} & \cdots & x_{1,n} \\ \vdots & \ddots & \vdots \\ x_{m,1} & \cdots & x_{m,n} \end{bmatrix}$$

1. Review
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3. Limitations of linear regression
4. History of neural networks
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- *The causal effects of education on health outcomes in the UK Biobank.* Davies et al. *Nature Human Behaviour.*
- By staying in school, you are likely to live longer
- Being rich also helps, but education alone has a **causal** relationship with life expectancy

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$$f : X \times \Theta \mapsto Y$$

Approach: Learn the parameters θ such that

$$f(x, \theta) = y; \quad x \in X, y \in Y$$

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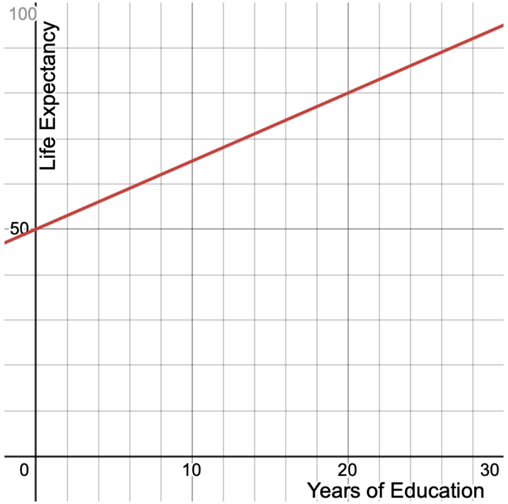
$$f(x, \boldsymbol{\theta}) = f\left(x, \begin{bmatrix} \theta_1 \\ \theta_0 \end{bmatrix}\right) = \theta_1 x + \theta_0$$



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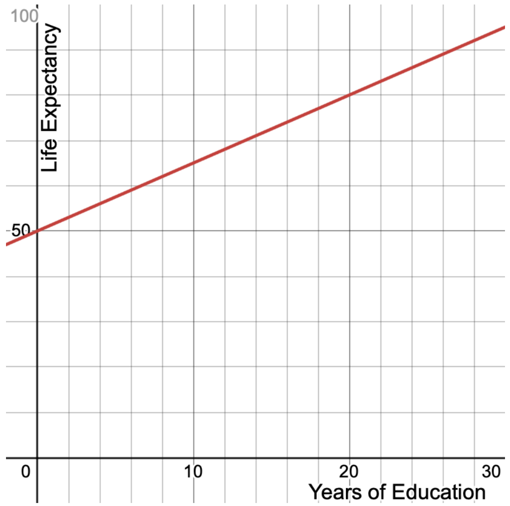

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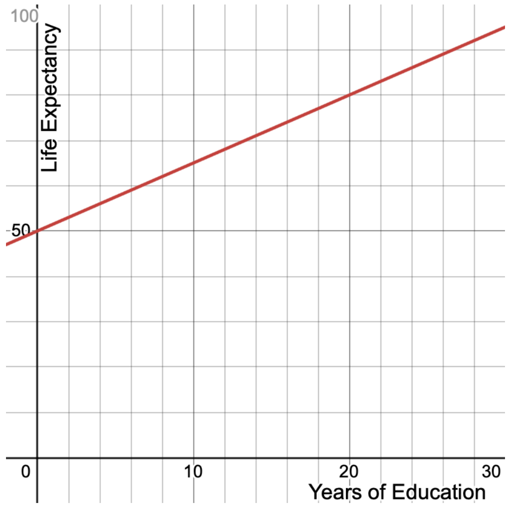

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$$\text{error}(f(x, \boldsymbol{\theta}), y) = (f(x, \boldsymbol{\theta}) - y)^2$$

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We wrote the loss function for a single datapoint $x_{[i]}, y_{[i]}$ using the square error

$$\mathcal{L}\left(x_{[i]}, y_{[i]}, \boldsymbol{\theta}\right) = \text{error}\left(f\left(x_{[i]}, \boldsymbol{\theta}\right), y_{[i]}\right) = \left(f\left(x_{[i]}, \boldsymbol{\theta}\right) - y_{[i]}\right)^2$$

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$$\mathcal{L}(\boldsymbol{x}, \boldsymbol{y}, \boldsymbol{\theta}) = \sum_{i=1}^{n} \text{error}\left(f\left(x_{[i]}, \boldsymbol{\theta}\right), y_{[i]}\right) = \sum_{i=1}^{n} \left(f\left(x_{[i]}, \boldsymbol{\theta}\right) - y_{[i]}\right)^2$$

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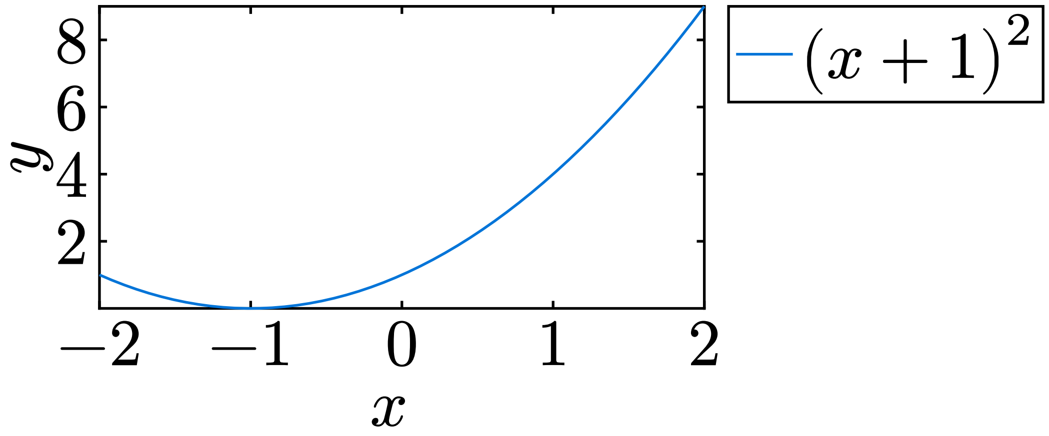

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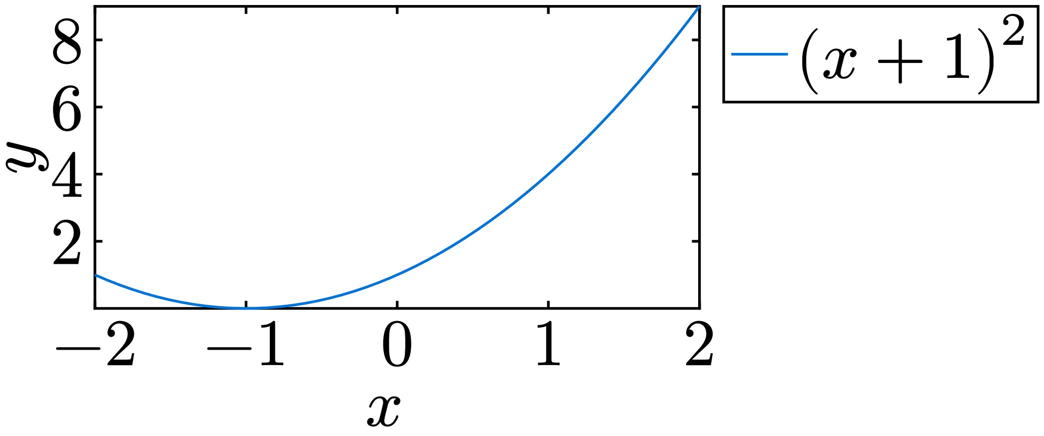

$$\arg\min_x f(x) = -1$$

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$$\arg\min_{\boldsymbol{\theta}} \mathcal{L}(\boldsymbol{x}, \boldsymbol{y}, \boldsymbol{\theta}) = \arg\min_{\boldsymbol{\theta}} \sum_{i=1}^{n} \text{error}\left(f\left(x_{[i]}, \boldsymbol{\theta}\right), y_{[i]}\right)$$

$$= \arg\min_{\boldsymbol{\theta}} \sum_{i=1}^{n} \left(f\left(x_{[i]}, \boldsymbol{\theta}\right) - y_{[i]}\right)^2$$

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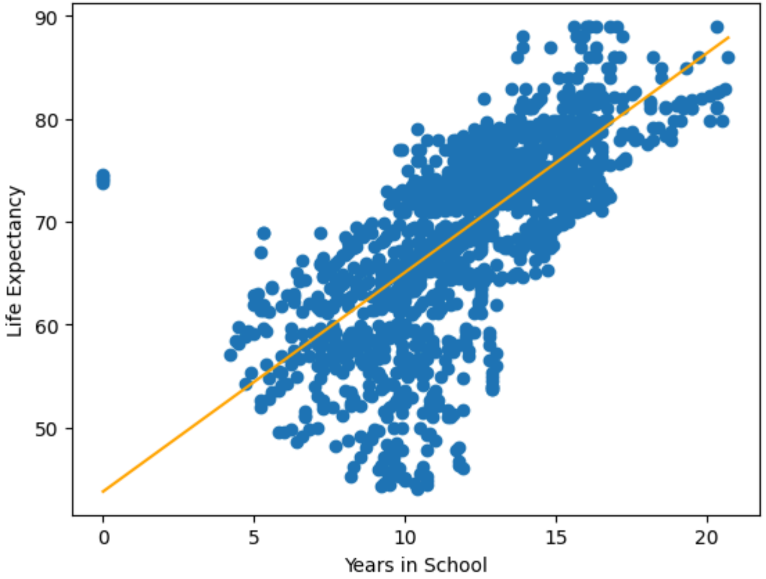

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$$\boldsymbol{X}_D = \begin{bmatrix} x_{[1]} & 1 \\ x_{[2]} & 1 \\ \vdots & \vdots \\ x_{[n]} & 1 \end{bmatrix} \Rightarrow \boldsymbol{X}_D = \begin{bmatrix} \log\left(1 + x_{[1]}\right) & 1 \\ \log\left(1 + x_{[2]}\right) & 1 \\ \vdots & \vdots \\ \log\left(1 + x_{[n]}\right) & 1 \end{bmatrix}$$

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$$\boldsymbol{X}_D = \begin{bmatrix} x_{[1]} & 1 \\ x_{[2]} & 1 \\ \vdots & \vdots \\ x_{[n]} & 1 \end{bmatrix} \Rightarrow \boldsymbol{X}_D = \begin{bmatrix} x_{[1]}^m & x_{[1]}^{m-1} & \ldots & x_{[1]} & 1 \\ x_{[2]}^m & x_{[2]}^{m-1} & \ldots & x_{[2]} & 1 \\ \vdots & \vdots & \ddots & & \\ x_{[n]}^m & x_{[n]}^{m-1} & \ldots & x_{[n]} & 1 \end{bmatrix}$$

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$$\Theta \in \mathbb{R}^2 \Rightarrow \Theta \in \mathbb{R}^{m+1}$$

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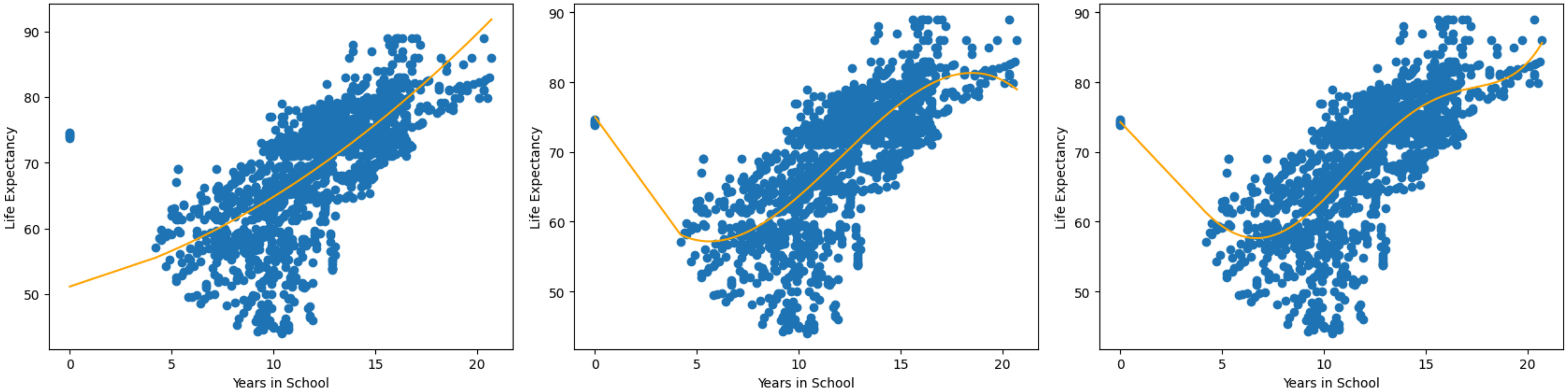

$m = 2$ $\quad$ $m = 3$ $\quad$ $m = 5$

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We can solve these problems using linear regression too

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$x_{[i],1}$ refers to the first dimension of training data i

The design matrix for a **multivariate** linear system is

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The solution is the same as before

$$\boldsymbol{\theta} = \left(\boldsymbol{X}_D^\top \boldsymbol{X}_D \right)^{-1} \boldsymbol{X}_D^\top \boldsymbol{y}$$

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Combine them to create multi-dimensional polynomial functions

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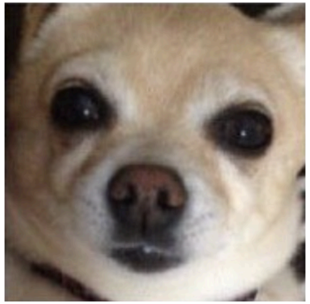
Task: predict how many ♥ a photo gets on social media



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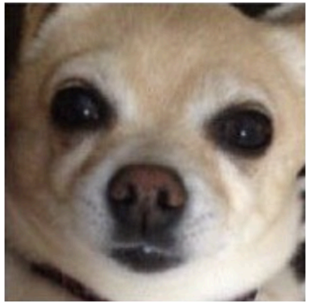

$$f : X \times \Theta \mapsto Y; \quad X : \text{Image}, \quad Y : \text{Number of } ♥$$

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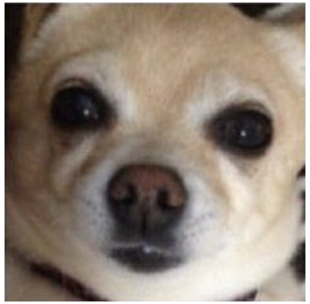

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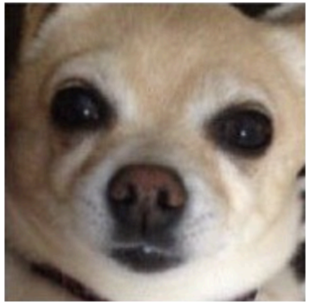

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Highly nonlinear task, use a polynomial with order $m = 20$

$$\boldsymbol{X}_D = \begin{bmatrix} \boldsymbol{x}_{D,[1]} & \cdots & \boldsymbol{x}_{D,[n]} \end{bmatrix}^\top$$

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$$\boldsymbol{x}_{D,[i]} =$$

$$\begin{bmatrix} \underbrace{x_{[i],d_x}^m x_{[i],d_x-1}^m \dots x_{[i],1}^m}_{(d_x \Rightarrow 1, x^m)} & \underbrace{x_{[i],d_x}^m x_{[i],d_x-1}^m \dots x_{[i],2}^m}_{(d_x \Rightarrow 2, x^m)} & \cdots & \underbrace{x_{[i],d_x}^{m-1} x_{[i],d_x-1}^{m-1} \dots x_{[i],1}^m}_{(d_x \Rightarrow 1, x^{m-1})} & \cdots \end{bmatrix}$$

Question: How many columns in this matrix?

$$\boldsymbol{X}_D = \begin{bmatrix} \boldsymbol{x}_{D,[1]} & \cdots & \boldsymbol{x}_{D,[n]} \end{bmatrix}^\top$$

$$\boldsymbol{x}_{D,[i]} =$$

$$\begin{bmatrix} \underbrace{x_{[i],d_x}^m x_{[i],d_x-1}^m \dots x_{[i],1}^m}_{(d_x \Rightarrow 1, x^m)} & \underbrace{x_{[i],d_x}^m x_{[i],d_x-1}^m \dots x_{[i],2}^m}_{(d_x \Rightarrow 2, x^m)} & \cdots & \underbrace{x_{[i],d_x}^{m-1} x_{[i],d_x-1}^{m-1} \dots x_{[i],1}^m}_{(d_x \Rightarrow 1, x^{m-1})} & \cdots \end{bmatrix}$$

Question: How many columns in this matrix?

Hint: $d_x = 2, m = 3$: $x^3 + y^3 + x^2 y + y^2 x + xy + x + y + 1$

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Answer: $(d_x)^m = 65536^{20} + 1 \approx 10^{96}$

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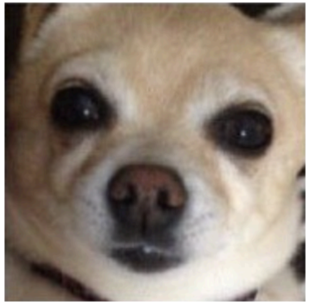

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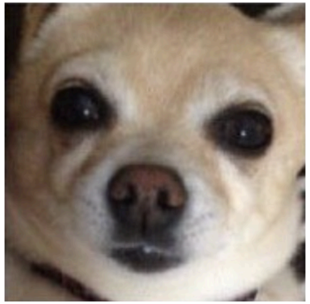

Polynomial regression does not scale to large inputs

Issues arise with other problems

1. **Poor scalability**
2. Polynomials do not generalize well

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$$\theta_m \lim_{x \to \infty} x^m = \infty$$

If $\theta_m > 0$

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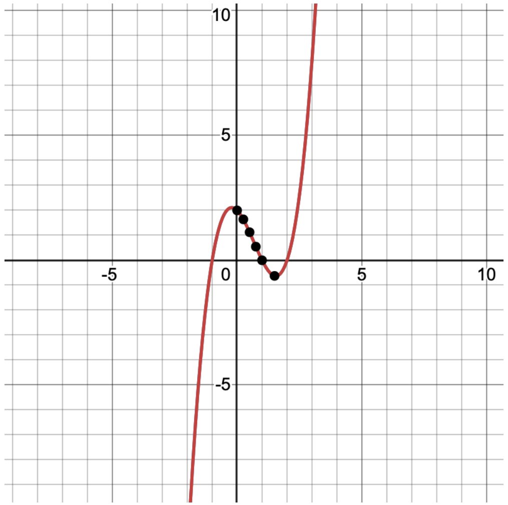

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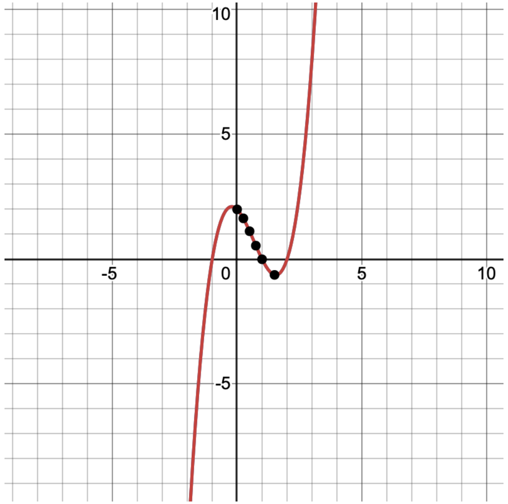

Remember, to predict new data we want our functions to generalize

Linear regression has issues

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We can use neural networks as an alternative to linear regression

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1. No analytical solution
2. High data requirement

1. Review
2. Multivariate linear regression
3. **Limitations of linear regression**
4. History of neural networks
5. Biological neurons
6. Artificial neurons
7. Wide neural networks
8. Deep neural networks
9. Practical considerations

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In 1939-1945, there was a World War

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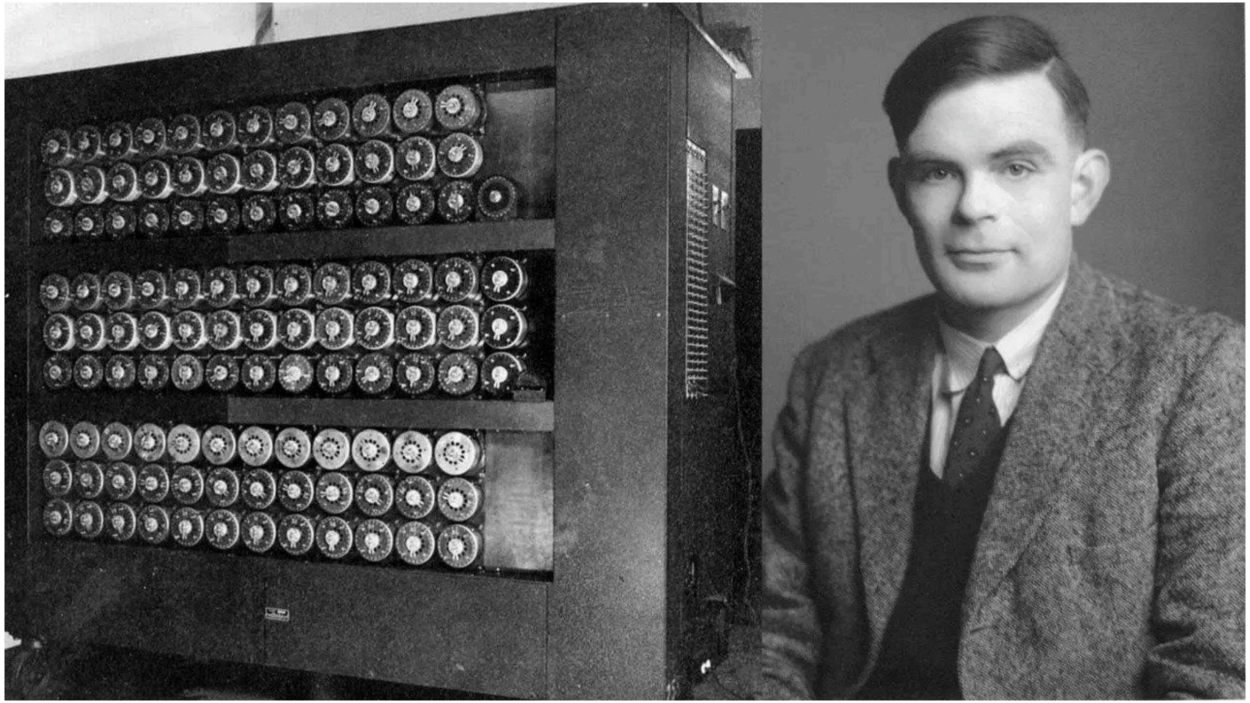
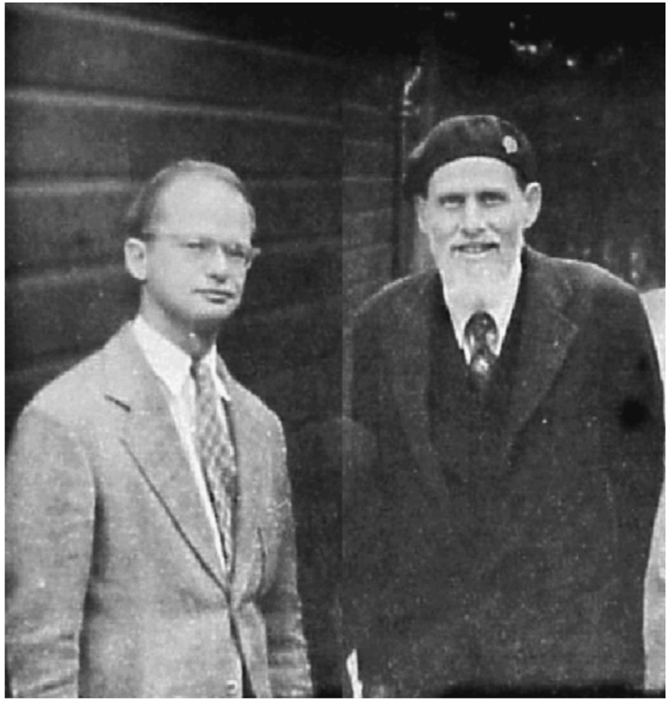


Meanwhile, a neuroscientist and mathematician (McCullough and Pitts) were trying to understand the human brain



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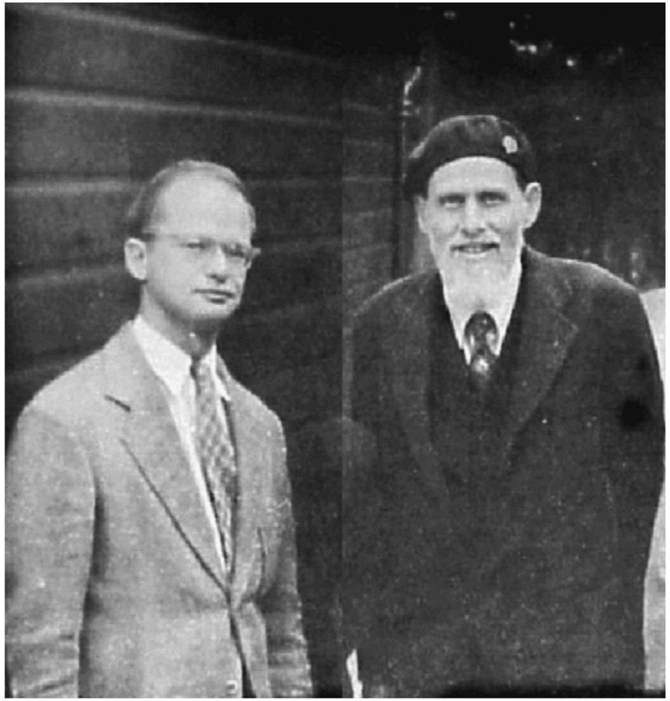

They designed the theory for the first neural network

Rosenblatt implemented this neural network theory on a computer a few years later

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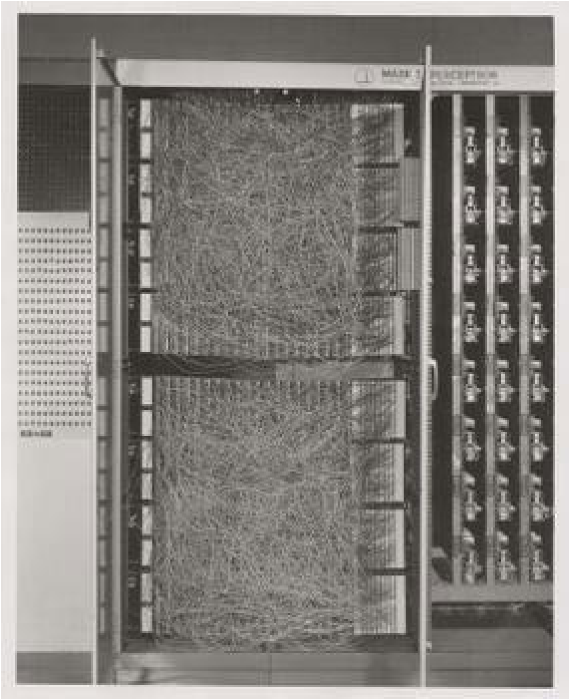
At the time, computers were very slow and expensive



Through advances in theory and hardware, neural networks became slightly better

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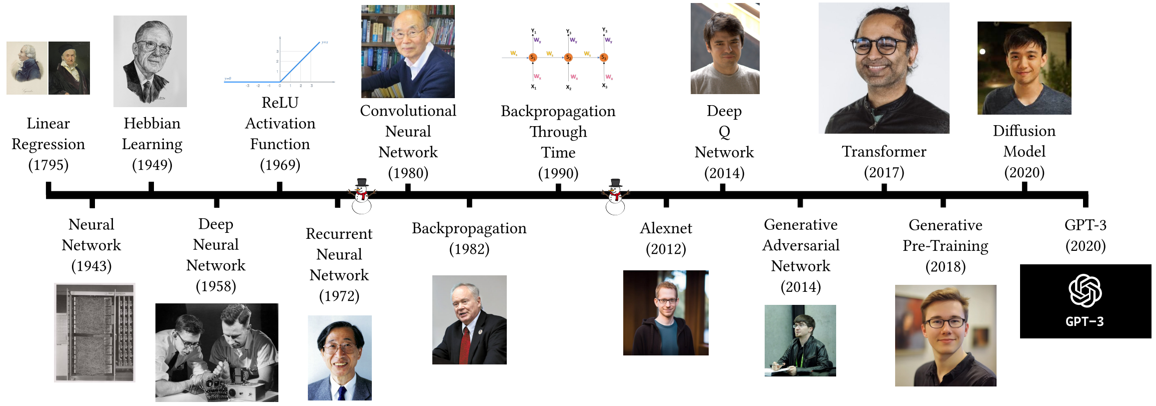
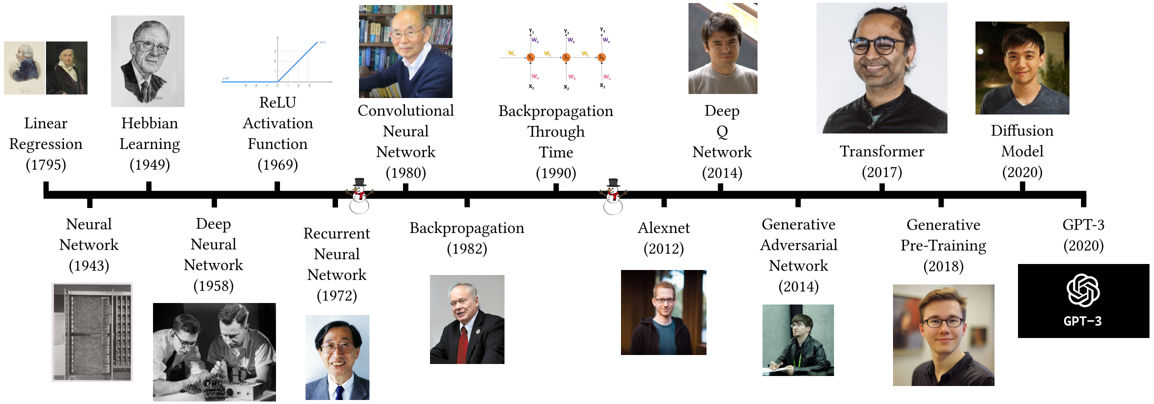


Through advances in theory and hardware, neural networks became slightly better



Around 2012, these improvements culminated in neural networks that perform like humans

So what is a neural network?

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It is a function, inspired by how the brain works

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It is a function, inspired by how the brain works

$$f : X \times \Theta \mapsto Y$$

Brains and neural networks rely on **neurons**

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First, let us review biological neurons

Brains and neural networks rely on **neurons**

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First, let us review biological neurons

Note: I am not a neuroscientist! I may make simplifications or errors with biology

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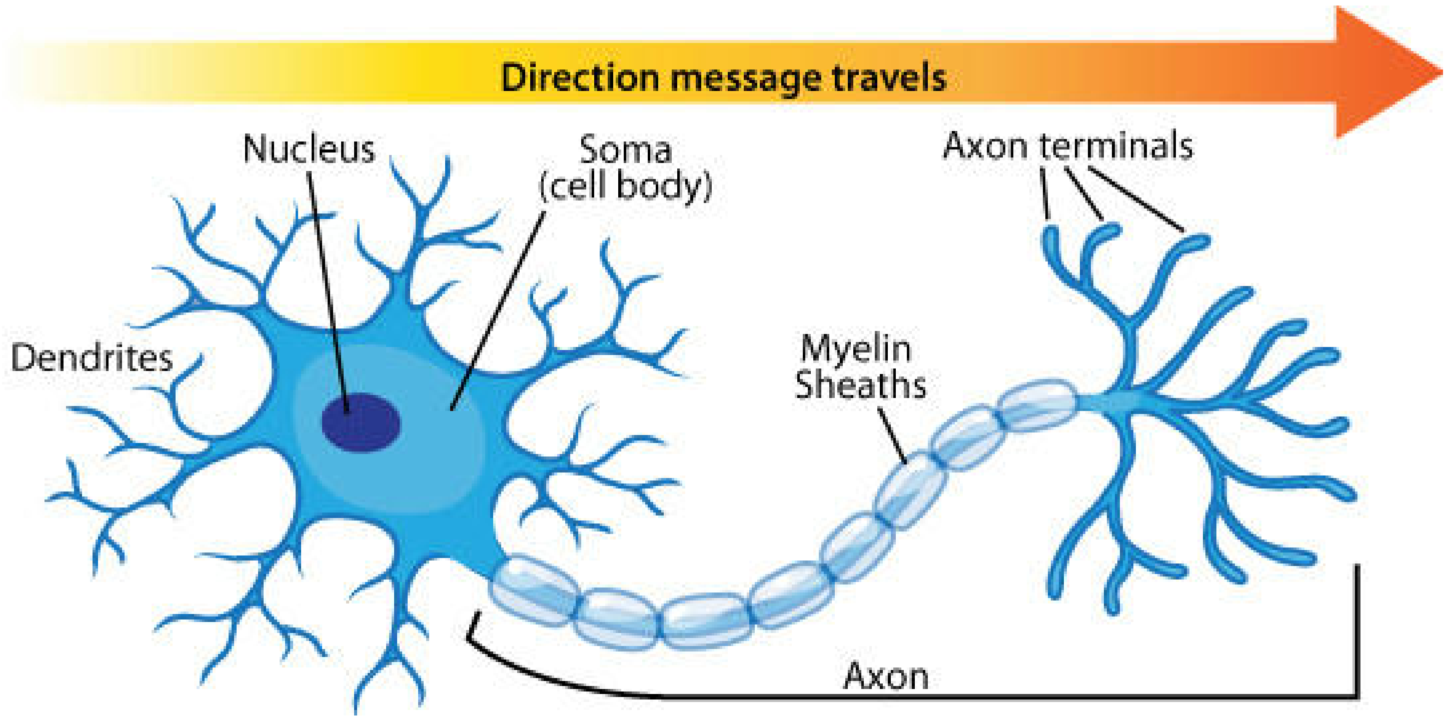
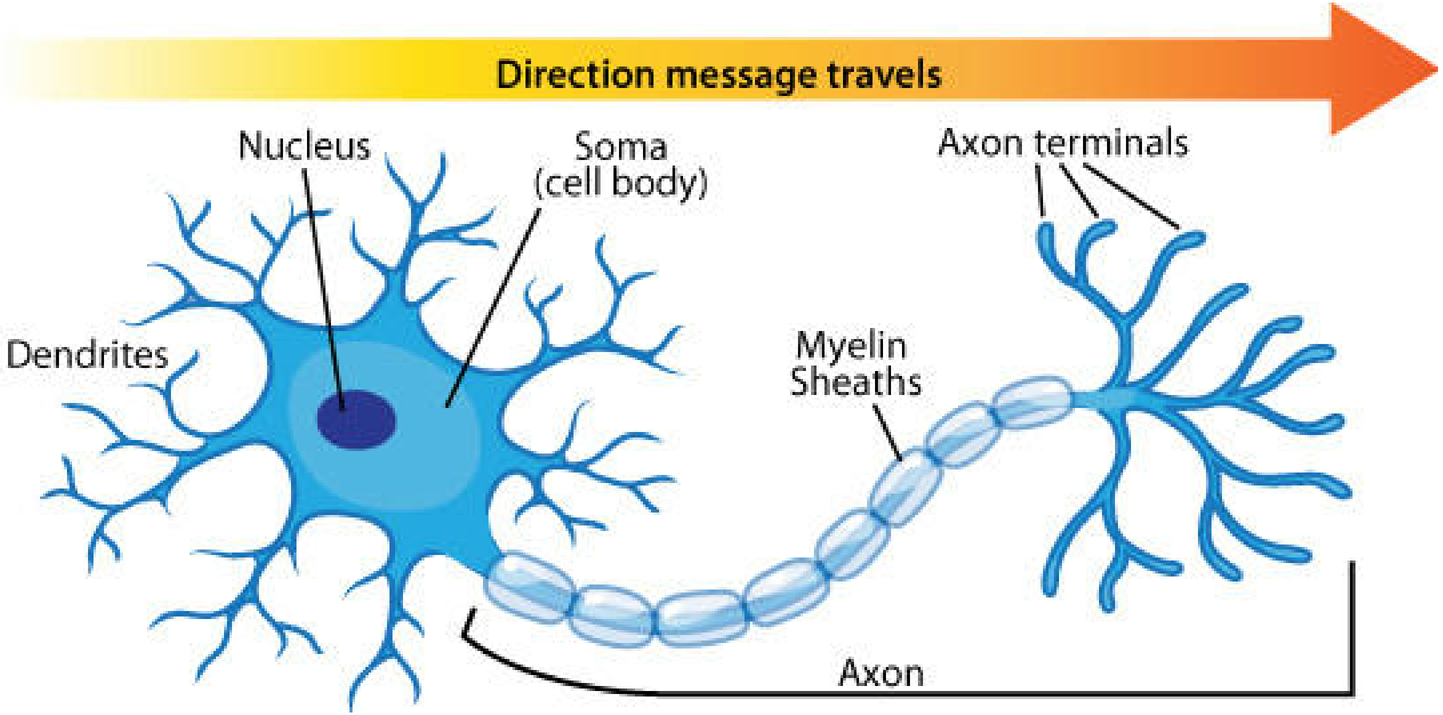
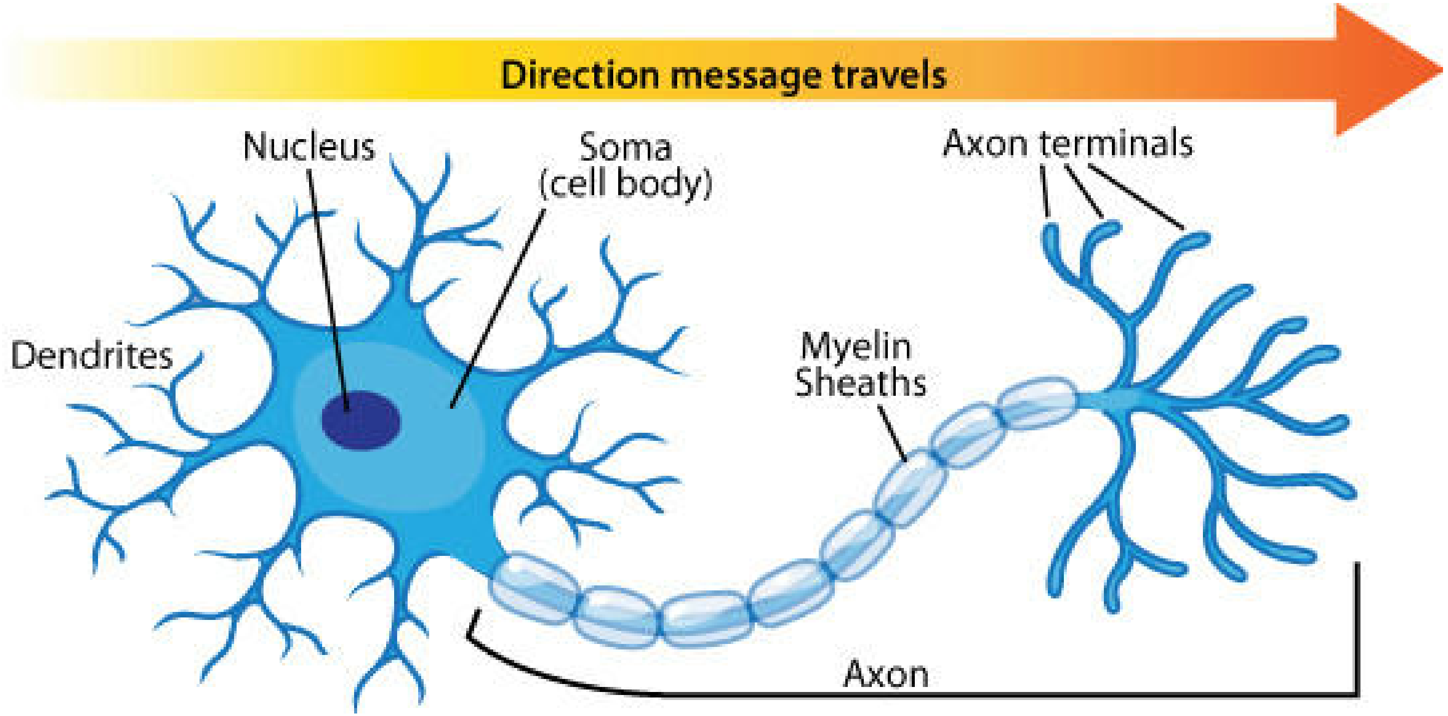


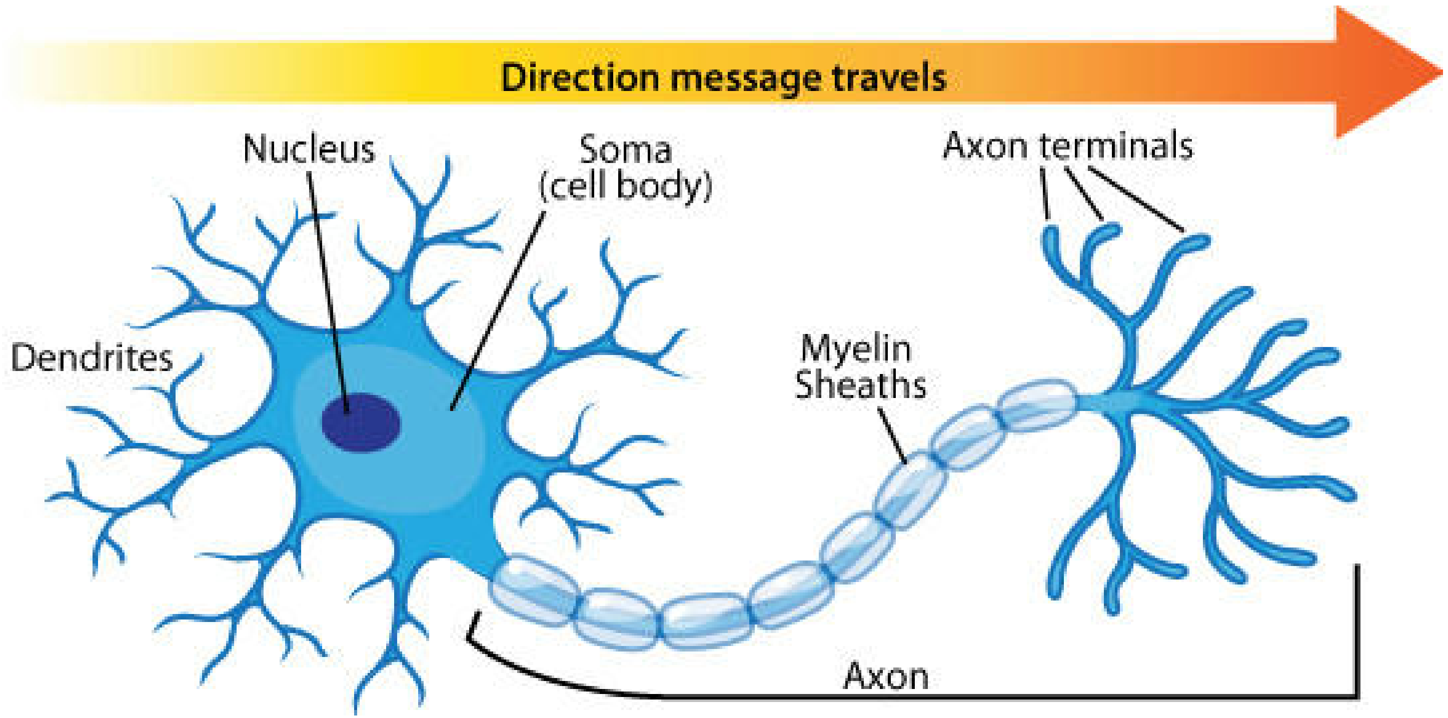
A simplified neuron consists of many parts



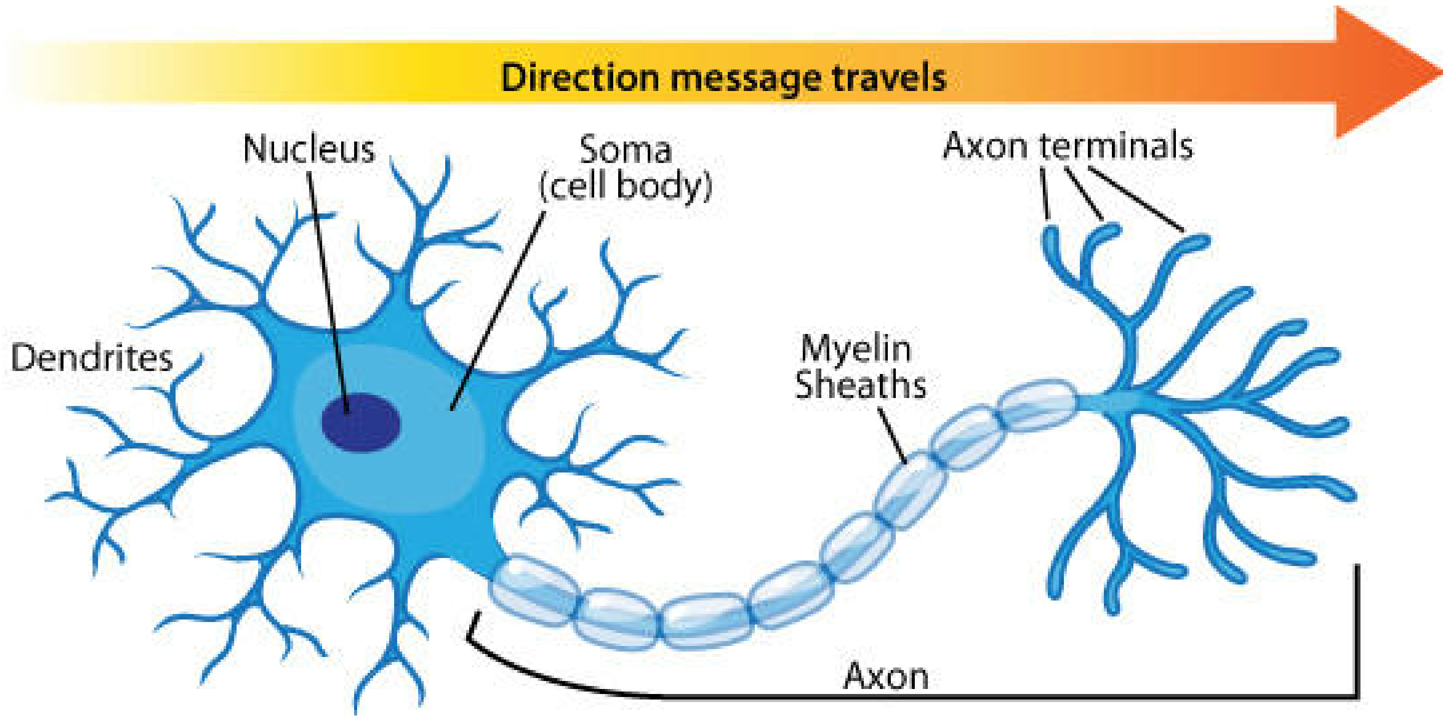
Neurons send messages based on messages received from other neurons



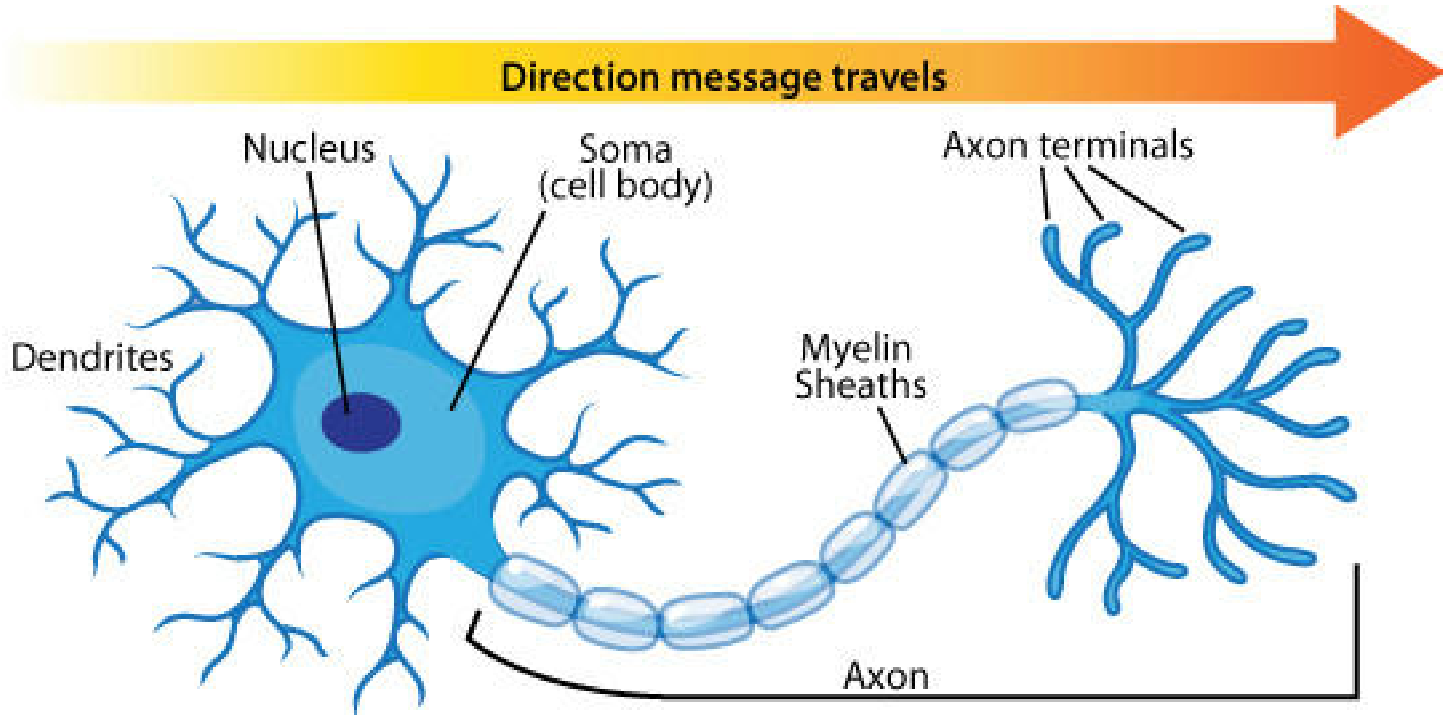
Incoming electrical signals travel along dendrites



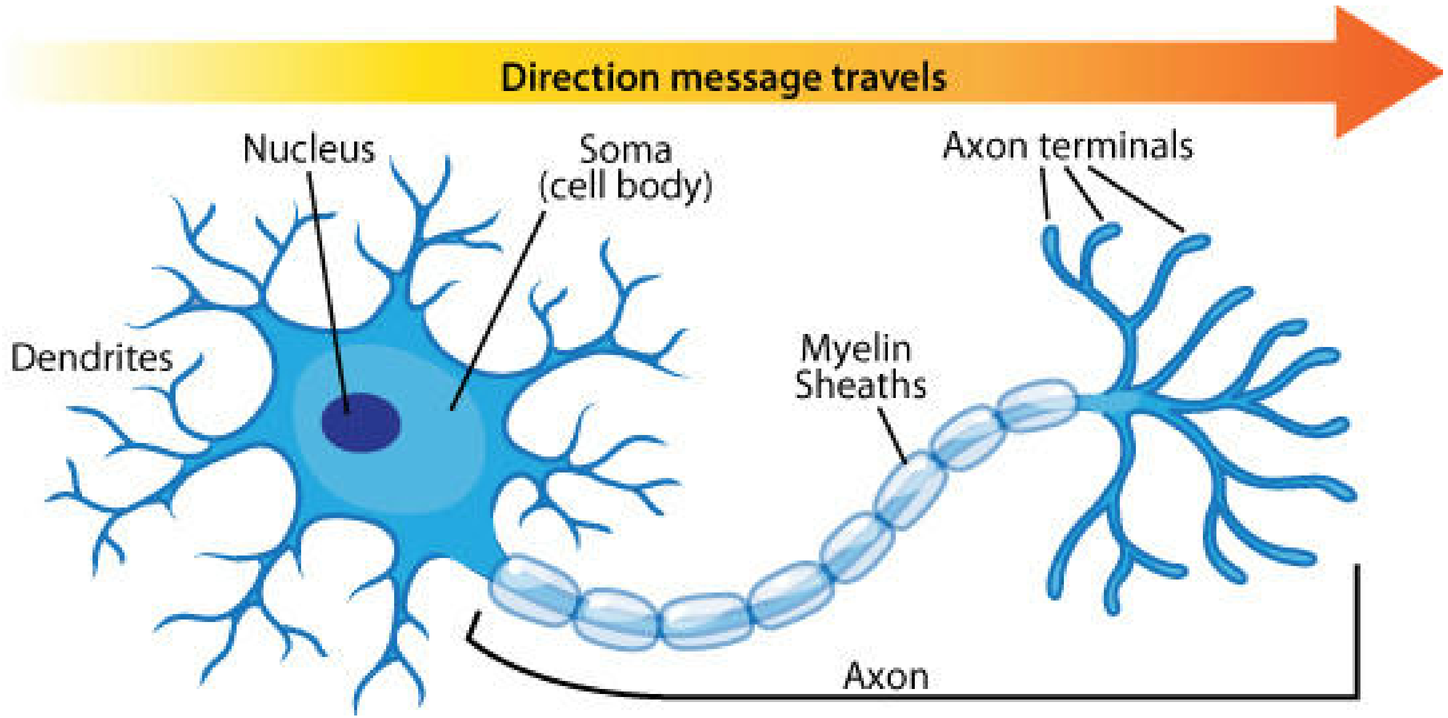
Dendrites are not all equal! Different dendrites have different diameters and structures



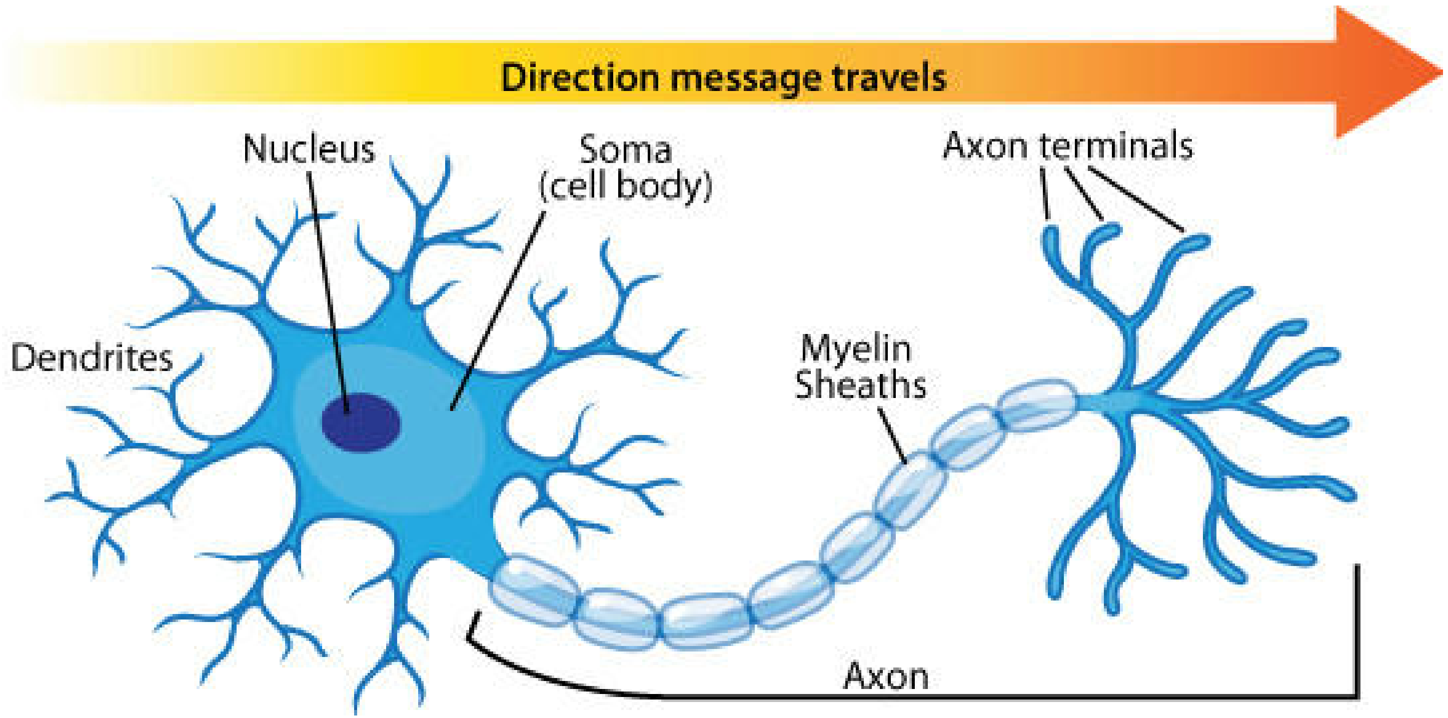
Electrical charges collect in the Soma (cell body)



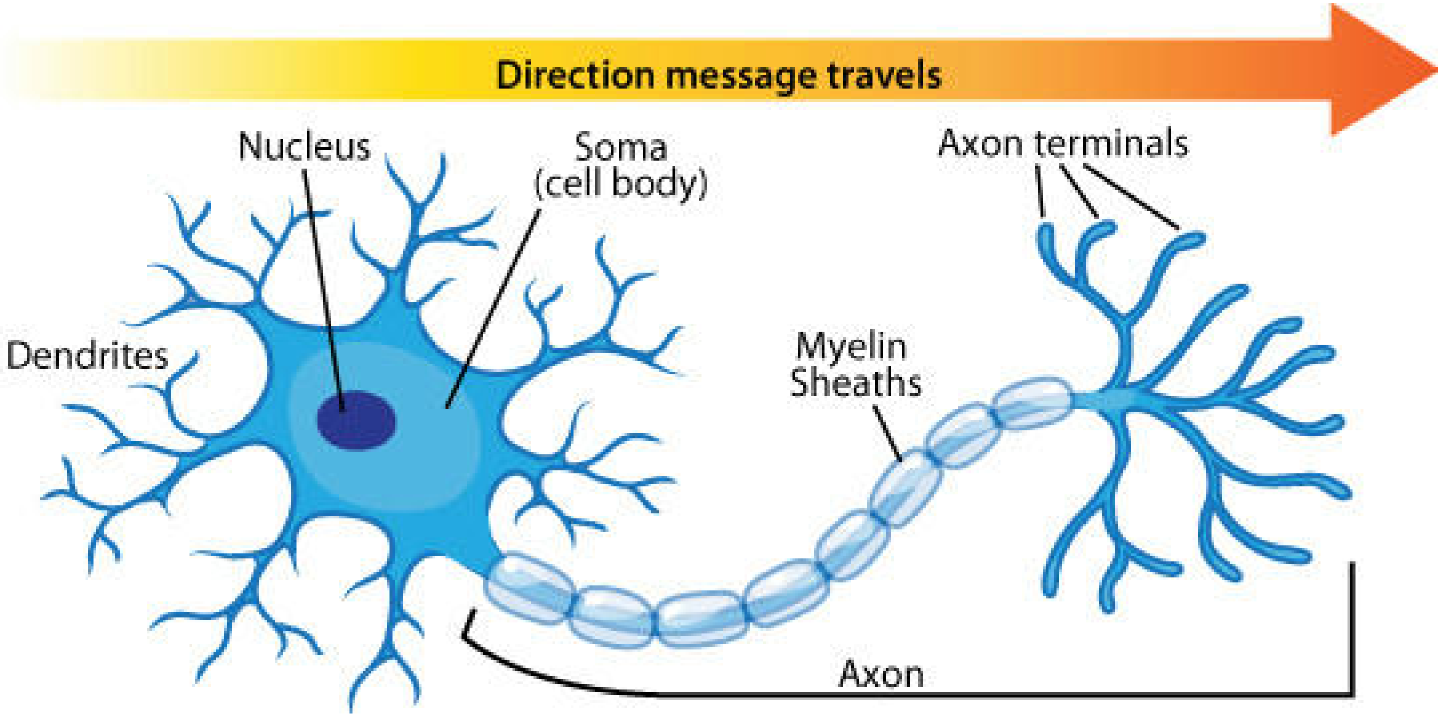
The axon outputs an electrical signal to other neurons



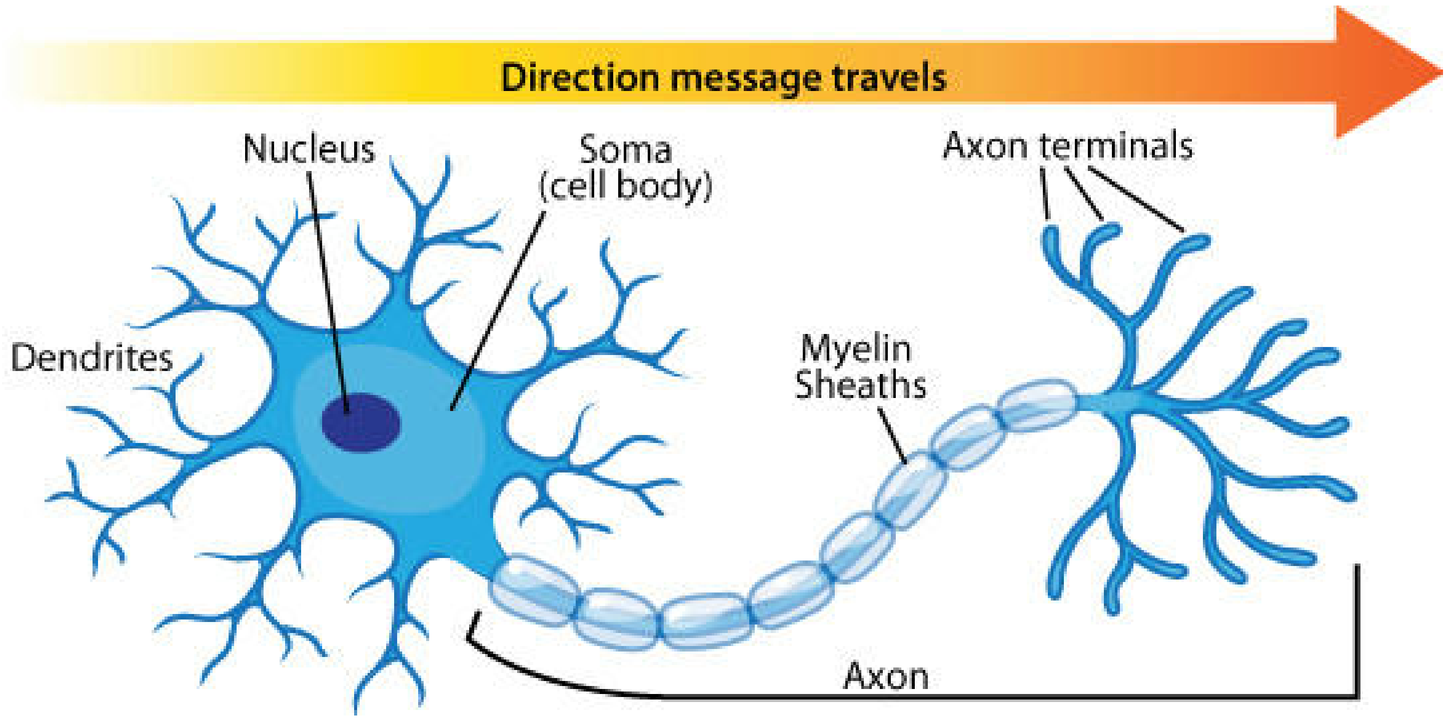
The axon terminals will connect to dendrites of other neurons



For our purposes, we can consider the axon terminals and dendrites to be the same thing



The neuron takes many inputs, and produces a single output



The neuron will only output a signal down the axon (“fire”) at certain times

How does a neuron decide to send an impulse (“fire”)?

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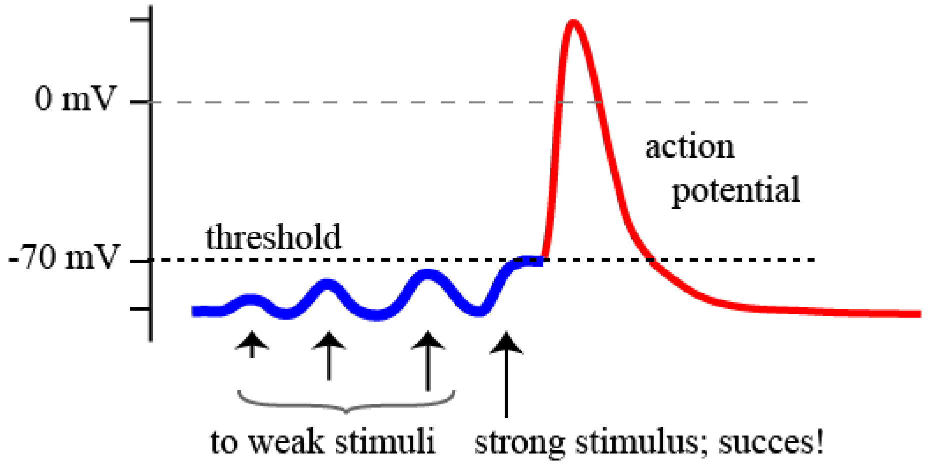
Incoming impulses (via dendrites) change the electric potential of the neuron



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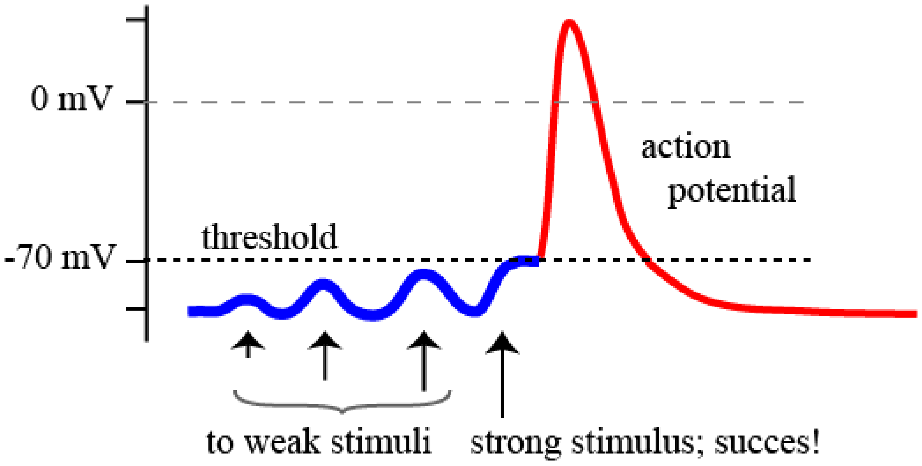

In a parallel circuit, we can sum voltages together

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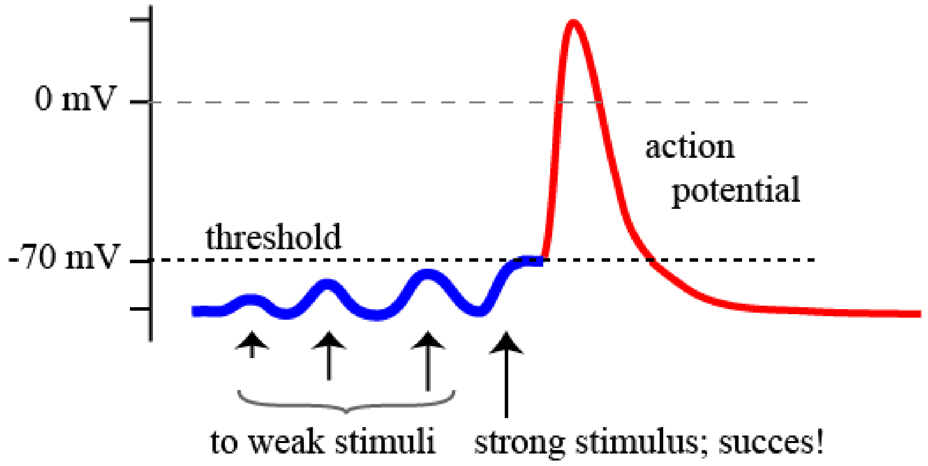
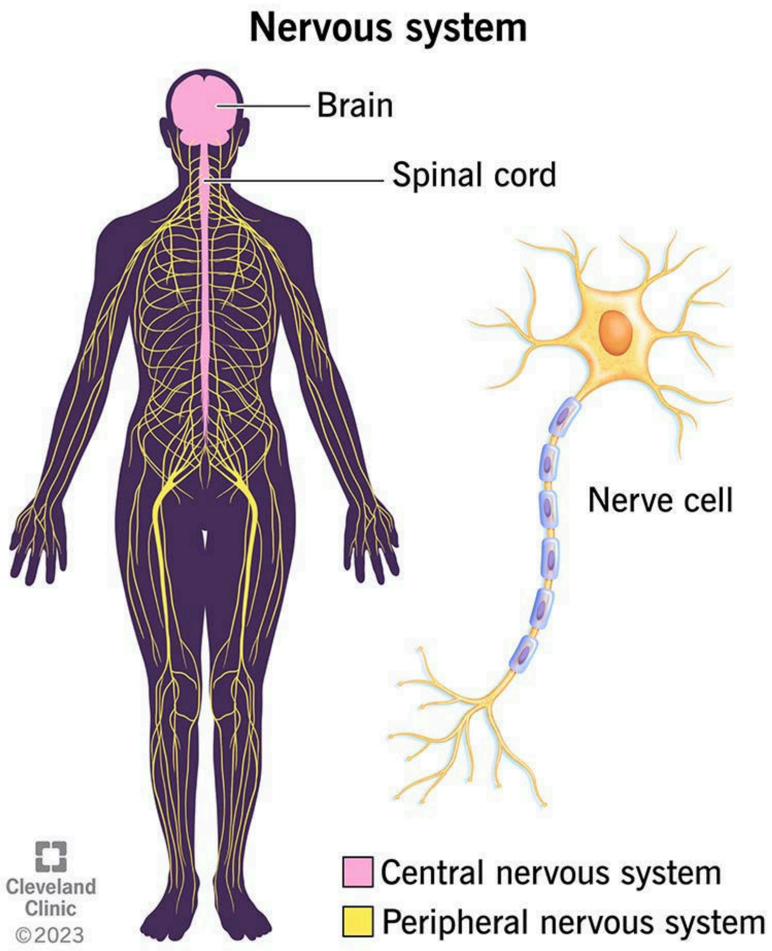


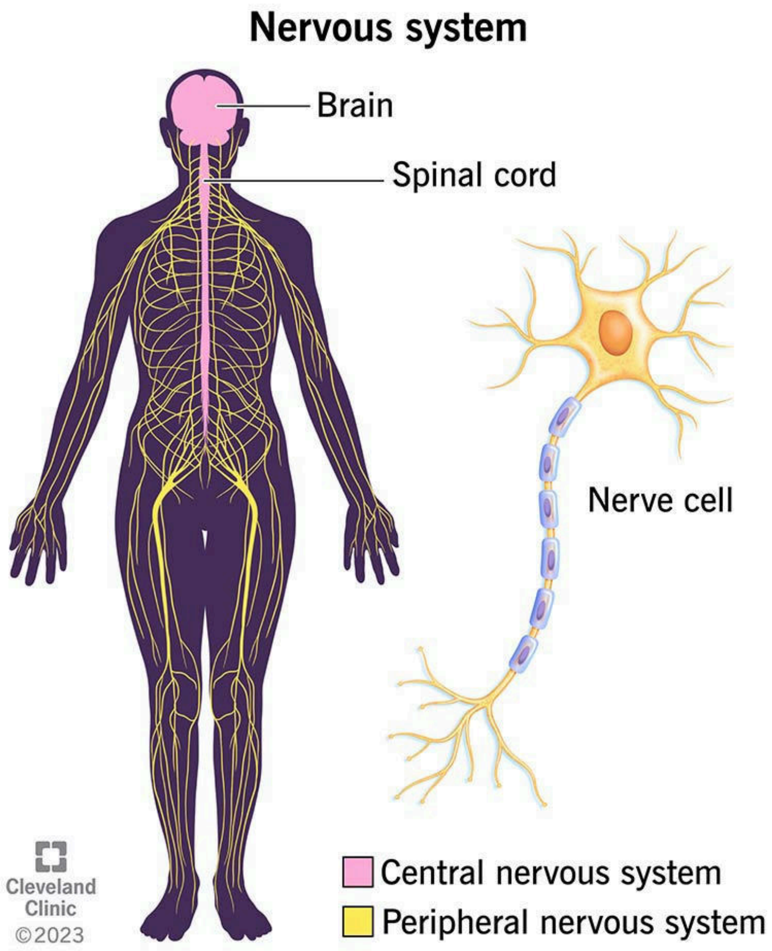
In a parallel circuit, we can sum voltages together

Many active dendrites will add together and trigger an impulse

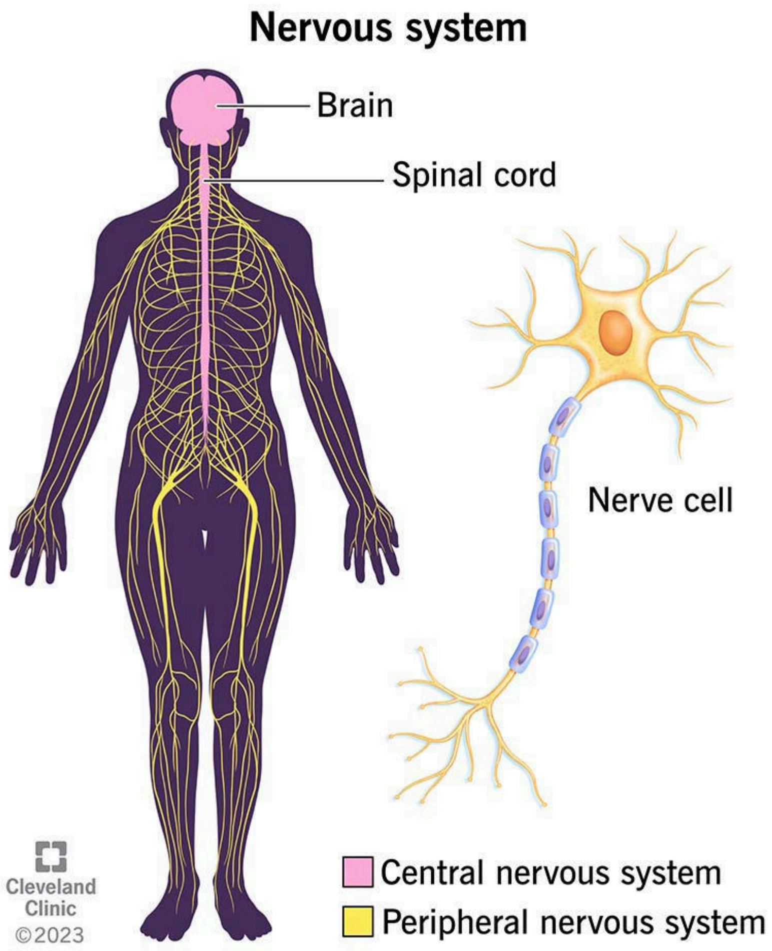
Pain triggers initial nerve impulse, starts a chain reaction into the brain



When the signal reaches the brain,
we will think



After thinking, we will take action



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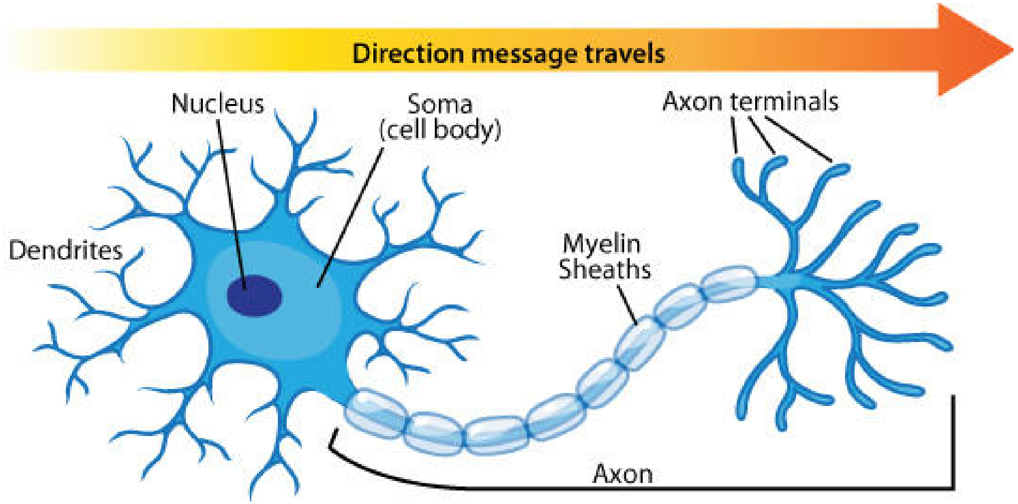
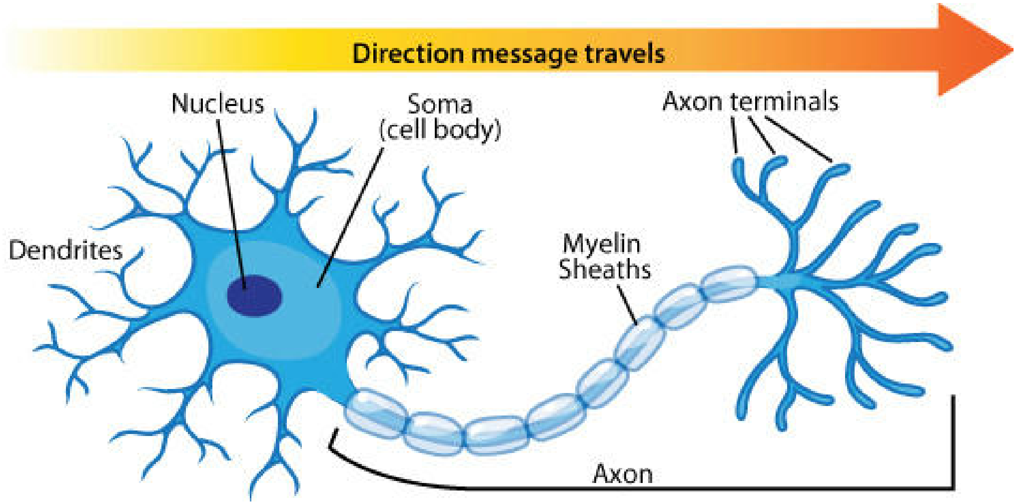
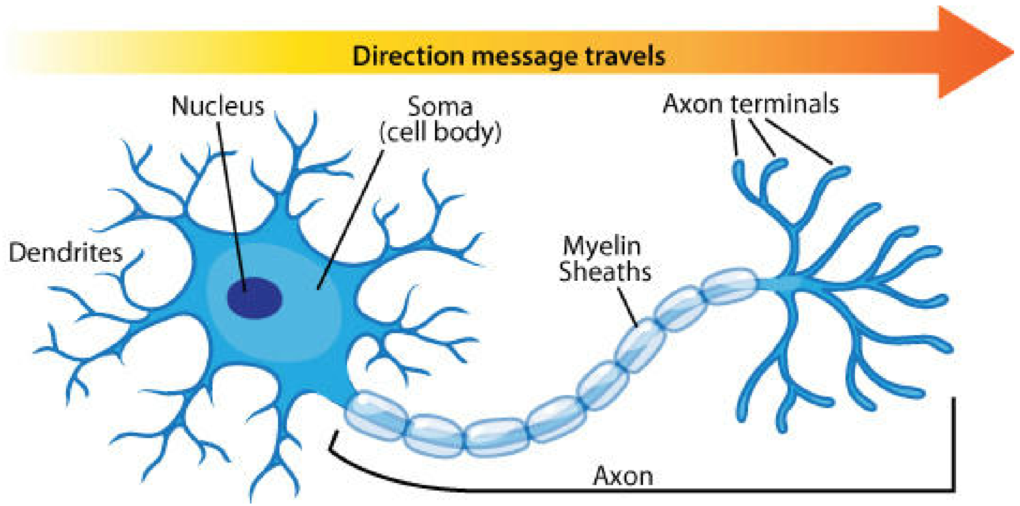

Direction message travels
Nucleus
Soma
(cell body)
Axon terminals
Dendrites
Myelin
Sheaths
Axon



Question: How could we write a neuron as a function? $f : \_\_ \mapsto \_\_$



Question: How could we write a neuron as a function? $f : \_\_ \mapsto \_\_$

Answer:

$$f : \underbrace{\mathbb{R}^{d_x}}_{\text{Dendrite voltages}} \times \underbrace{\mathbb{R}^{d_x}}_{\text{Dendrite size}} \mapsto \underbrace{\mathbb{R}}_{\text{Axon voltage}}$$

Let us implement an artifical neuron as a function

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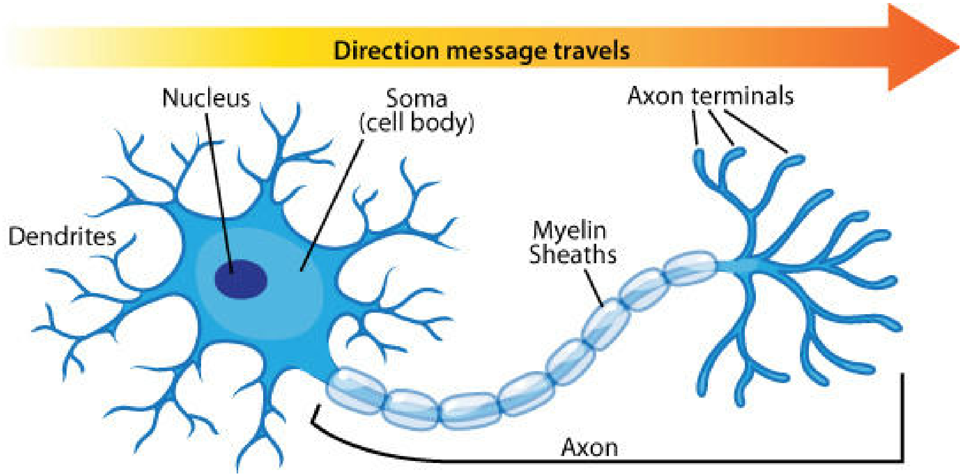

Neuron has a structure of dendrites

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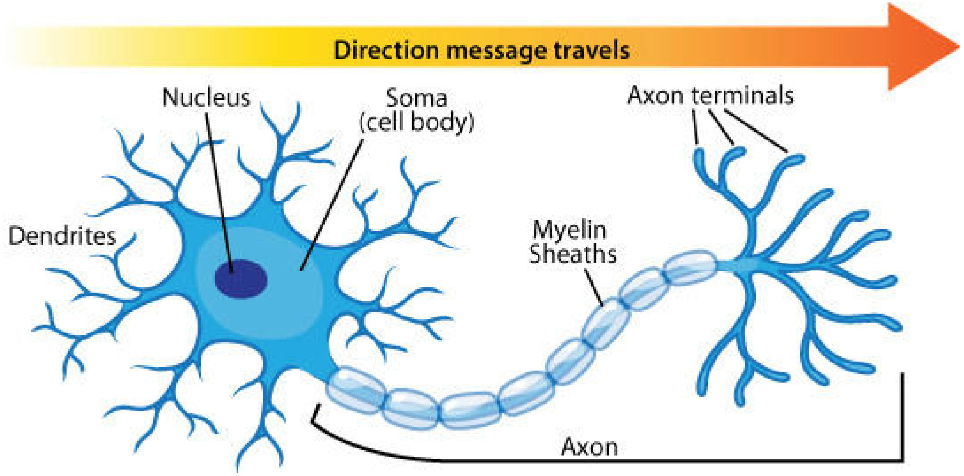
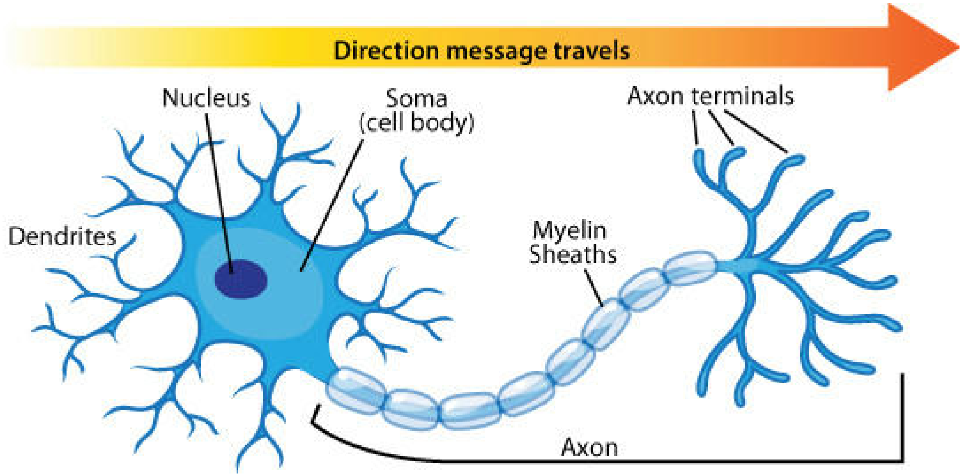


Neuron has a structure of dendrites

$$f\left(\begin{bmatrix} \theta_1 \\ \theta_2 \\ \vdots \\ \theta_{d_x} \end{bmatrix}\right)$$

$$f(\boldsymbol{\theta})$$

Let us implement an artifical neuron as a function



Each incoming dendrite has some voltage potential

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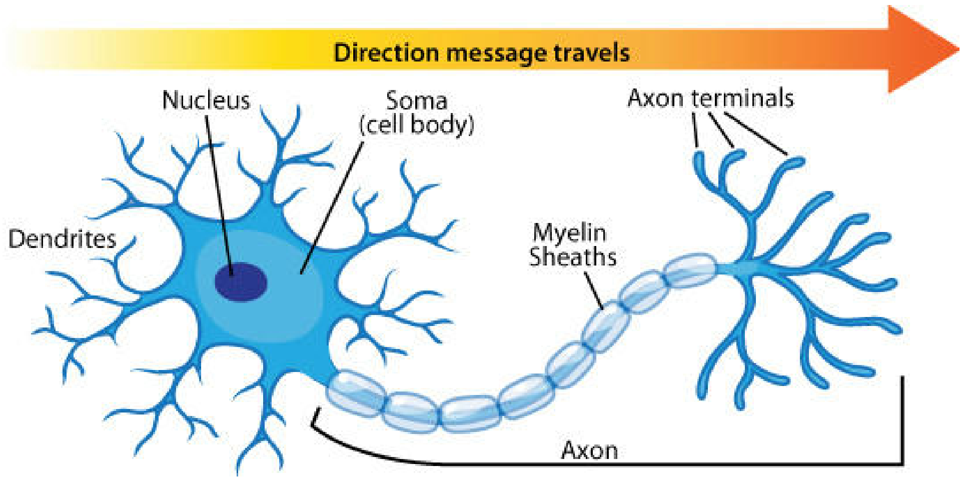

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$$f\left(\begin{bmatrix} x_1 \\ \vdots \\ x_{d_x} \end{bmatrix}, \begin{bmatrix} \theta_1 \\ \vdots \\ \theta_{d_x} \end{bmatrix}\right)$$

$$f(\boldsymbol{x}, \boldsymbol{\theta})$$

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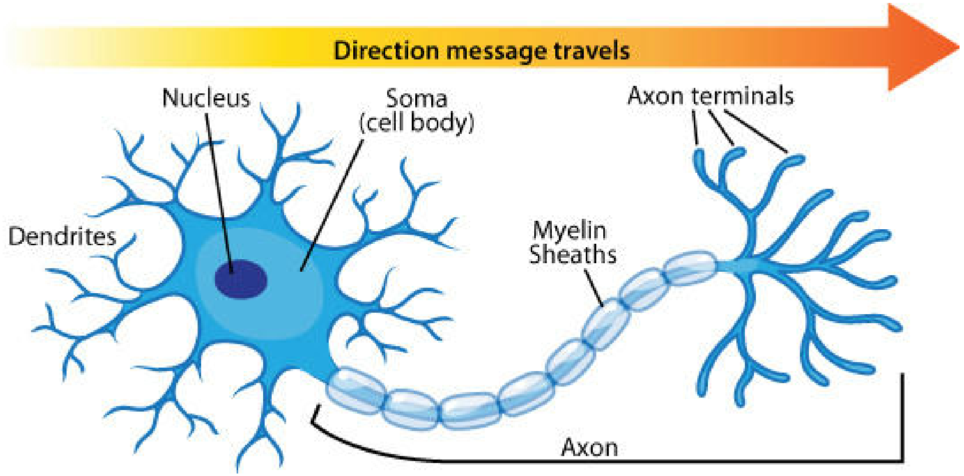

Voltage potentials sum together to give us the voltage in the cell body

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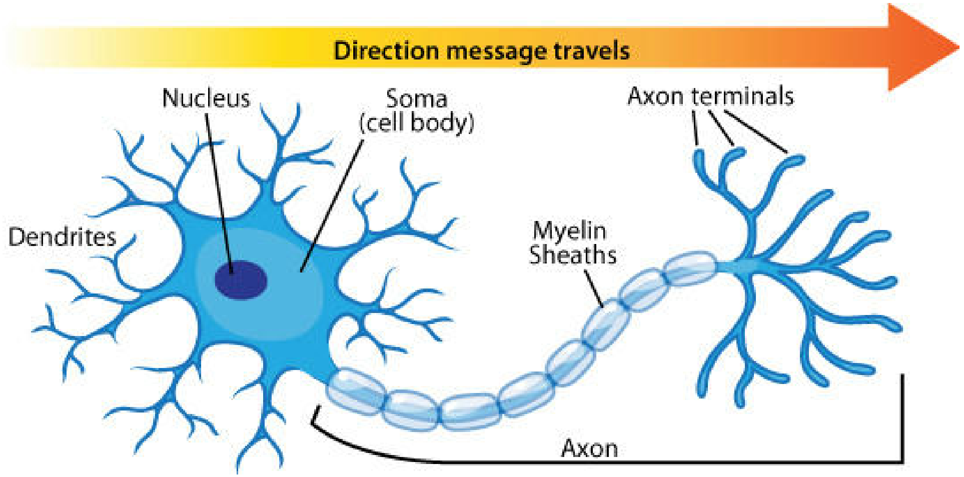

Voltage potentials sum together to give us the voltage in the cell body

$$f\left(\begin{bmatrix} x_1 \\ \vdots \\ x_{d_x} \end{bmatrix}, \begin{bmatrix} \theta_1 \\ \vdots \\ \theta_{d_x} \end{bmatrix} \right) = \sum_{j=1}^{d_x} \theta_j x_j$$

$$f(\boldsymbol{x}, \boldsymbol{\theta}) = \boldsymbol{\theta}^\top \boldsymbol{x}$$

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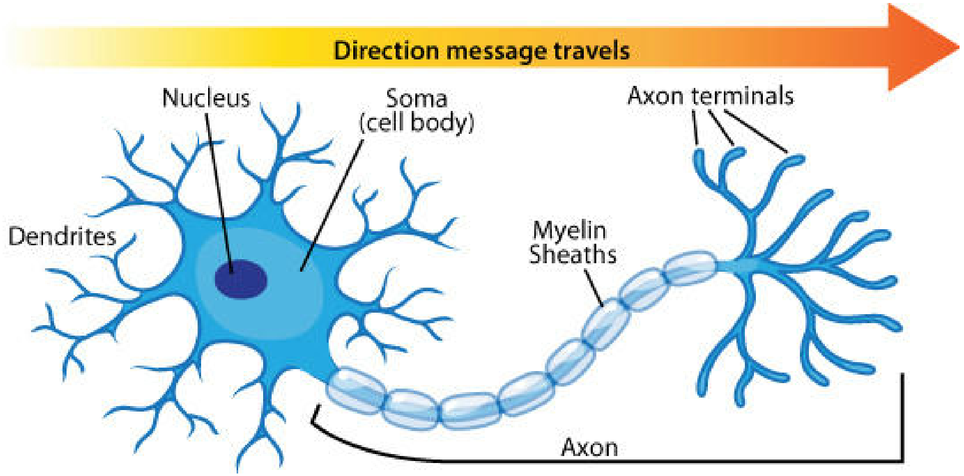

The axon fires only if the voltage is over a threshold

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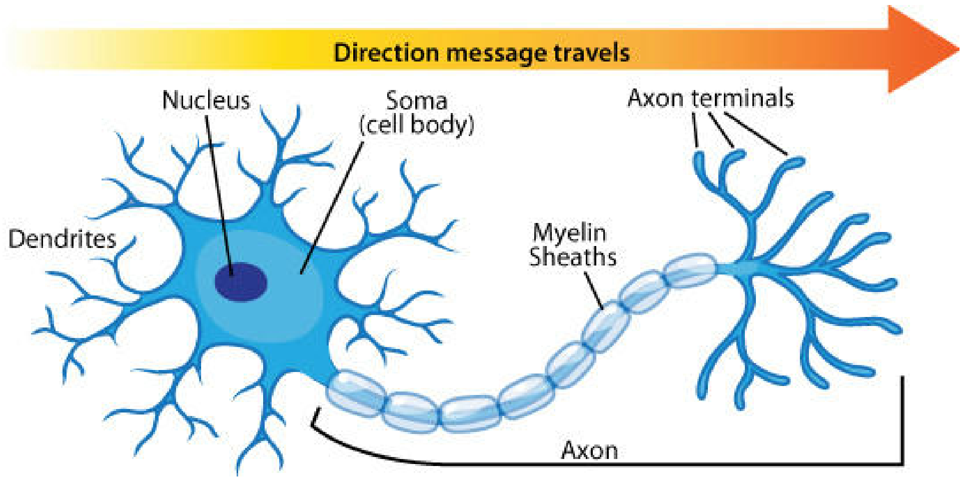

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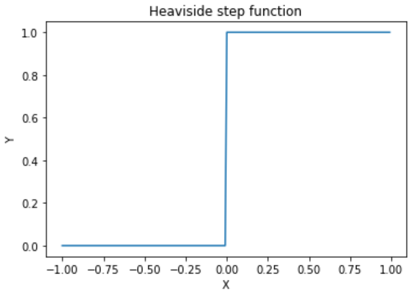
$$\sigma(x) = H(x) =$$



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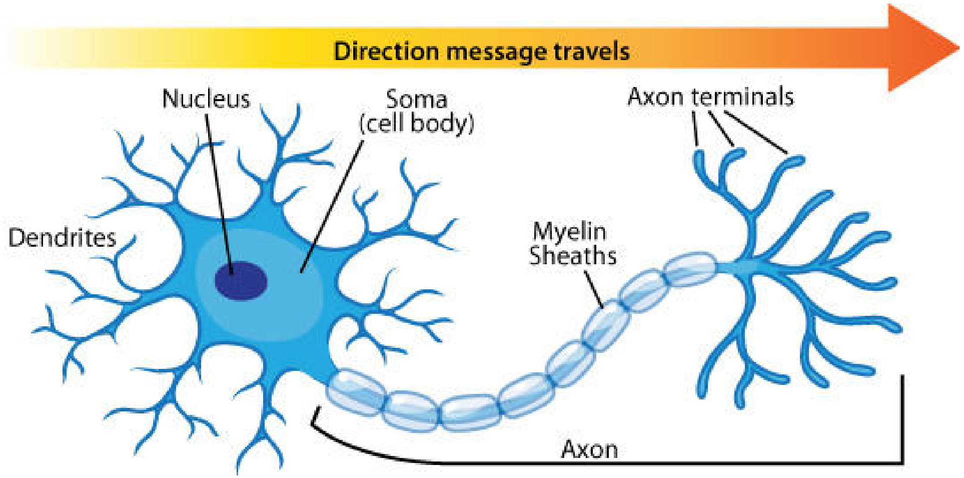

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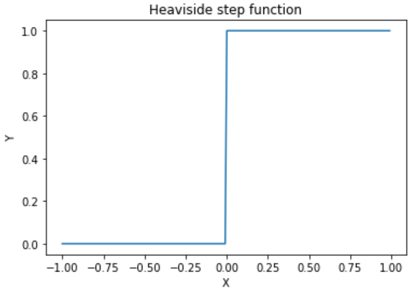
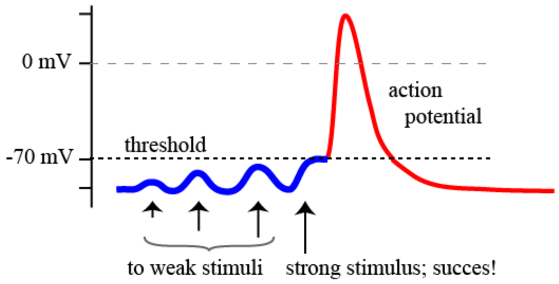
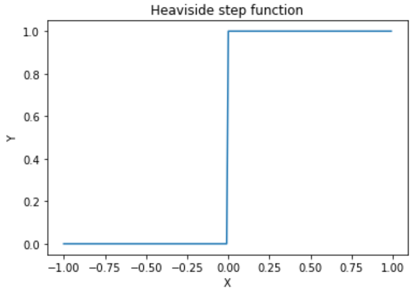


$$f\left(\begin{bmatrix} x_1 \\ \vdots \\ x_n \end{bmatrix}, \begin{bmatrix} \theta_1 \\ \vdots \\ \theta_n \end{bmatrix} \right) = \sigma \left(\sum_{j=1}^{d_x} \theta_j x_j \right)$$

Maybe we want to vary the activation threshold





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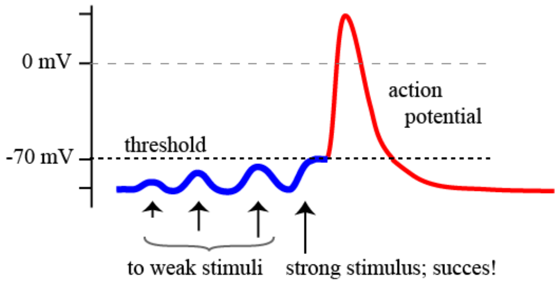

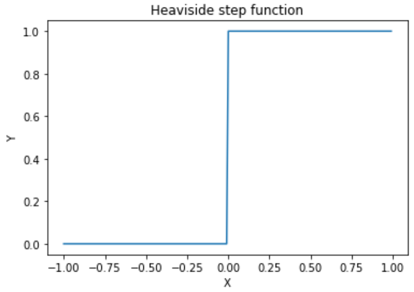

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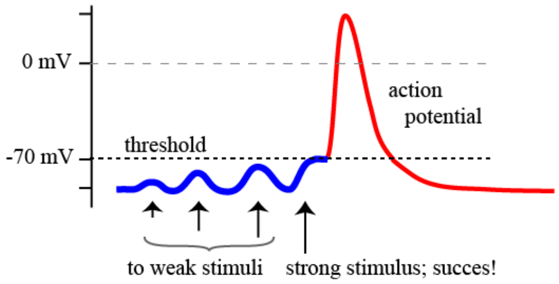

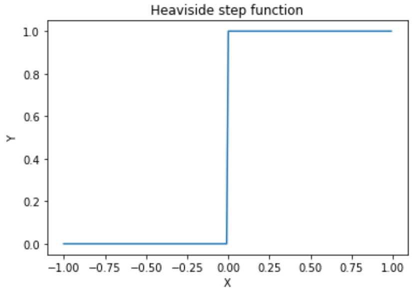

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Question: Does this look familiar to anyone?

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Question: Does this look familiar to anyone?

Answer: Inside σ is the multivariate linear model!

$$f(\boldsymbol{x}, \boldsymbol{\theta}) = \theta_{d_x} x_{d_x} + \theta_{d_x - 1} x_{d_x - 1} + \ldots + \theta_0$$

We model a neuron using a linear model and activation function

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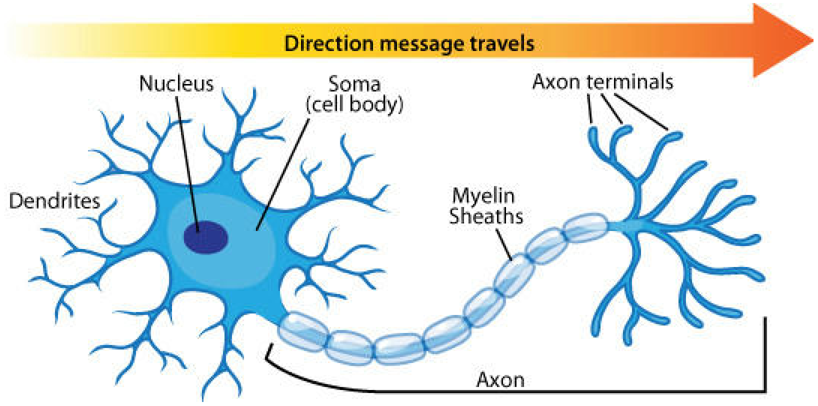

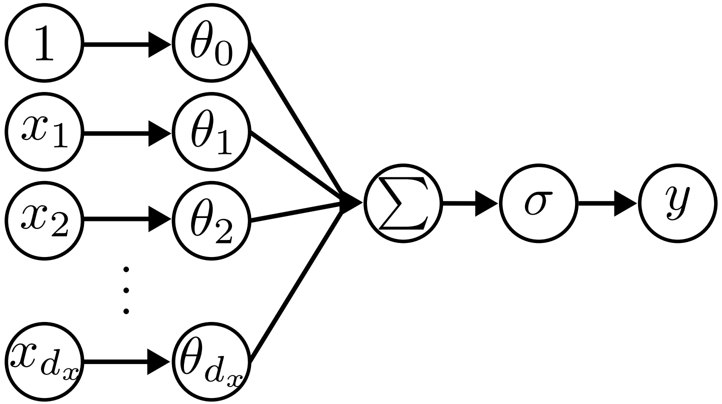

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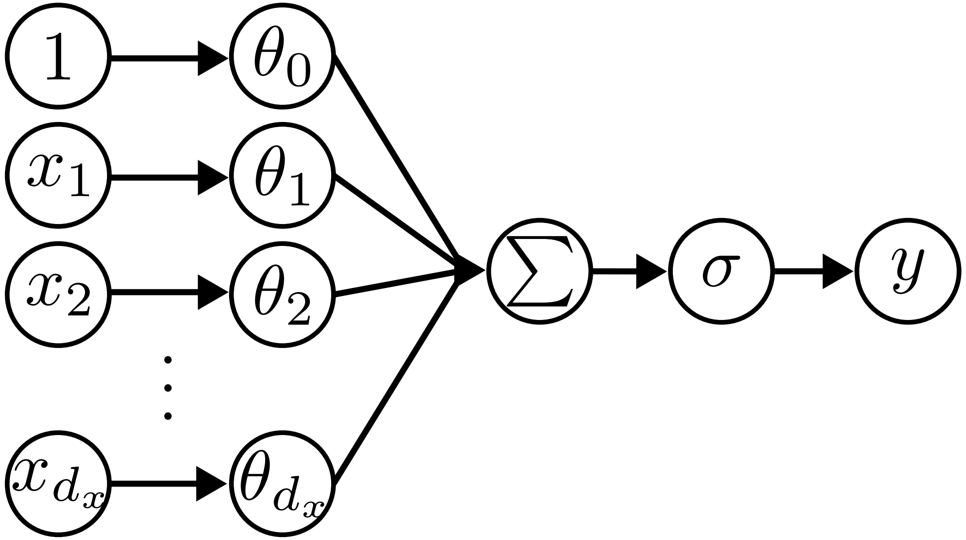
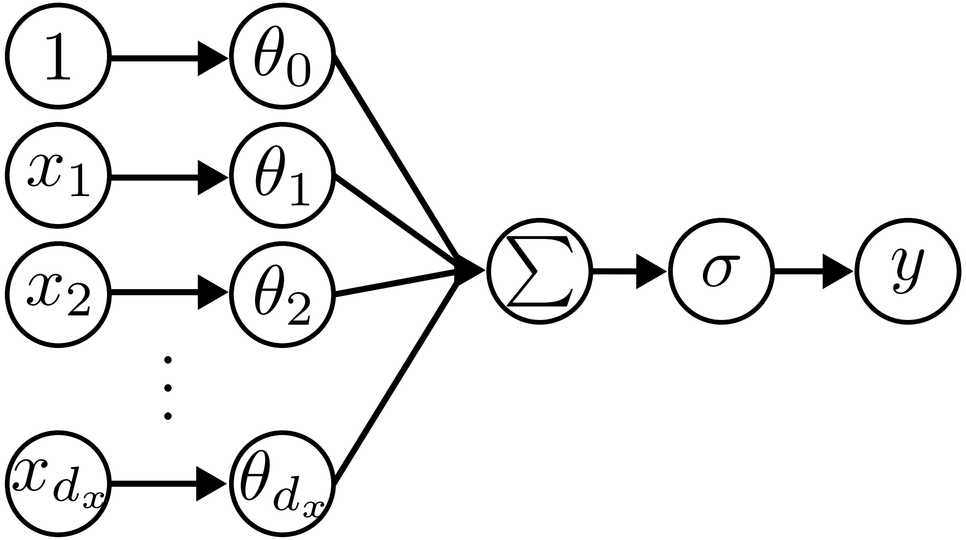
$$f\left(\boldsymbol{x}, \begin{bmatrix} b \\ \boldsymbol{w} \end{bmatrix}\right) = b + \boldsymbol{w}^\top \boldsymbol{x}$$

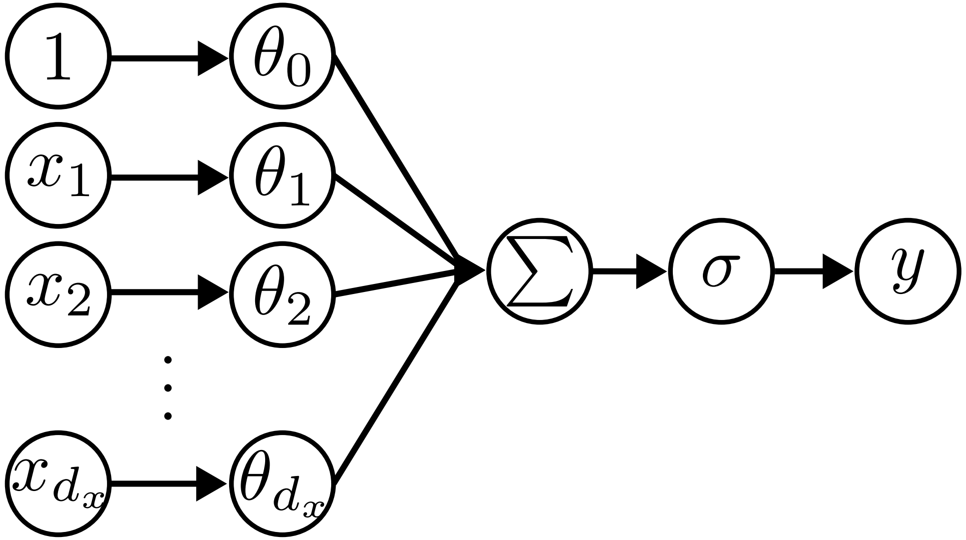
Relax



1
θ_0
x_1
θ_1
x_2
θ_2
x_{d_x}
θ_{d_x}
$\sum$
σ
y



In machine learning, we represent functions



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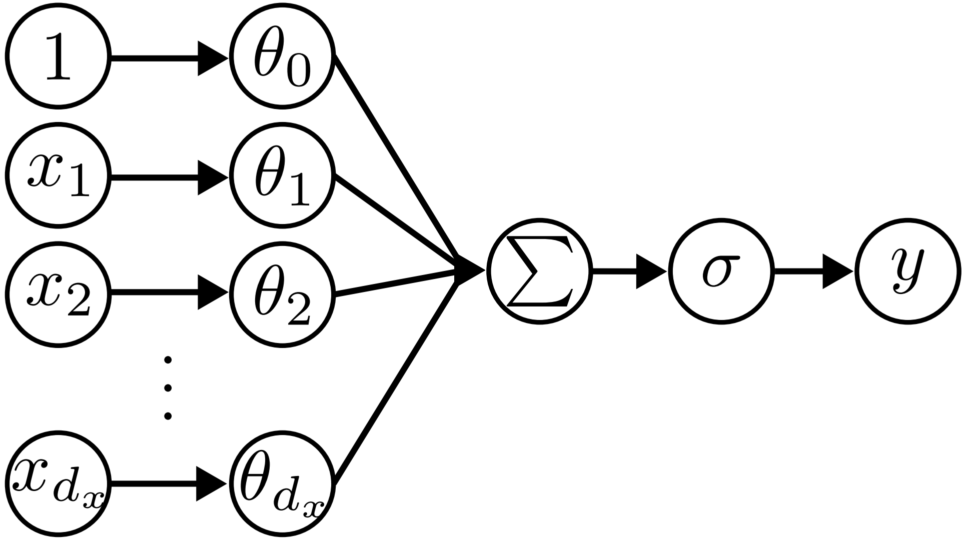
What kinds of functions can our neuron represent?



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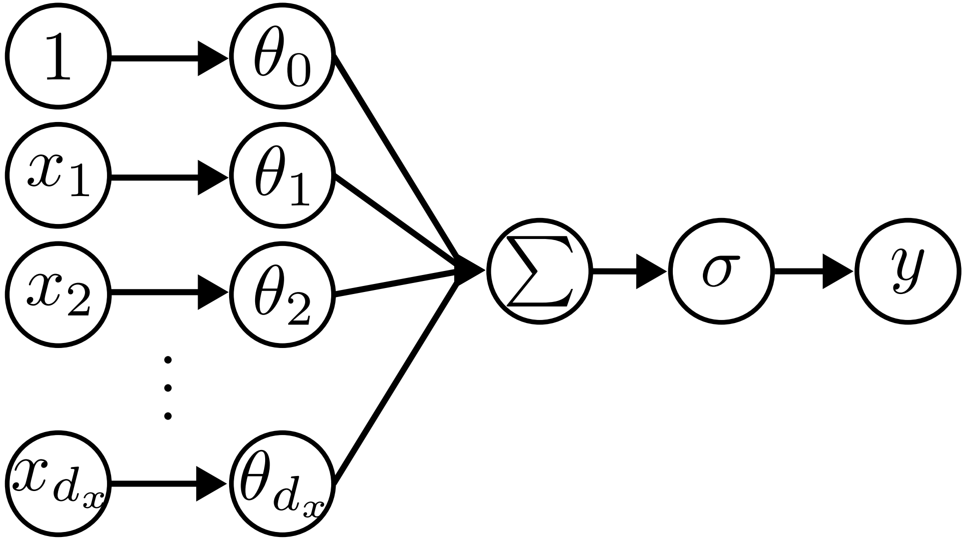

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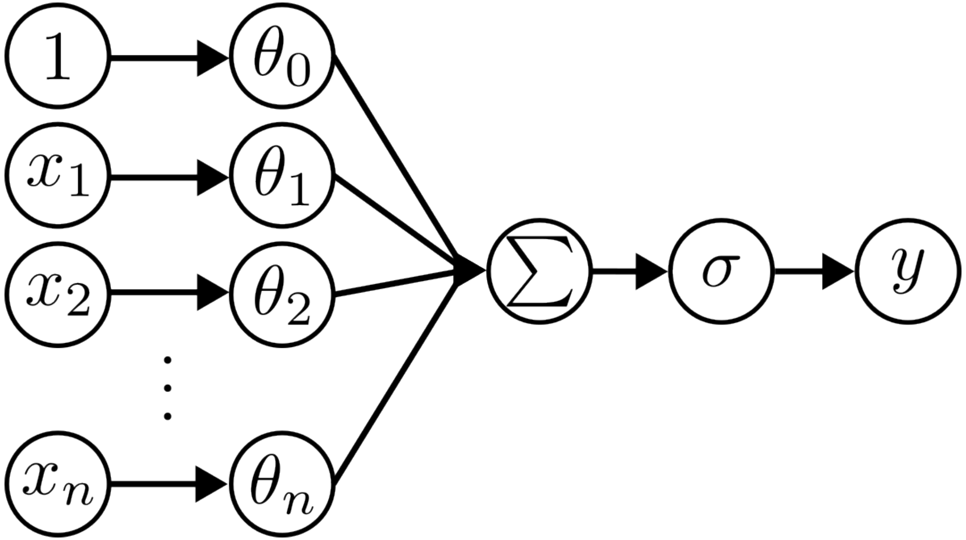
Let us start with a logical AND function

Review: Activation function (Heaviside step function)



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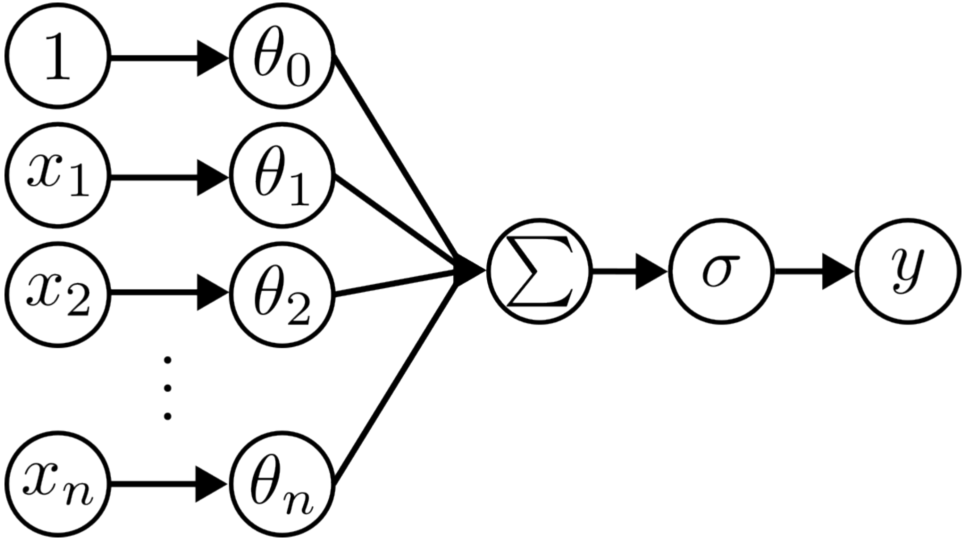

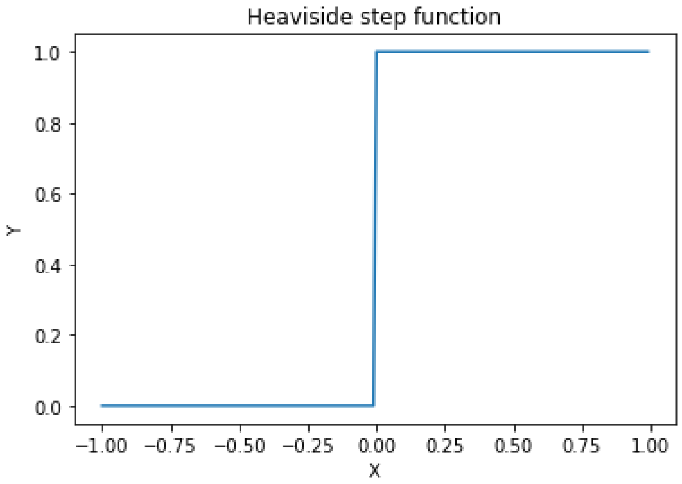

$$\sigma(x) = H(x) = \begin{cases} 1 \text{ if } x > 0 \\ 0 \text{ if } x \leq 0 \end{cases}$$

Implement AND using an artificial neuron

Implement AND using an artificial neuron

$$f\left([x_1 \ \ x_2]^\top, [\theta_0 \ \ \theta_1 \ \ \theta_2]^\top\right) = \sigma(\theta_0 + x_1\theta_1 + x_2\theta_2)$$

Implement AND using an artificial neuron

$$f\left(\begin{bmatrix} x_1 & x_2 \end{bmatrix}^\top, \begin{bmatrix} \theta_0 & \theta_1 & \theta_2 \end{bmatrix}^\top\right) = \sigma(\theta_0 + x_1\theta_1 + x_2\theta_2)$$

$$\boldsymbol{\theta} = \begin{bmatrix} \theta_0 & \theta_1 & \theta_2 \end{bmatrix}^\top = \begin{bmatrix} -1 & 1 & 1 \end{bmatrix}^\top$$

Implement AND using an artificial neuron

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x_1	x_2	y	$f(x_1, x_2, \boldsymbol{\theta})$	$\hat{y}$
0	0	0	$\sigma(-1 + 1 \cdot 0 + 1 \cdot 0) = \sigma(-1)$	0
0	1	0	$\sigma(-1 + 1 \cdot 0 + 1 \cdot 1) = \sigma(0)$	0
1	0	0	$\sigma(-1 + 1 \cdot 1 + 1 \cdot 0) = \sigma(0)$	0
1	1	1	$\sigma(-1 + 1 \cdot 1 + 1 \cdot 1) = \sigma(1)$	1

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x_1	x_2	y	$f(x_1, x_2, \boldsymbol{\theta})$	$\hat{y}$
0	0	0	$\sigma(0 + 1 \cdot 0 + 1 \cdot 0) = \sigma(0)$	0
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1	1	1	$\sigma(1 + 1 \cdot 1 + 1 \cdot 1) = \sigma(2)$	1

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x_1	x_2	y	$f(x_1, x_2, \boldsymbol{\theta})$	$\hat{y}$
0	0	0	This is IMPOSSIBLE!	
0	1	1		
1	0	1		
1	1	0		

Why can’t we represent XOR using a neuron?

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Let us think back to biology, maybe it has an answer

Brain: Biological neurons $\rightarrow$ Biological neural network

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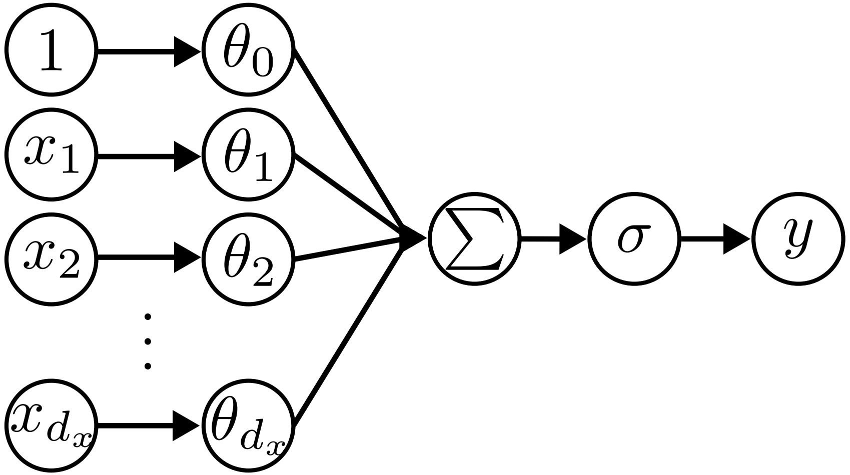
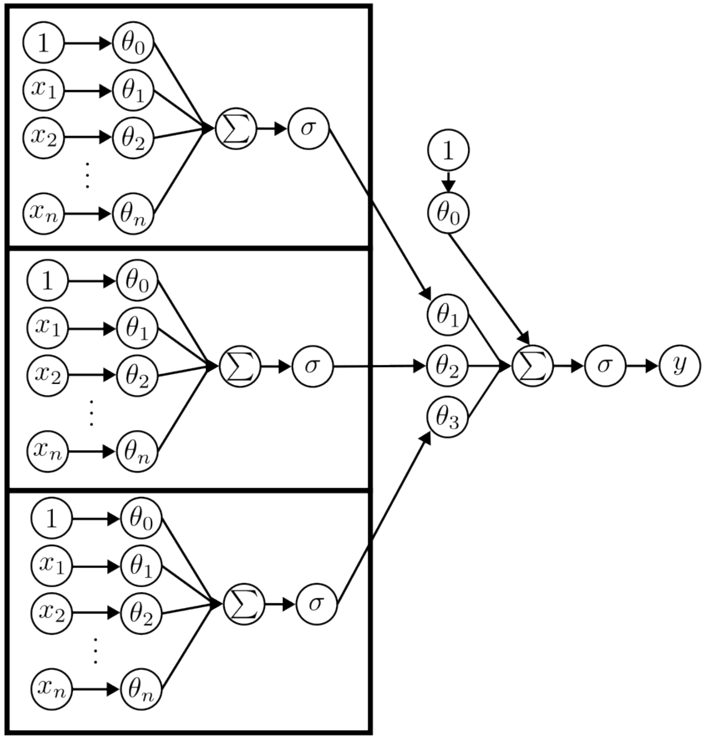
Computer: Artificial neurons $\rightarrow$ Artificial neural network

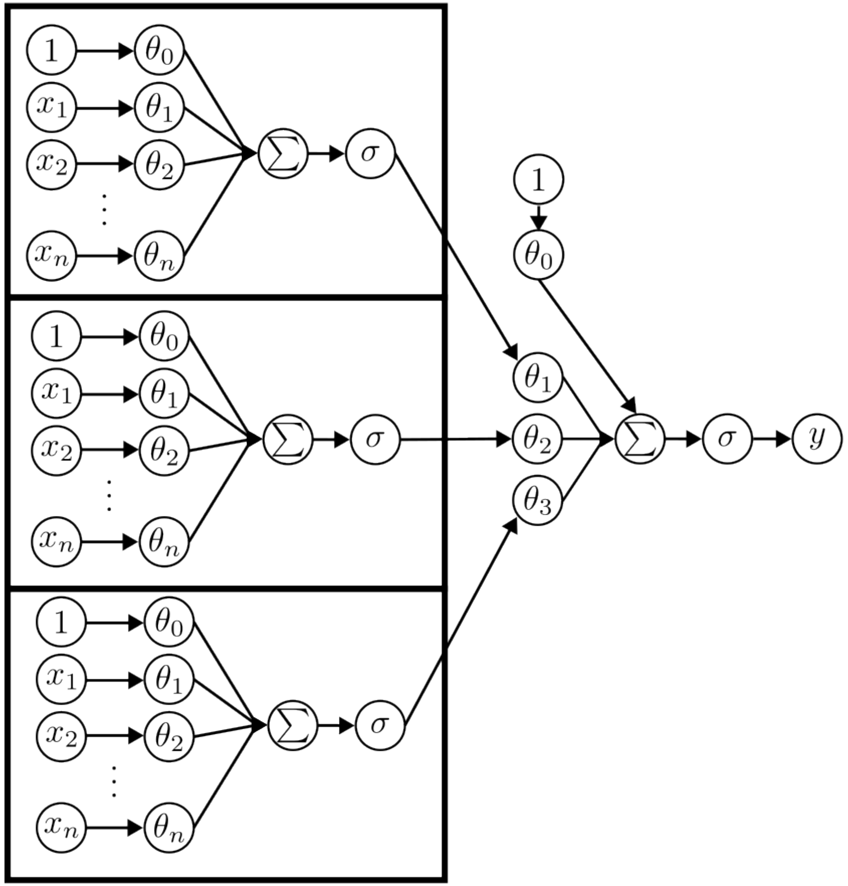
Connect artificial neurons into a network



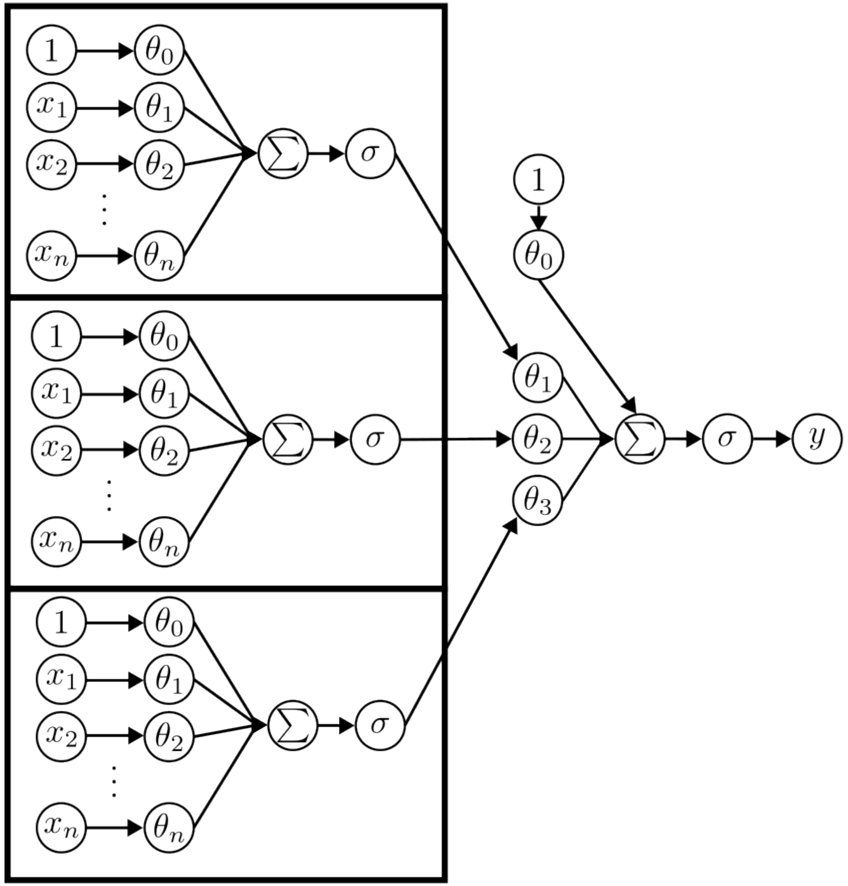
Neuron



Neural Network



Adding neurons in **parallel** creates a **wide** neural network



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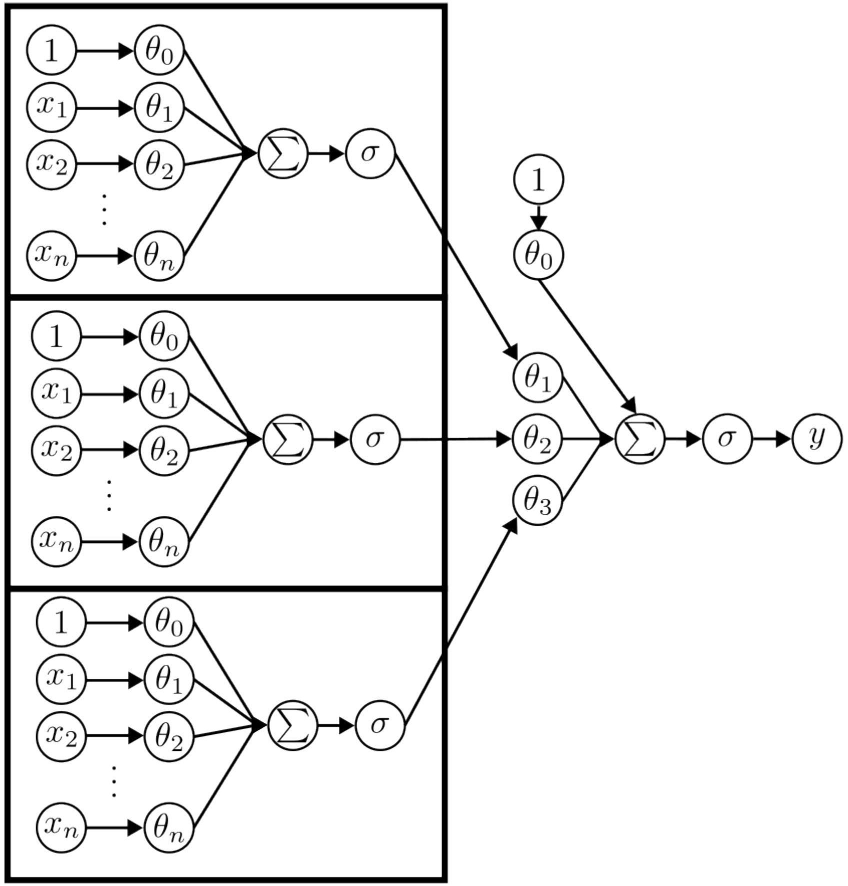

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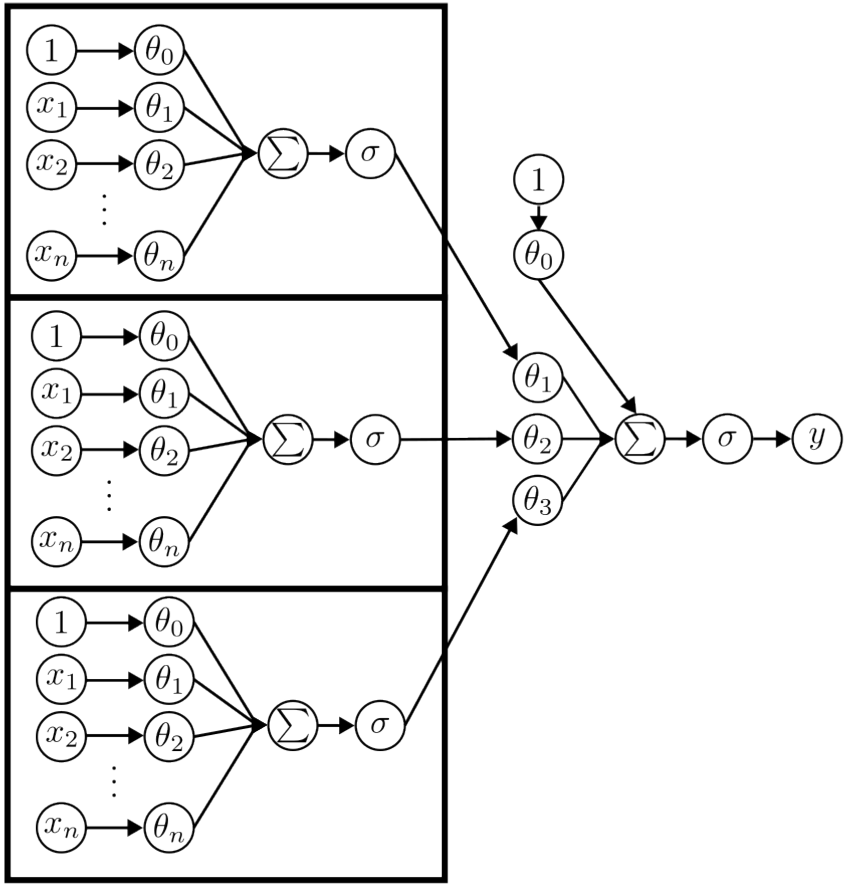
Today's powerful neural networks are both **wide** and **deep**



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Let us try to implement XOR using a wide and deep neural network

1. Review
2. Multivariate linear regression
3. Limitations of linear regression
4. History of neural networks
5. Biological neurons
6. Artificial neurons
7. **Wide neural networks**
8. Deep neural networks
9. Practical considerations

How do we express a **wide** neural network mathematically?

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$$f : \mathbb{R}^{d_x} \times \Theta \mapsto \mathbb{R}$$

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d_y neurons (wide):

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$$\Theta \in \mathbb{R}^{(d_x+1) \times d_y}$$

For a single neuron:

$$f\left(\begin{bmatrix} x_1 \\ \vdots \\ x_{d_x} \end{bmatrix}, \begin{bmatrix} \theta_0 \\ \vdots \\ \theta_{d_x} \end{bmatrix} \right) = \sigma\left(\theta_0 + \sum_{i=1}^{d_x} \theta_i x_i \right)$$

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For a wide network:

$$f\left(\begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_{d_x} \end{bmatrix}, \begin{bmatrix} \theta_{1,0} & \theta_{2,0} & \cdots & \theta_{d_x,0} \\ \theta_{1,1} & \theta_{2,1} & \cdots & \theta_{d_x,1} \\ \vdots & \vdots & \ddots & \vdots \\ \theta_{1,d_y} & \theta_{2,d_y} & \cdots & \theta_{d_y,d_x} \end{bmatrix}\right) = \begin{bmatrix} \sigma\left(\theta_{1,0} + \sum_{i=1}^{d_x} x_i \theta_{1,i}\right) \\ \sigma\left(\theta_{2,0} + \sum_{i=1}^{d_x} x_i \theta_{2,i}\right) \\ \vdots \\ \sigma\left(\theta_{d_y,0} + \sum_{i=1}^{d_x} x_i \theta_{d_y,i}\right) \end{bmatrix}$$

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Deep: $\Theta \in \mathbb{R}^{(d_x+1) \times d_h} \times \mathbb{R}^{(d_h+1) \times d_h} \times \ldots \times \mathbb{R}^{(d_h+1) \times d_y}$

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Wide: $\Theta \in \mathbb{R}^{(d_x+1) \times d_y}$

Deep: $\Theta \in \mathbb{R}^{(d_x+1) \times d_h} \times \mathbb{R}^{(d_h+1) \times d_h} \times \ldots \times \mathbb{R}^{(d_h+1) \times d_y}$

$$\boldsymbol{\theta} = \begin{bmatrix} \boldsymbol{\theta}_1 & \boldsymbol{\theta}_2 & \ldots & \boldsymbol{\theta}_\ell \end{bmatrix}^\top = \begin{bmatrix} \boldsymbol{\varphi} & \boldsymbol{\psi} & \ldots & \boldsymbol{\xi} \end{bmatrix}^\top$$

A wide network:

$$f(\boldsymbol{x}, \boldsymbol{\theta}) = \boldsymbol{\theta}_{\cdot, 0} + \boldsymbol{\theta}_{\cdot, 1:d_x} \boldsymbol{x}$$

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$$f(\boldsymbol{x}, \boldsymbol{\theta}) = f_\ell(\dots f_2(f_1(\boldsymbol{x}, \boldsymbol{\varphi}), \boldsymbol{\psi}) \dots \boldsymbol{\xi})$$

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We call each function a **layer**

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A deep neural network is made of many layers

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$$
\begin{aligned}
f(x_1, x_2, \boldsymbol{\theta}) = \sigma\big(\theta_{3,0} & \\
+\theta_{3,1} & \quad \cdot \quad \sigma\big(\theta_{1,0} + x_1 \theta_{1,1} + x_2 \theta_{1,2}\big) \\
+\theta_{3,2} & \quad \cdot \quad \sigma\big(\theta_{2,0} + x_1 \theta_{2,1} + x_2 \theta_{2,2}\big)\big)
\end{aligned}
$$

Proof Sketch: Approximate a function $g(x)$ using a linear combination of Heaviside functions

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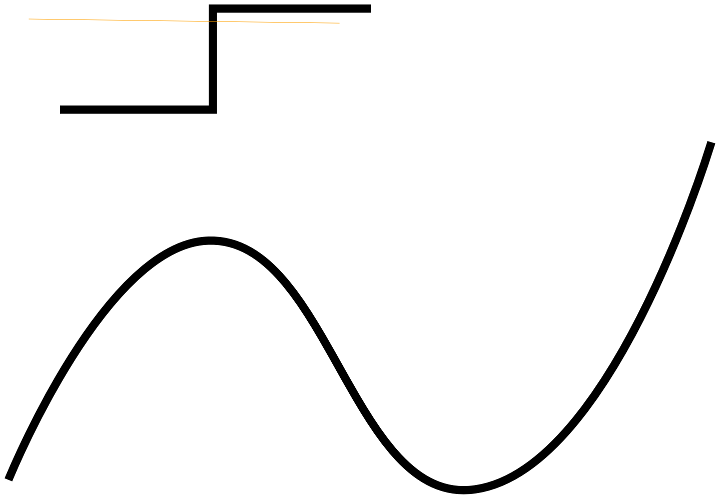

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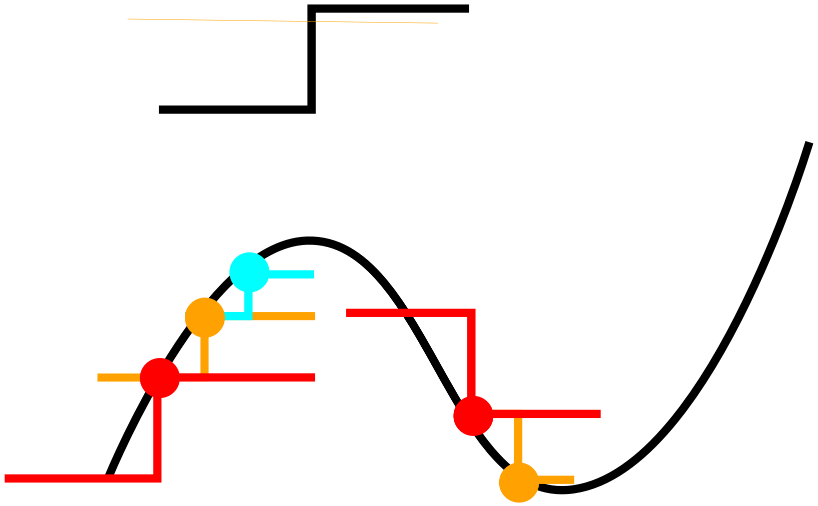

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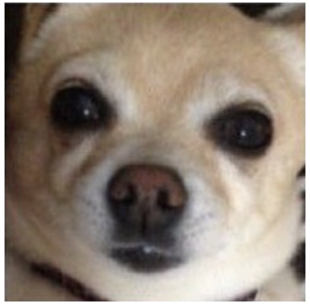
Very powerful finding! The basis of deep learning.

Task: predict how many ♥ a photo gets on social media



1. Review
2. Multivariate linear regression
3. Limitations of linear regression
4. History of neural networks
5. Biological neurons
6. Artificial neurons
7. Wide neural networks
8. Deep neural networks
9. **Practical considerations**

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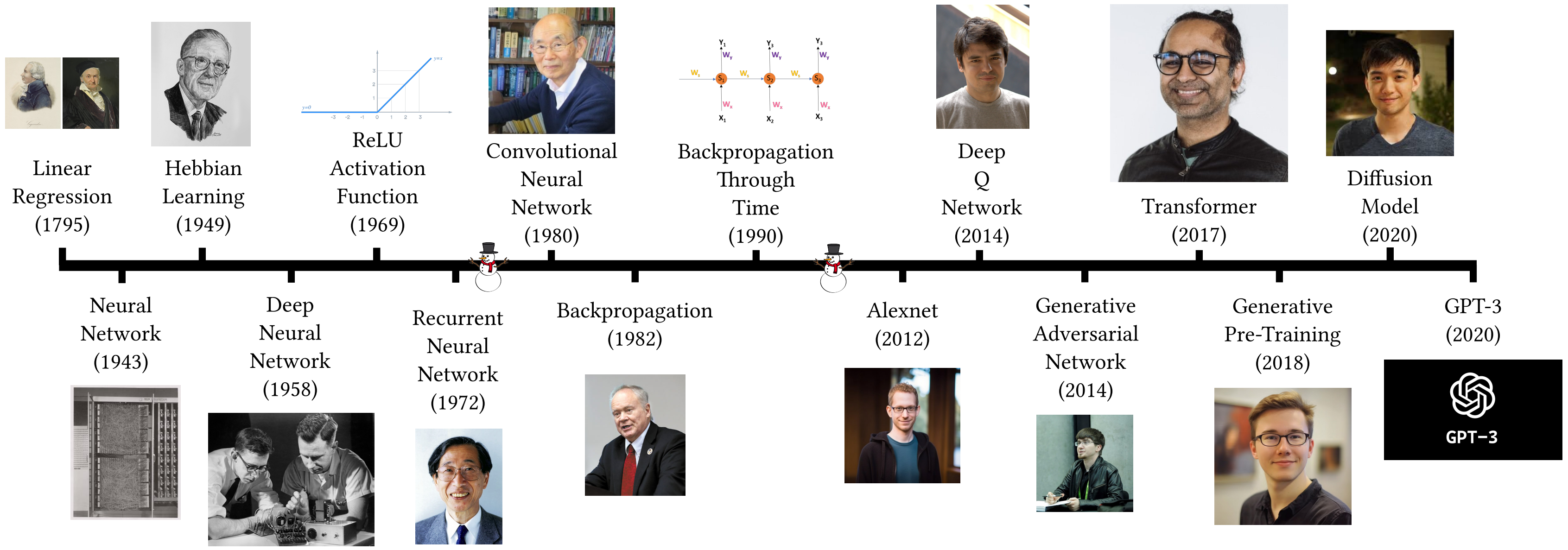

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I will explain them again very simply

A **layer** is a linear operation and an activation function

$$f\left(\boldsymbol{x}, \begin{bmatrix} \boldsymbol{b} \\ \boldsymbol{W} \end{bmatrix}\right) = \sigma(\boldsymbol{b} + \boldsymbol{W}\boldsymbol{x})$$

Many layers makes a deep neural network

$$\boldsymbol{z}_1 = f\left(\boldsymbol{x}, \begin{bmatrix} \boldsymbol{b}_1 \\ \boldsymbol{W}_1 \end{bmatrix}\right)$$

$$\boldsymbol{z}_2 = f\left(\boldsymbol{z}_1, \begin{bmatrix} \boldsymbol{b}_2 \\ \boldsymbol{W}_2 \end{bmatrix}\right)$$

$$\boldsymbol{y} = f\left(\boldsymbol{z}_2, \begin{bmatrix} \boldsymbol{b}_2 \\ \boldsymbol{W}_2 \end{bmatrix}\right)$$

Let us create a wide neural network in colab! https://colab.research.google.com/drive/1bLtf3QY-yROIif_EoQSU1WS7svd0q8j7?usp=sharing

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