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
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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- *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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Approach: Learn the parameters θ such that

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

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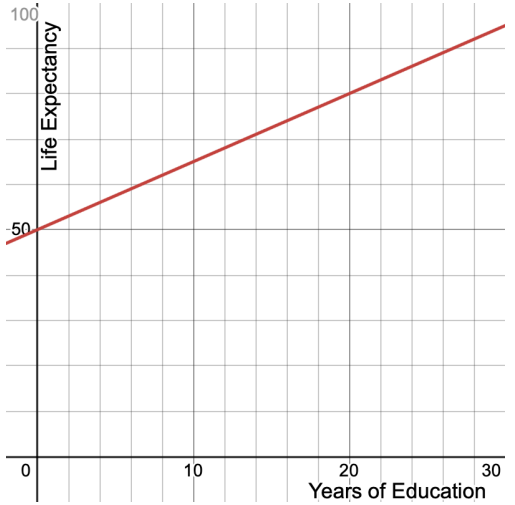
$$f(x, \boldsymbol{\theta}) = f\left(x, \begin{bmatrix} \theta_1 \\ \theta_0 \end{bmatrix}\right) = \theta_1 x + \theta_0$$



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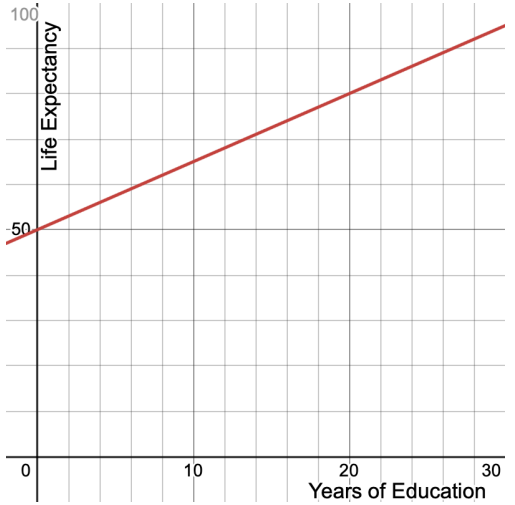

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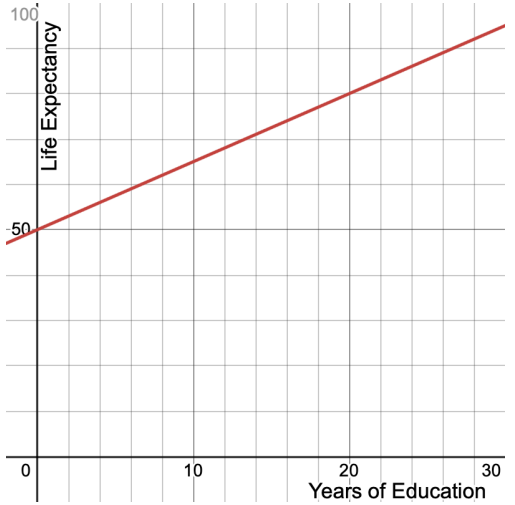

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$$\text{error}(f(x, \boldsymbol{\theta}), y) = (f(x, \boldsymbol{\theta}) - y)^2$$

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

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

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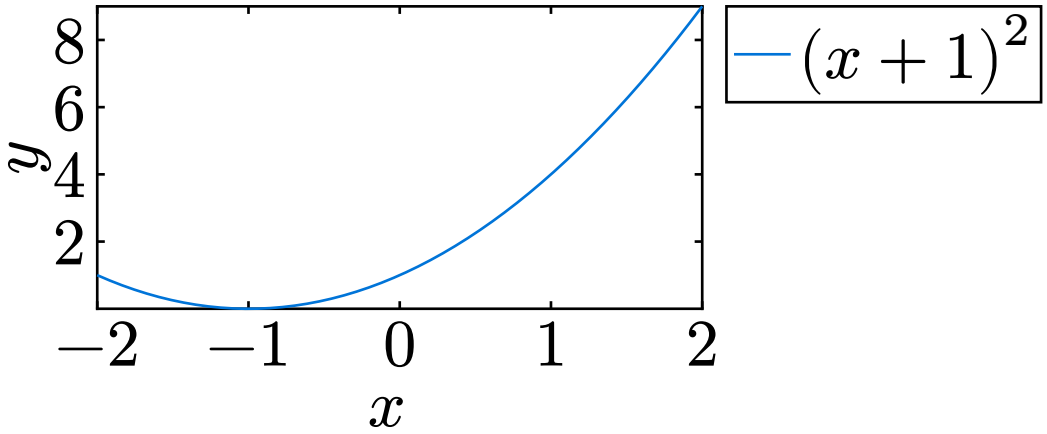

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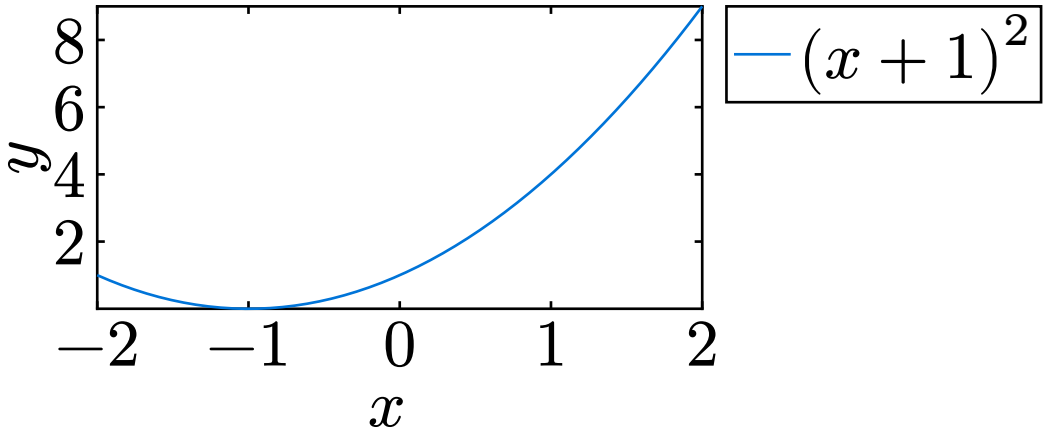

$$\arg\min_x f(x) = -1$$

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$$\begin{aligned}\arg\min_{\boldsymbol{\theta}} \mathcal{L}(\boldsymbol{x}, \boldsymbol{y}, \boldsymbol{\theta}) &= \arg\min_{\boldsymbol{\theta}} \sum_{i=1}^{n} \text{error}\Big(f\Big(x_{[i]}, \boldsymbol{\theta}\Big), y_{[i]}\Big) \\ &= \arg\min_{\boldsymbol{\theta}} \sum_{i=1}^{n} \Big(f\Big(x_{[i]}, \boldsymbol{\theta}\Big) - y_{[i]}\Big)^2\end{aligned}$$

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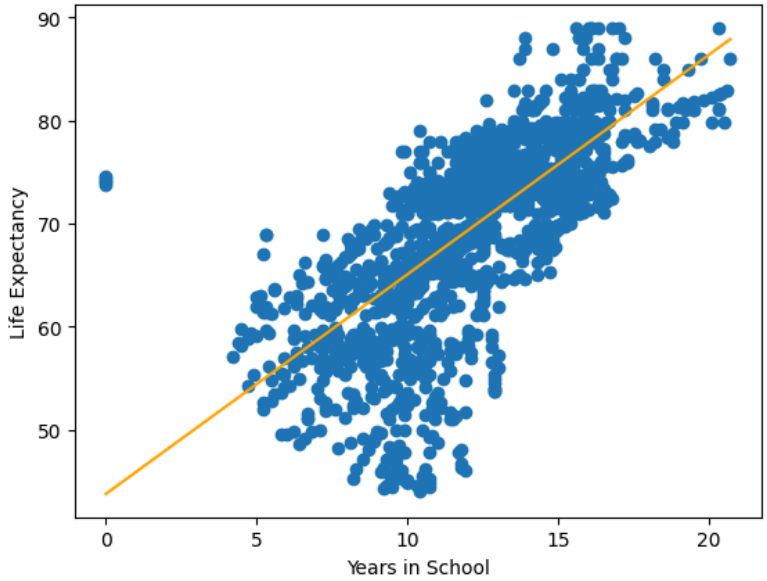

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Then, we used a trick to extend linear regression to nonlinear models

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

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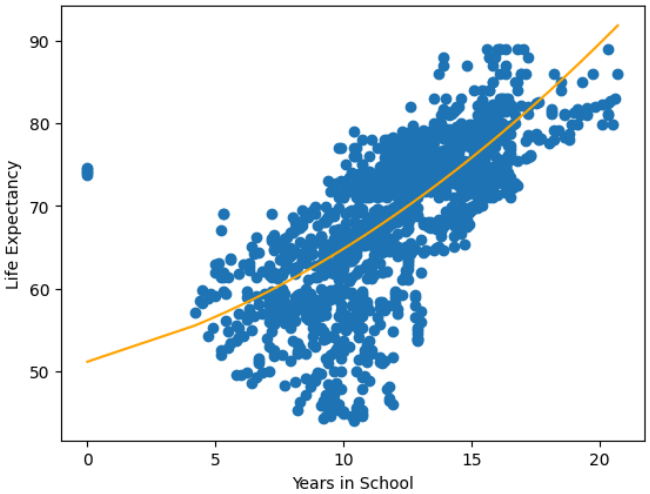
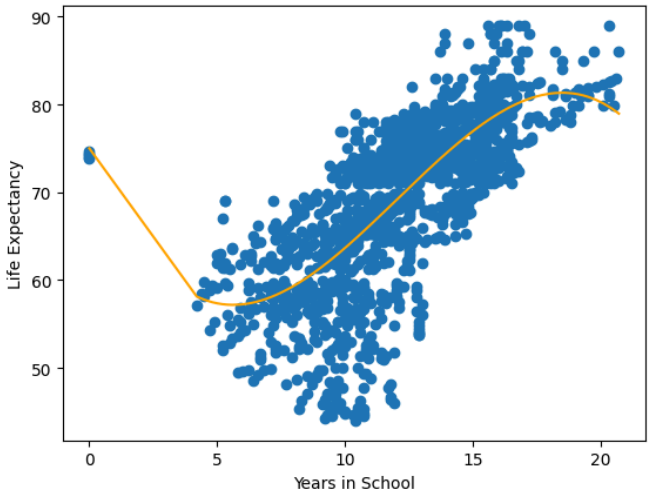
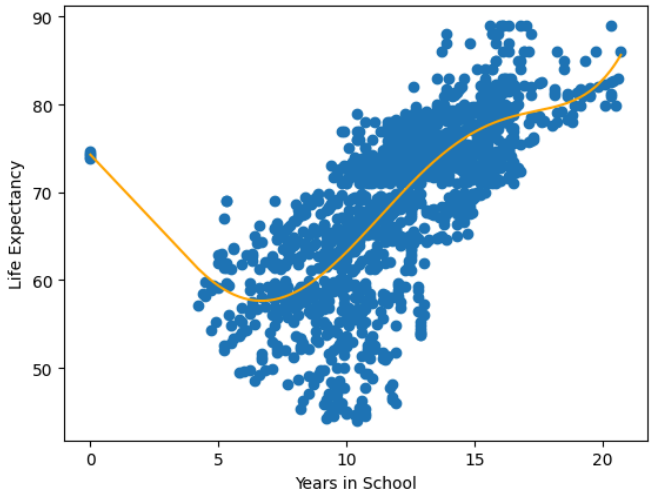


$m = 2$



$m = 3$



$m = 5$

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We care about **generalization** in machine learning

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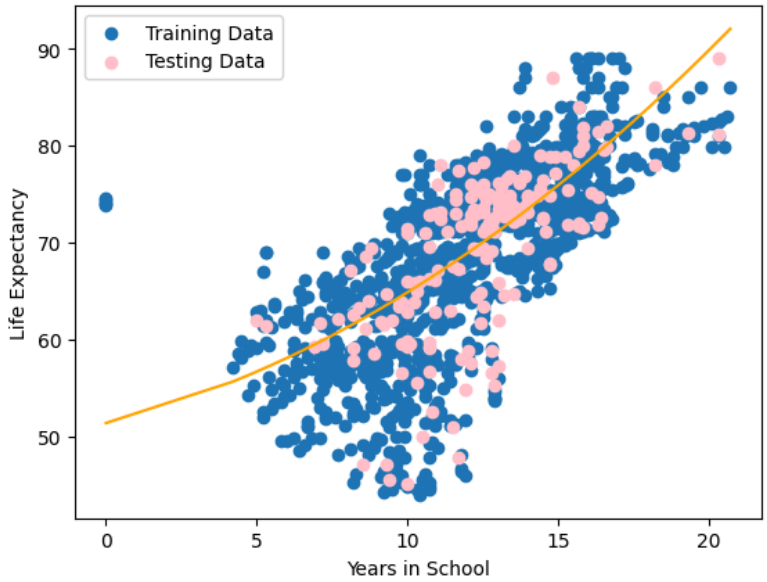

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We can solve these problems using linear regression too

For multivariate problems, we will define the input dimension as d_x

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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

$$\boldsymbol{X}_D = \begin{bmatrix} x_{[1],d_x} & x_{[1],d_x-1} & \cdots & x_{[1],1} & 1 \\ x_{[2],d_x} & x_{[2],d_x-1} & \cdots & x_{[2],1} & 1 \\ \vdots & \vdots & \ddots & \vdots & \\ x_{[n],d_x} & x_{[n],d_x-1} & \cdots & x_{[n],1} & 1 \end{bmatrix}$$

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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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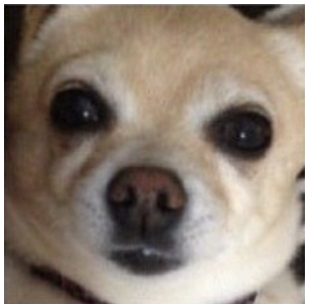

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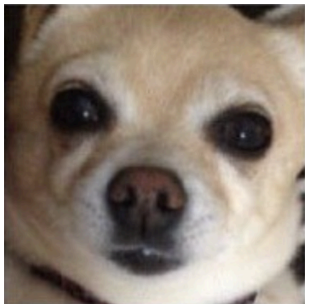

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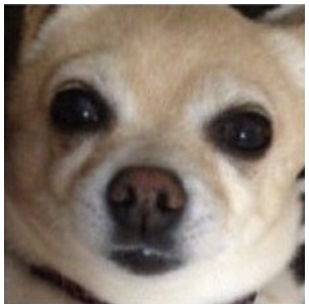

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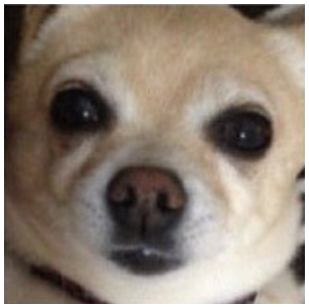

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Highly nonlinear task, use a polynomial with order $m = 20$

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

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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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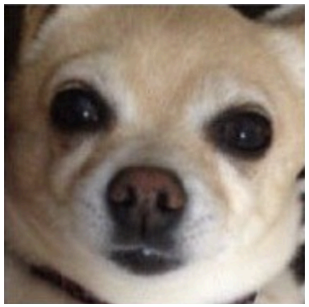

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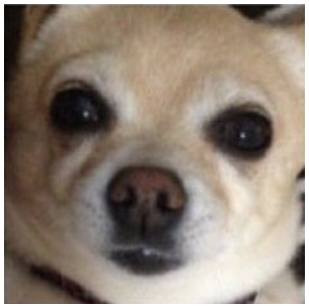

Polynomial regression does not scale to large inputs

Issues arise with other problems

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

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If $\theta_m > 0$

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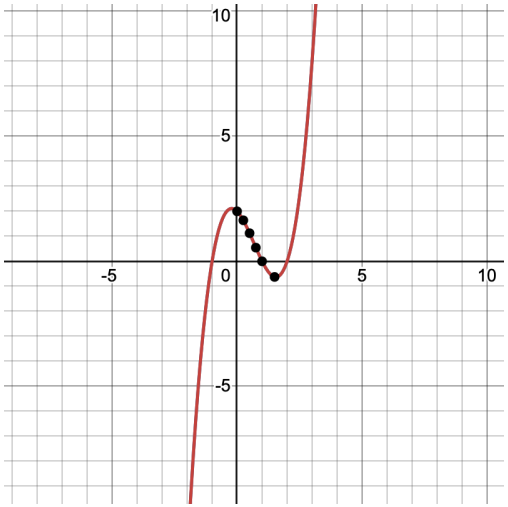

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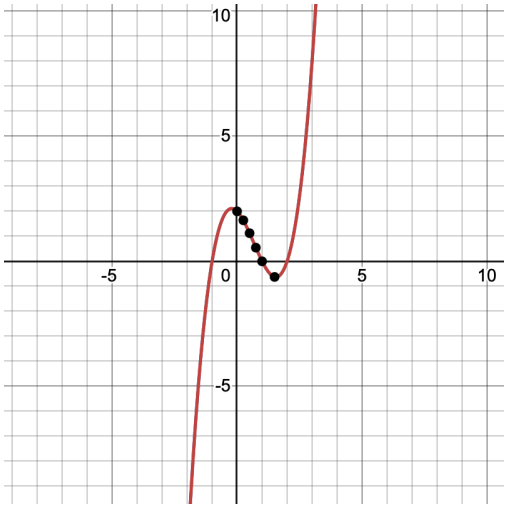

Remember, to predict new data we want our functions to generalize

Linear regression has issues

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1. No analytical solution
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1. Review
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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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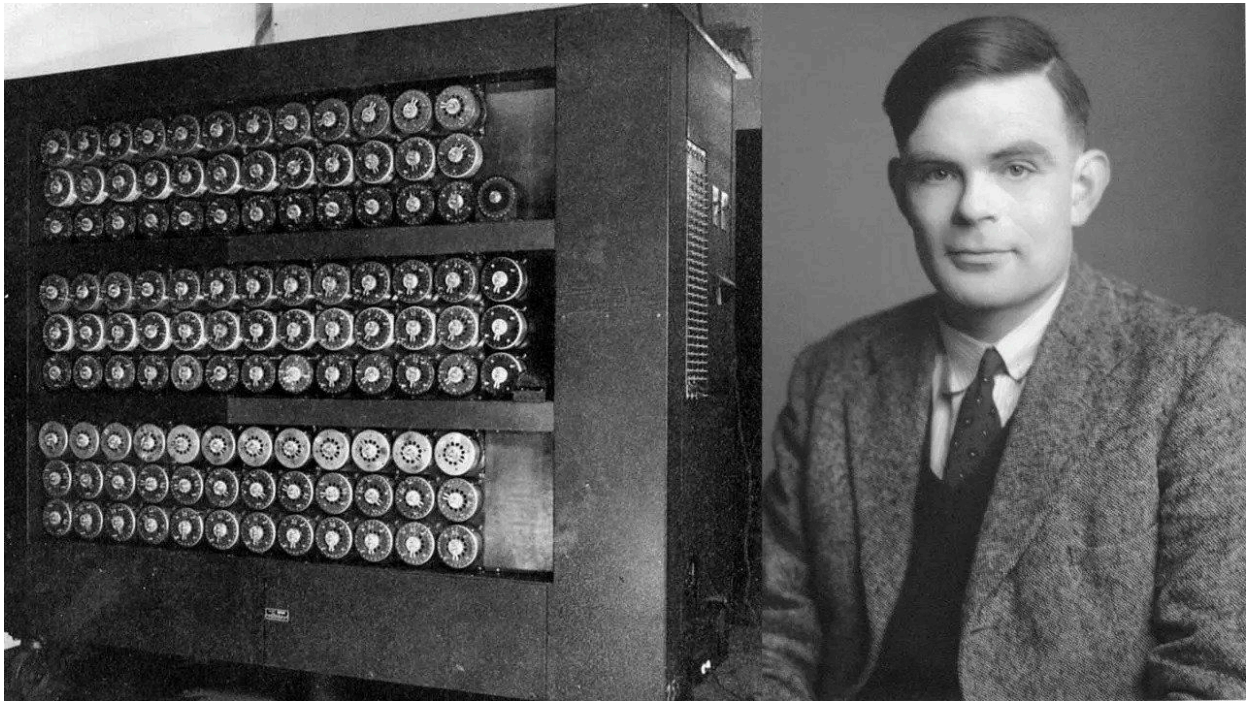
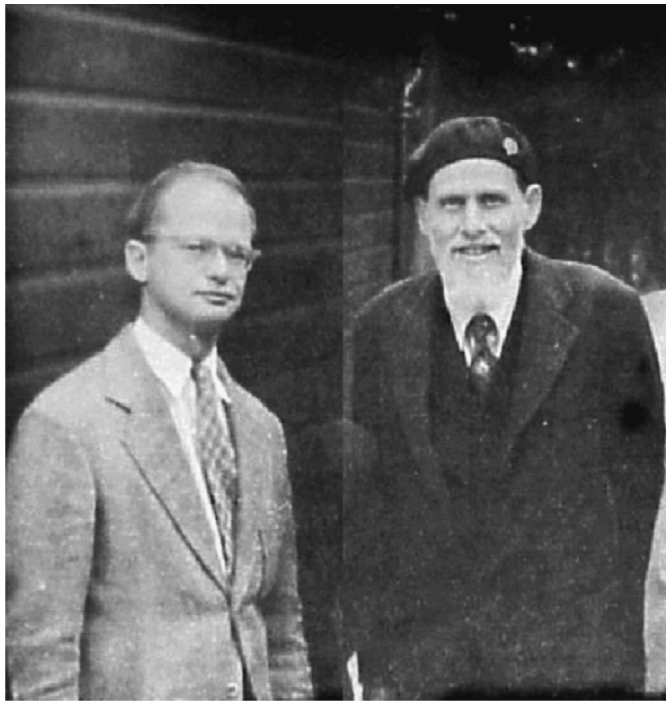


Meanwhile, a neuroscientist and mathematician (McCullough and Pitts) were trying to understand the human brain



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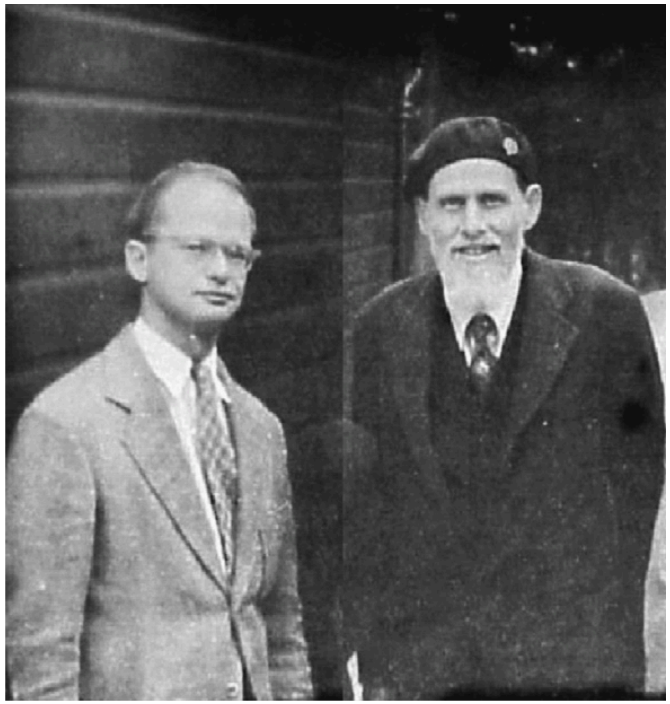

They designed the theory for the first neural network

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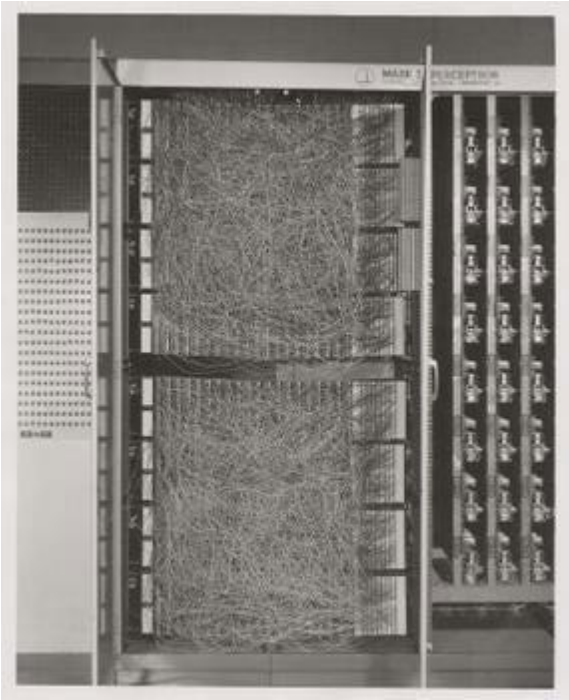
At the time, computers were very slow and expensive



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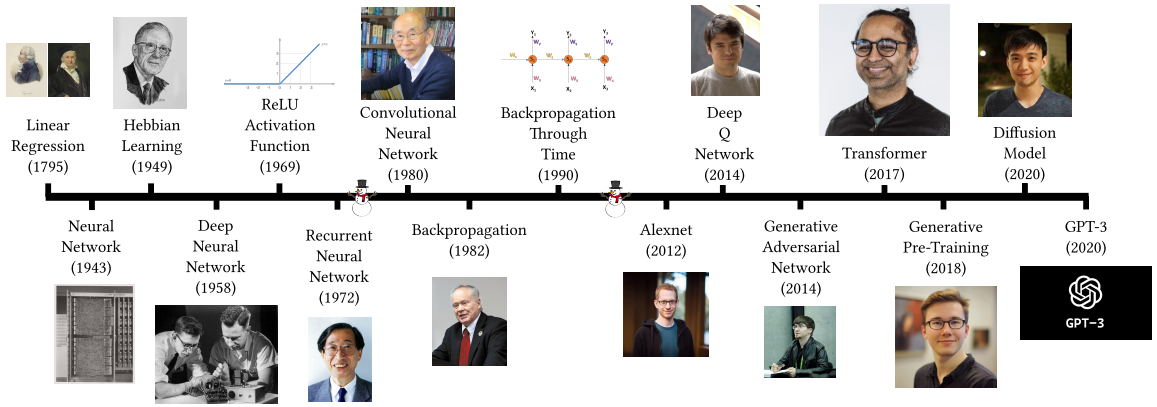

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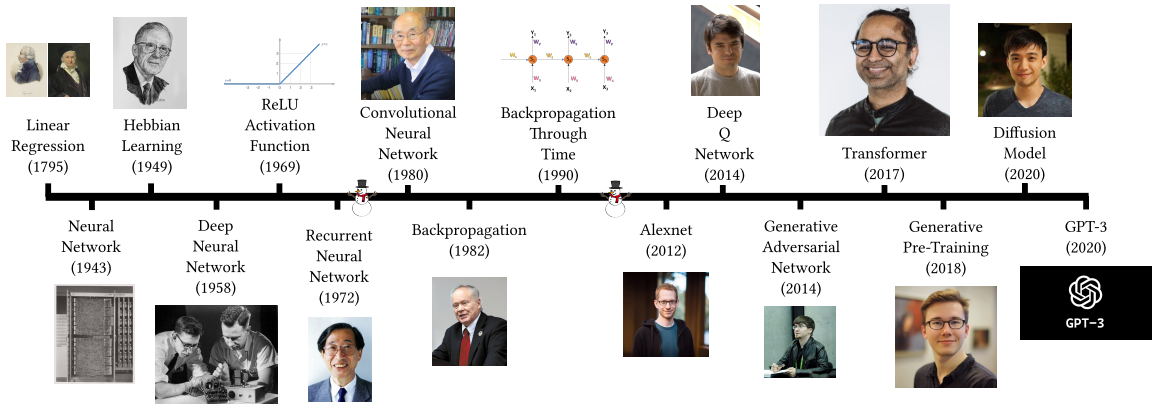

Around 2012, these improvements culminated in neural networks that perform like humans

So what is a neural network?

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First, let us review biological 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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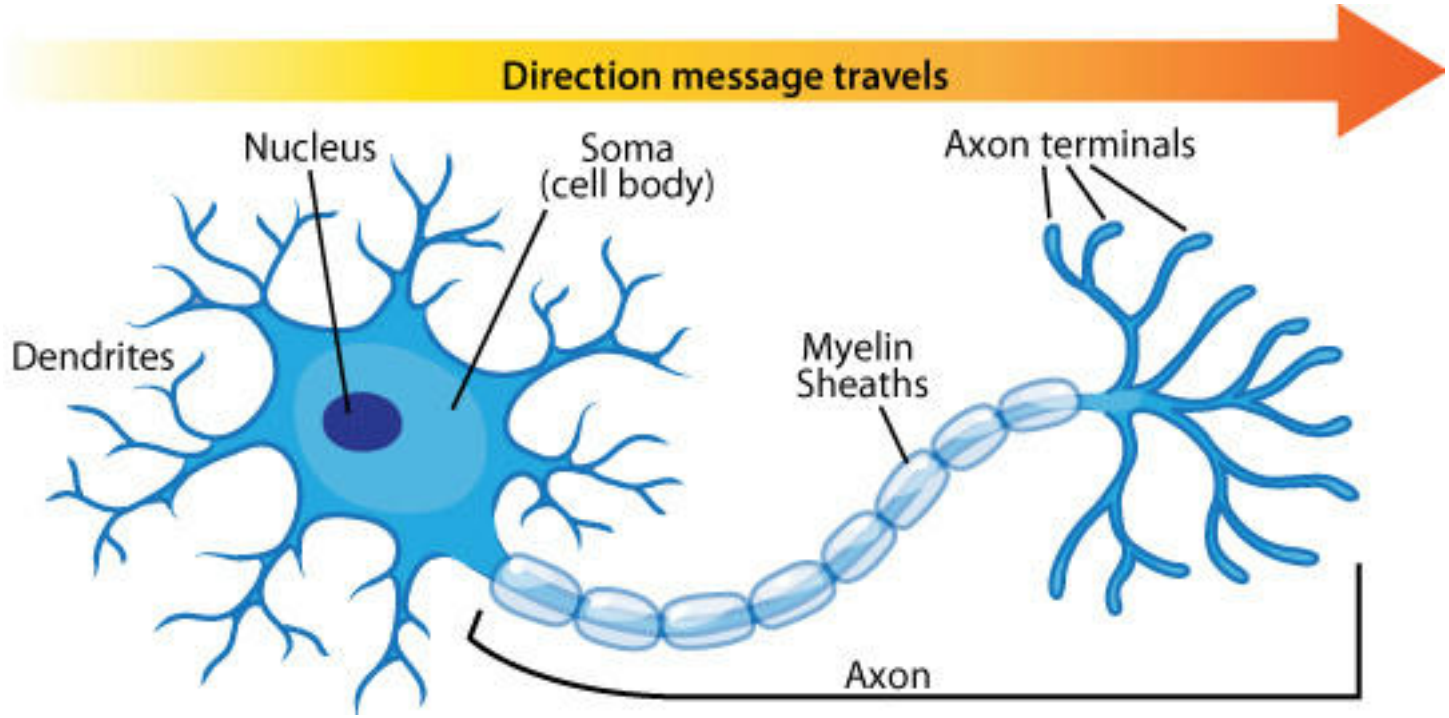
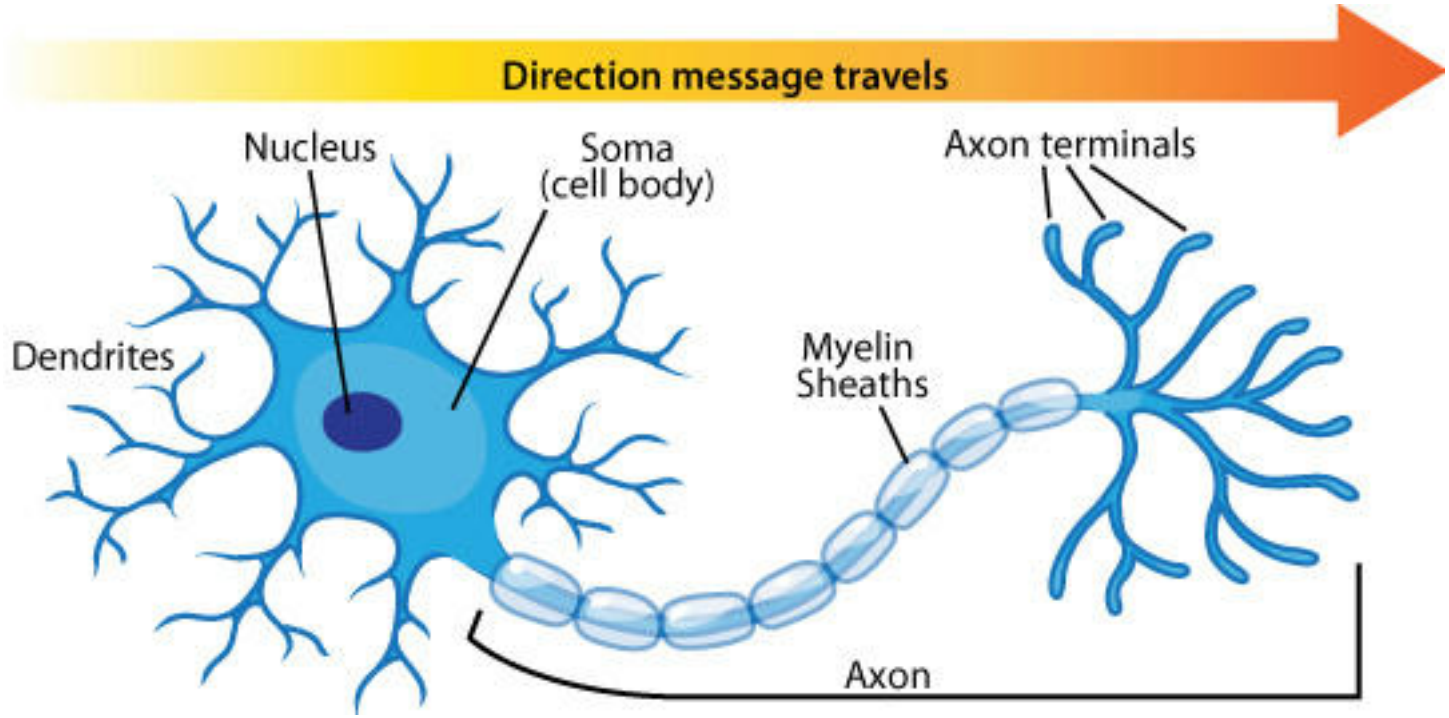
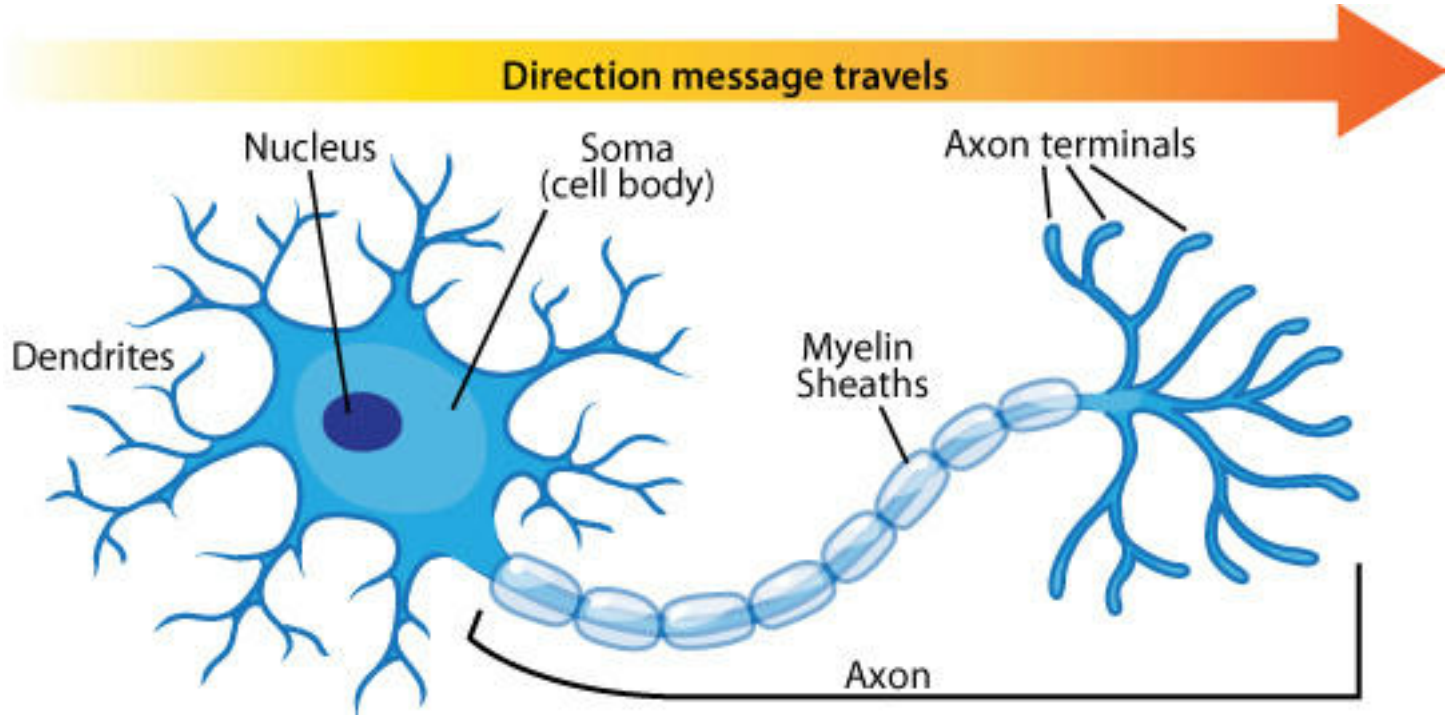


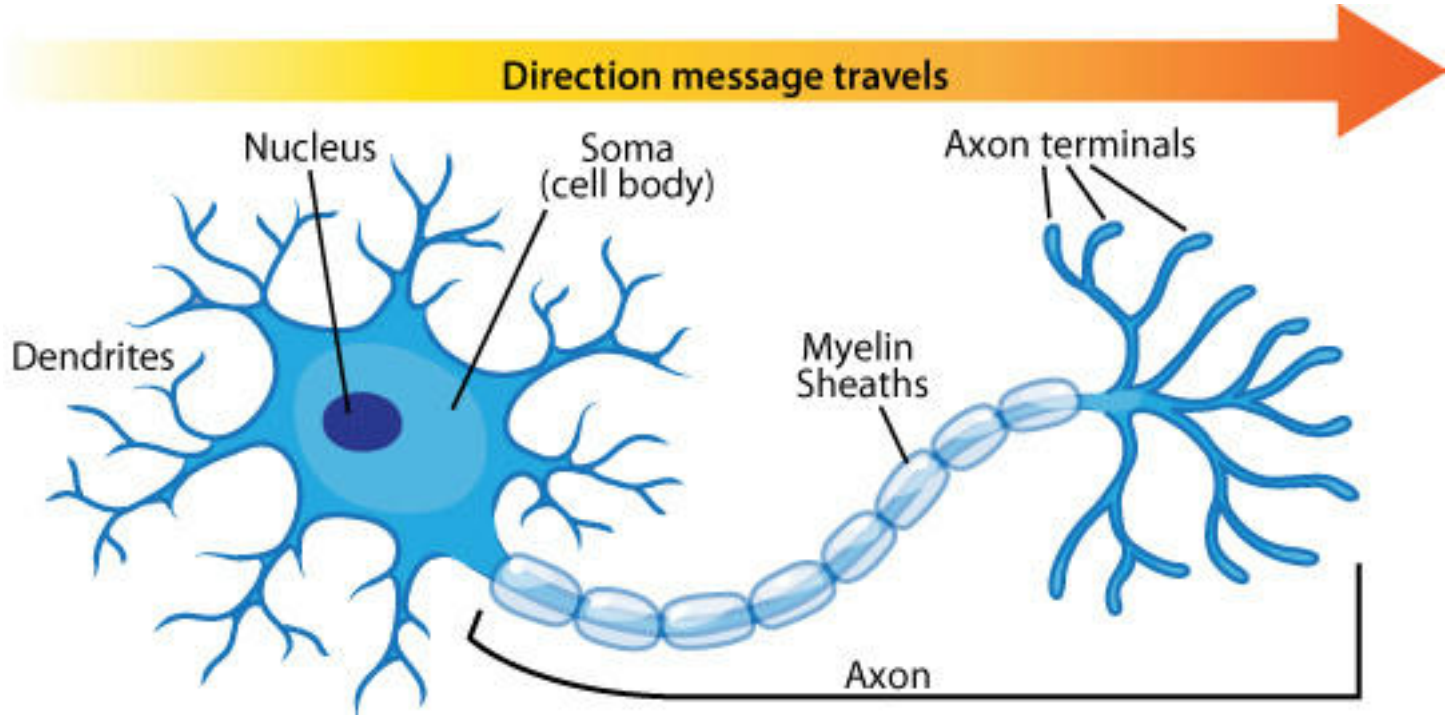
A simplified neuron consists of many parts



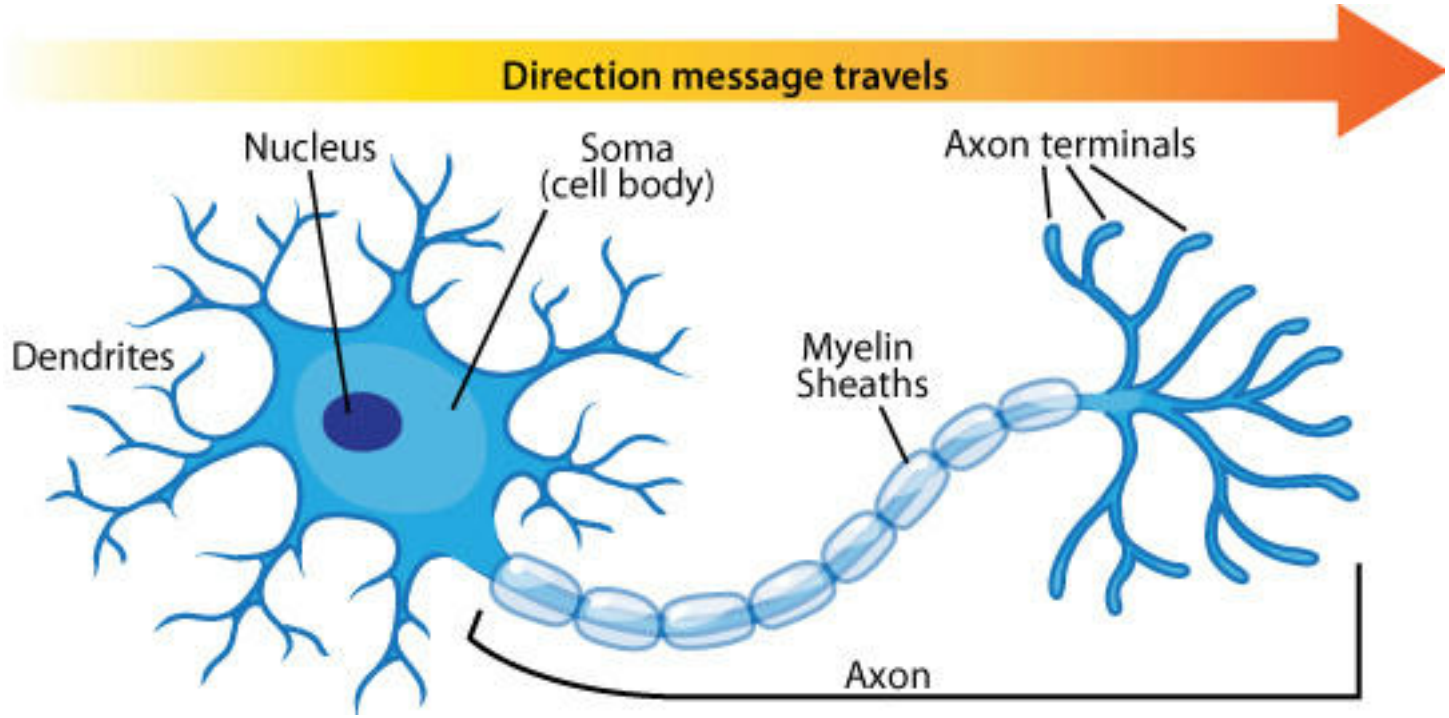
Neurons send messages based on messages received from other neurons



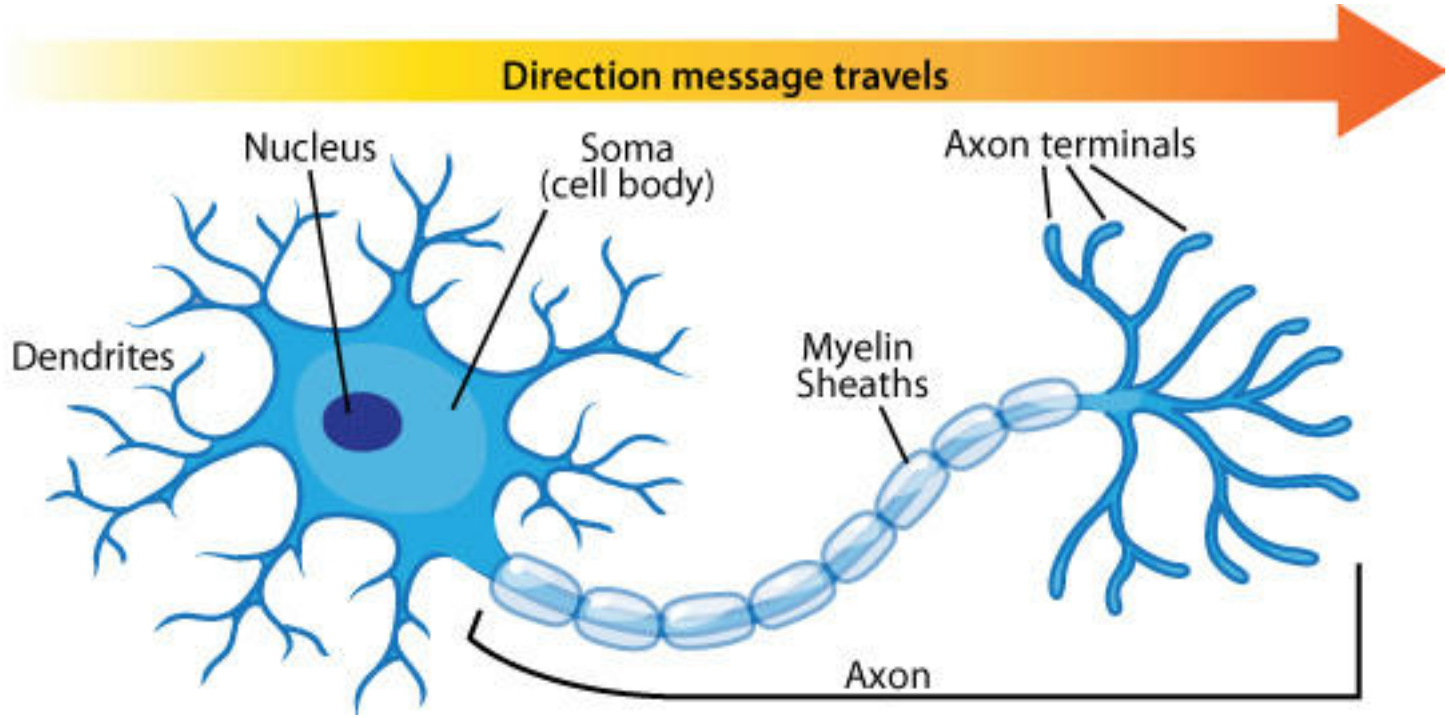
Incoming electrical signals travel along dendrites



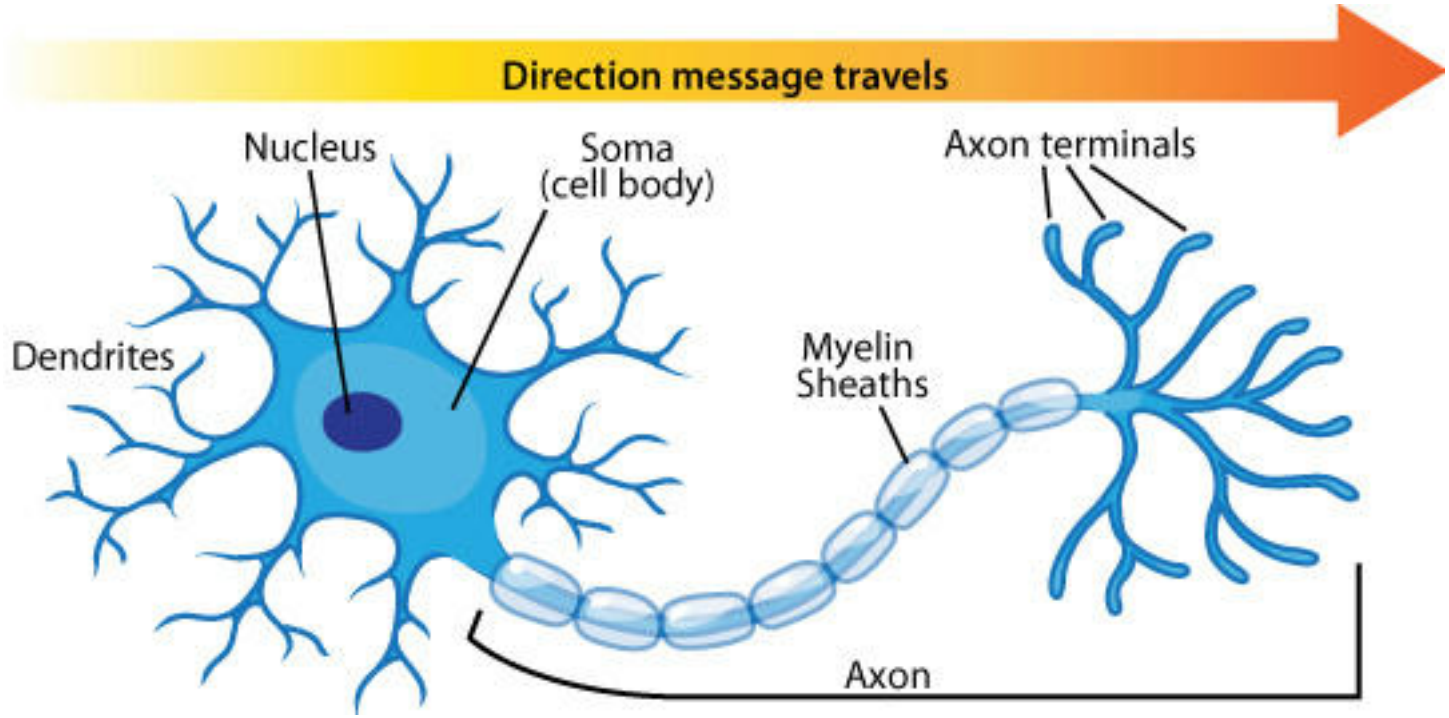
Dendrites are not all equal! Different dendrites have different diameters and structures



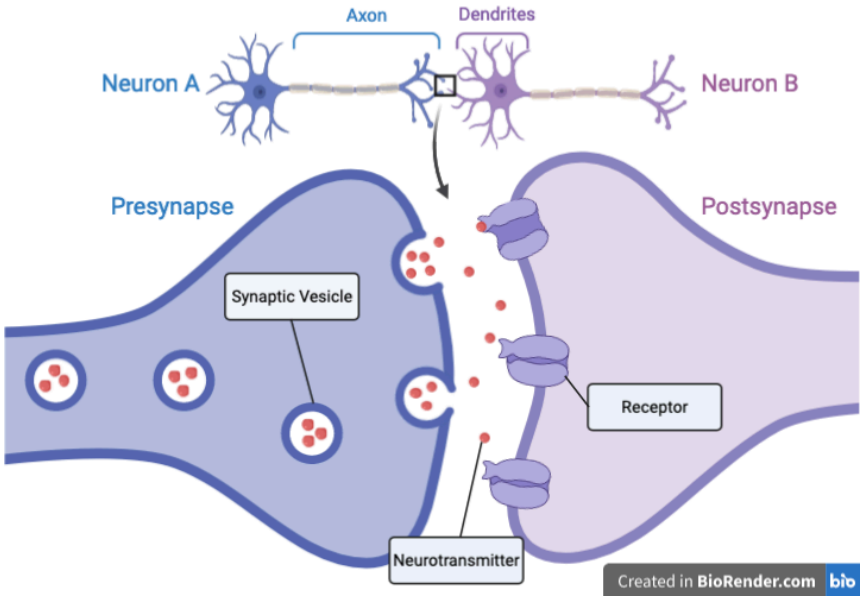
Electrical charges collect in the Soma (cell body)



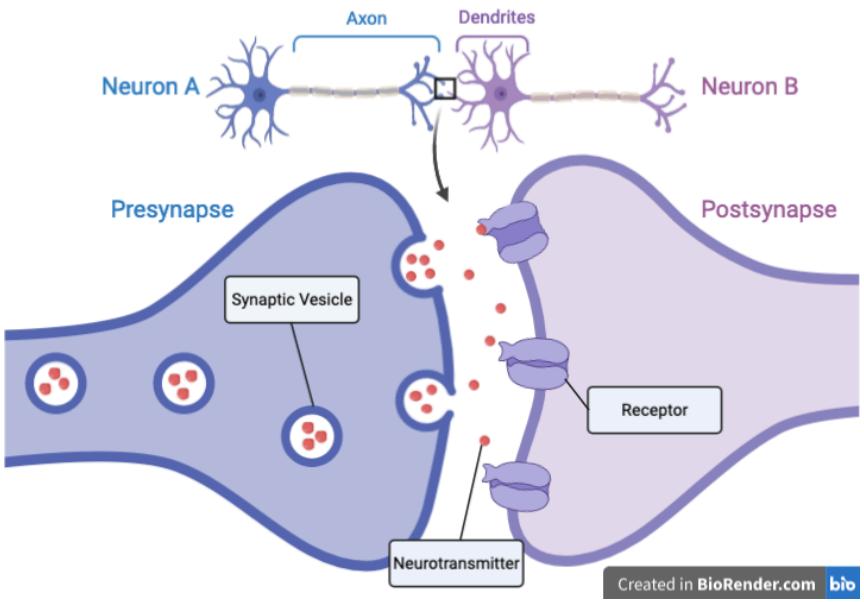
The axon outputs an electrical signal to other neurons



The axon terminals will connect to dendrites of other neurons through a synapse



The synapse converts electrical signal, to chemical signal, back to electrical signal



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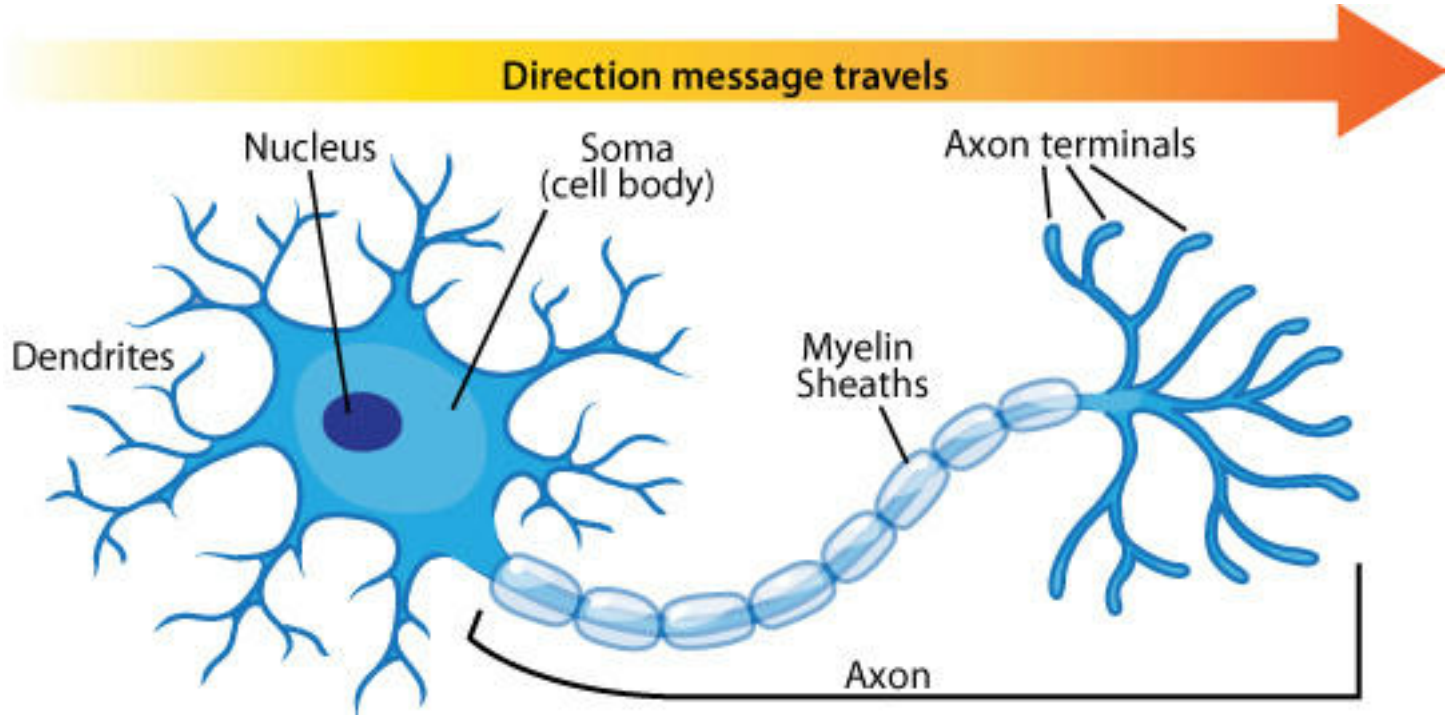
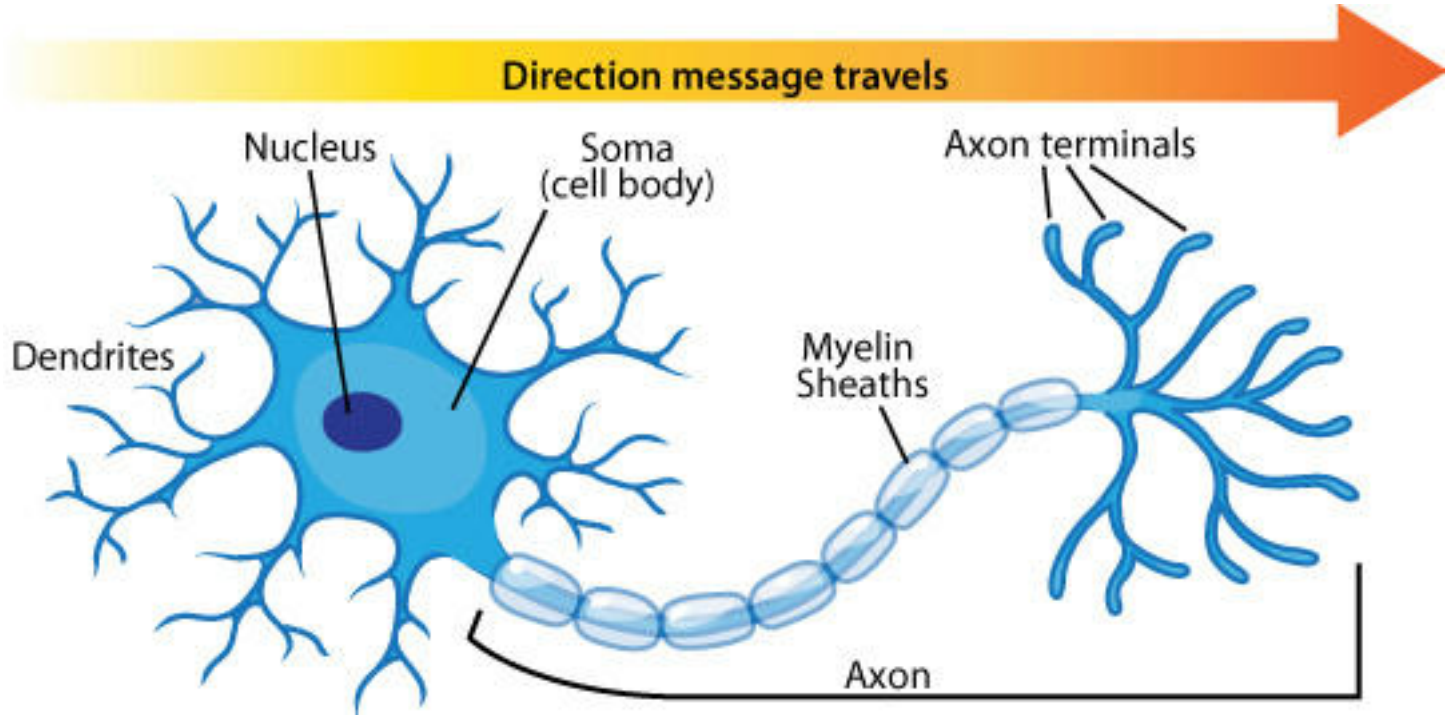
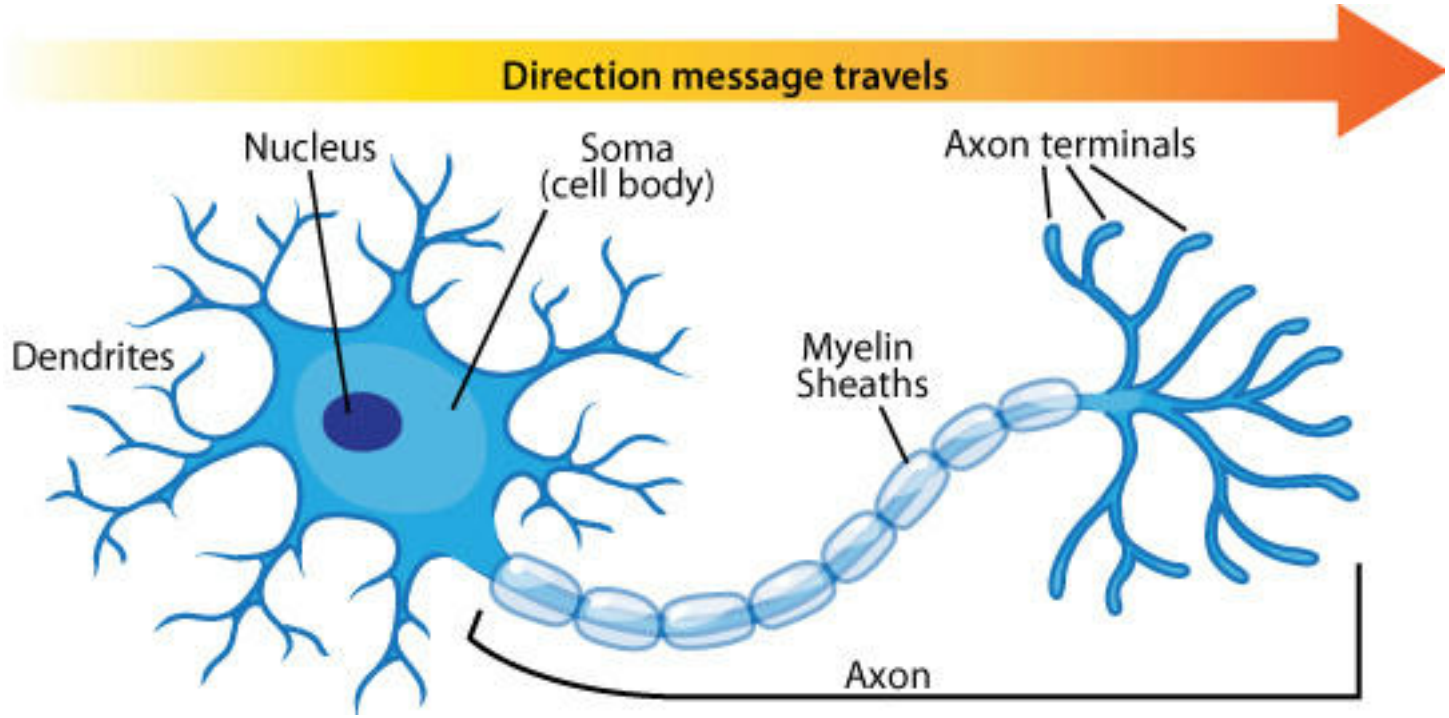
Synaptic weight determines how well a signal crosses the gap



For our purposes, we can model the axon terminals, dendrites, and synapses to be one 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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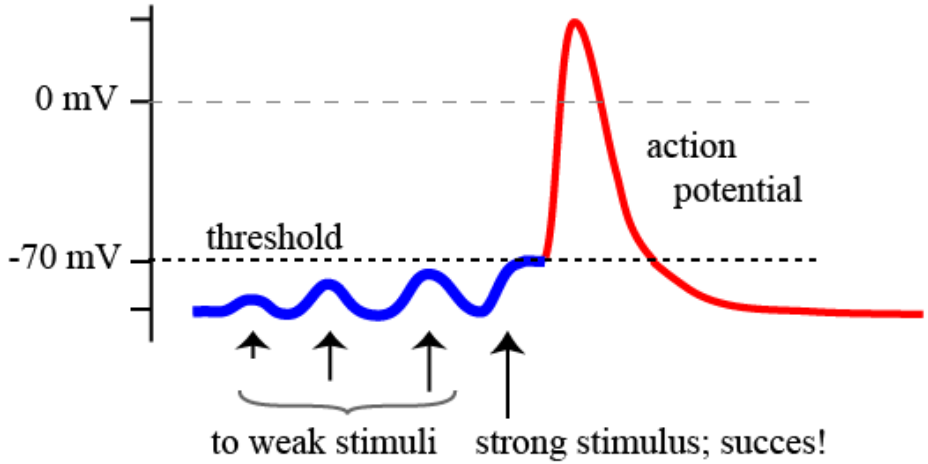
Incoming impulses (via dendrites) change the electric potential of the neuron



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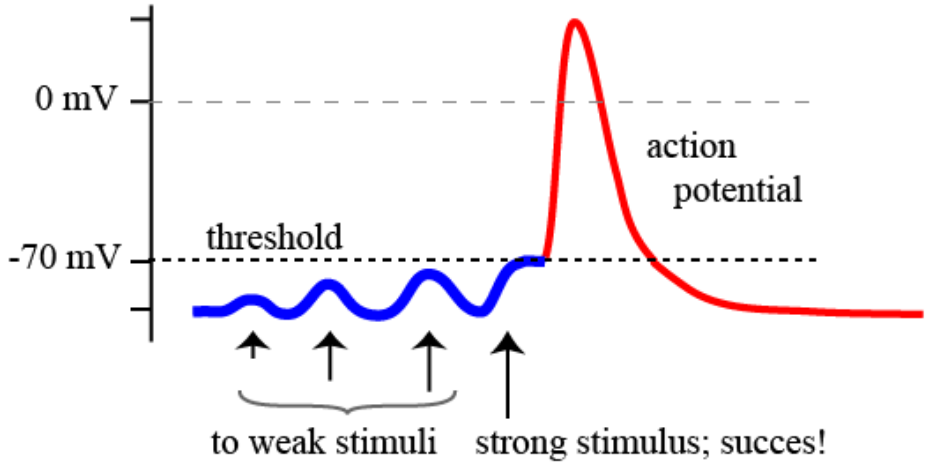

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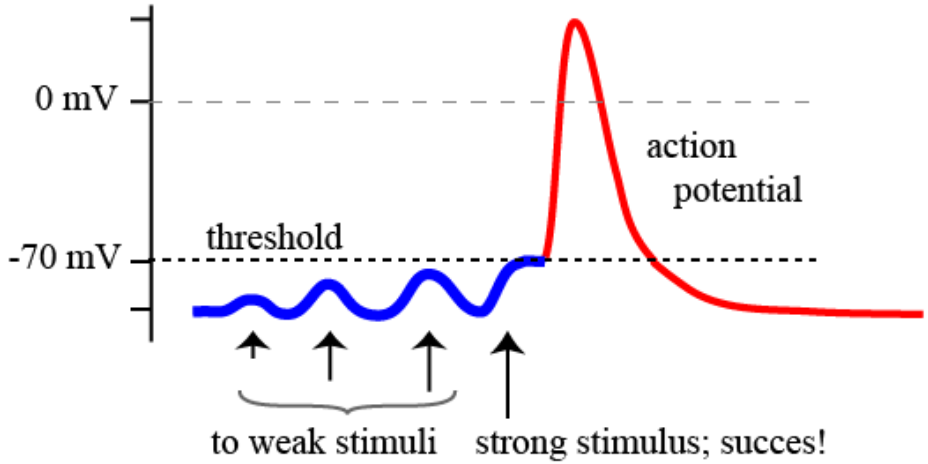

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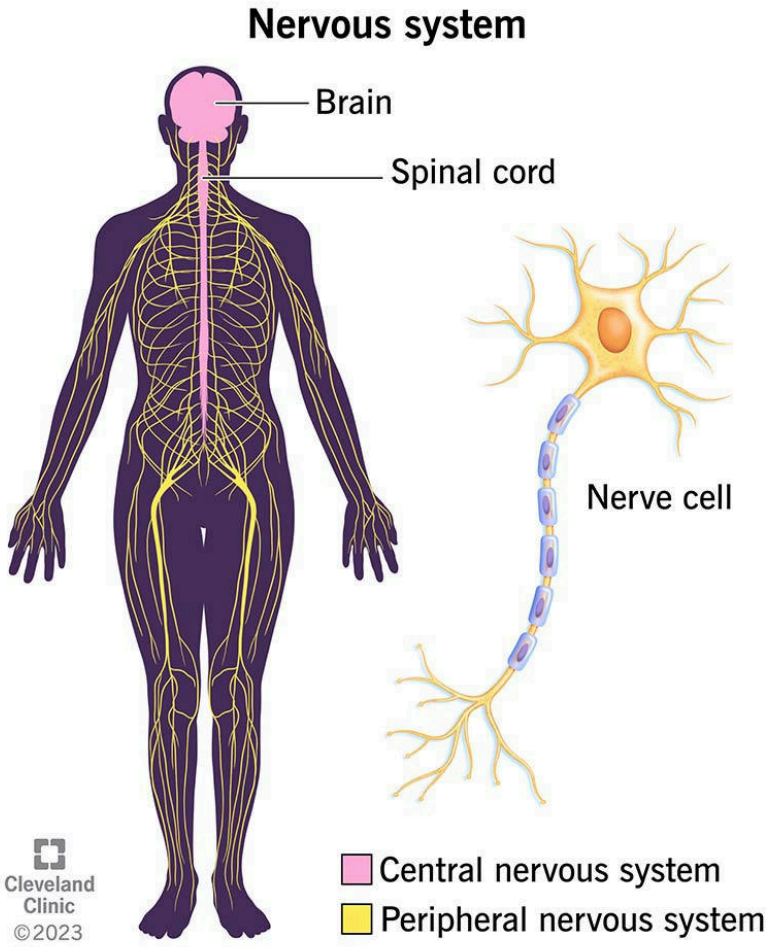
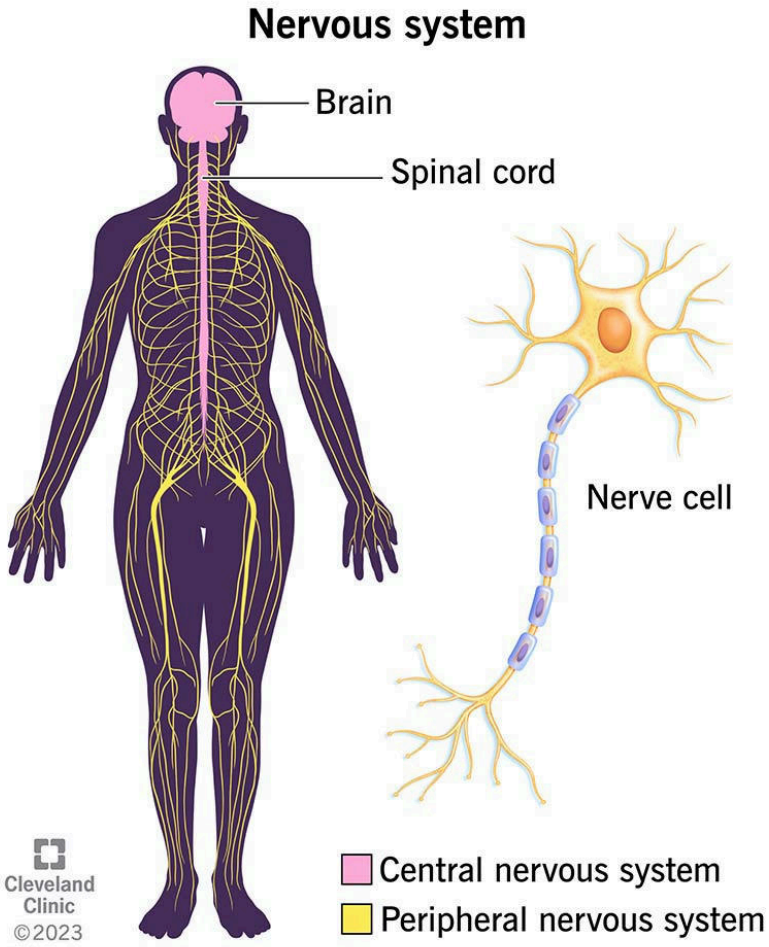
Many active dendrites will add together and trigger an impulse

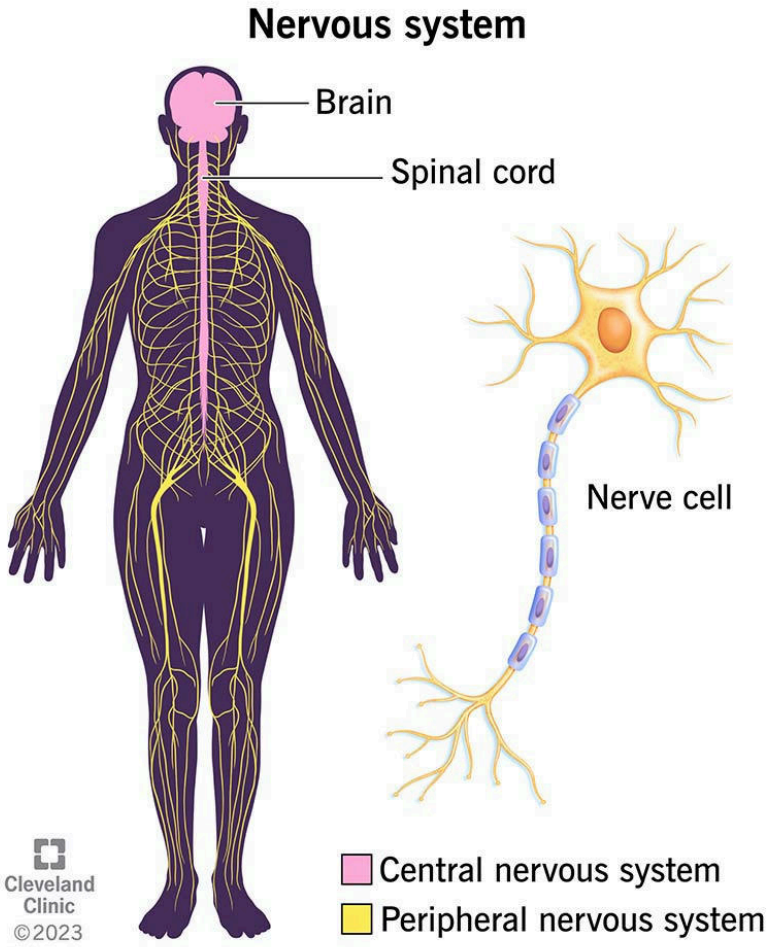
Pain triggers initial nerve impulse, starts a chain reaction into the brain



When the signal reaches the brain, we will think



After thinking, we will take action



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
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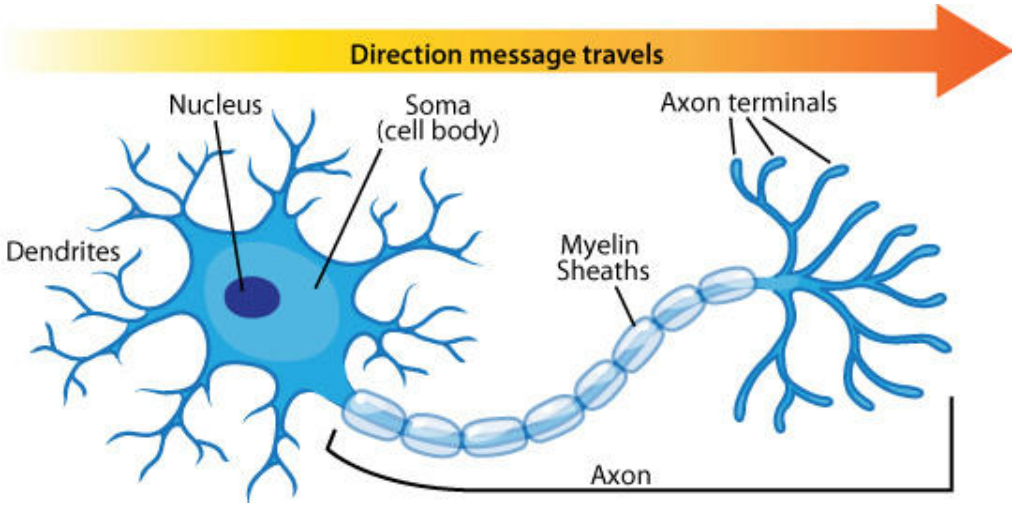
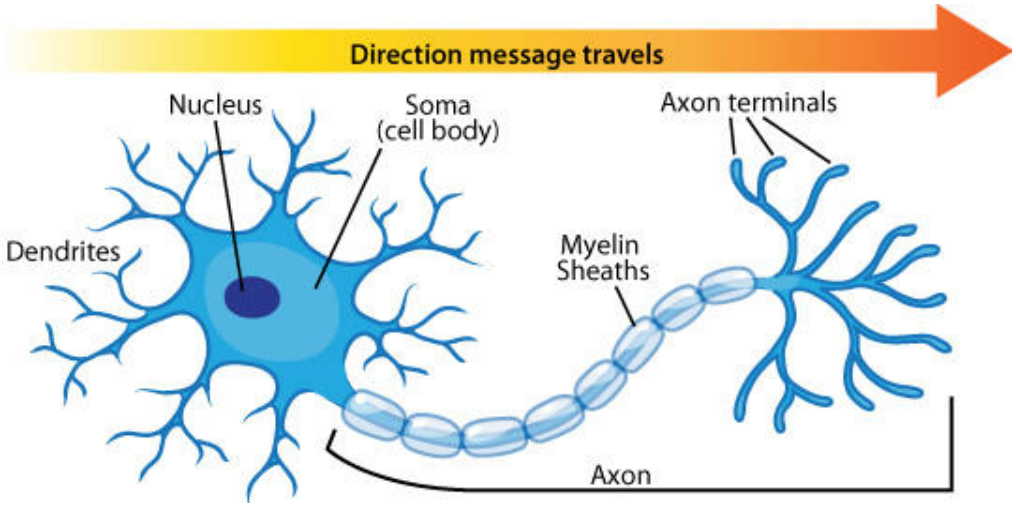
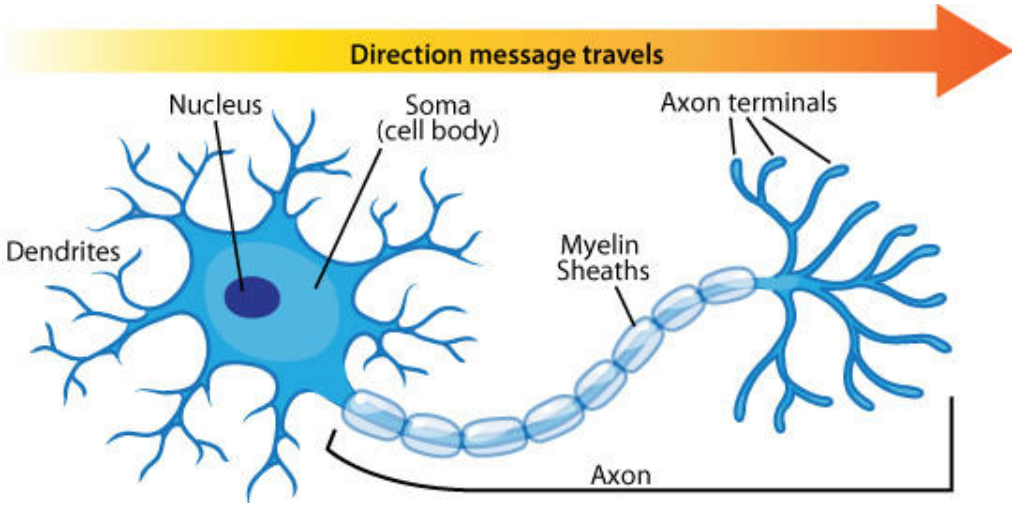

Direction message travels
Nucleus
Soma
(cell body)
Axon terminals
Dendrites
Myelin
Sheaths
Axon



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:

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

Let us implement an artifical neuron as a function

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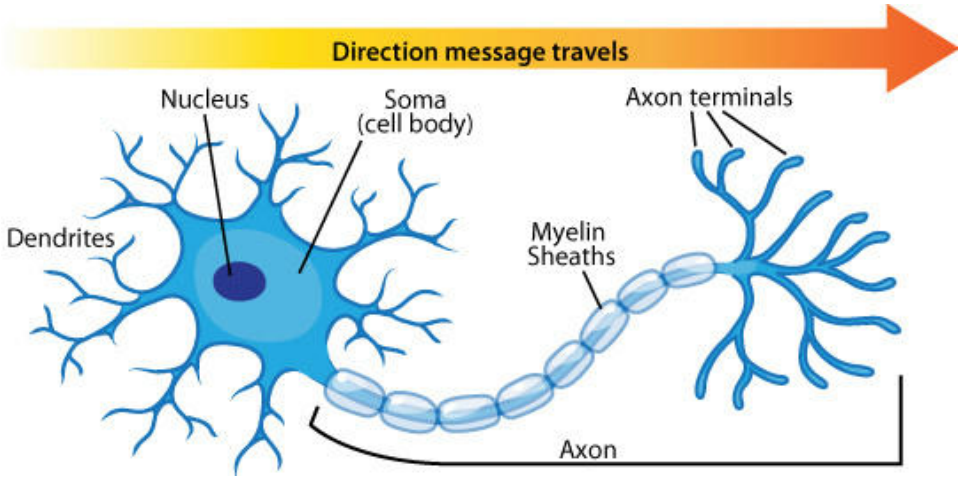

Neuron has a structure of dendrites with synaptic weights

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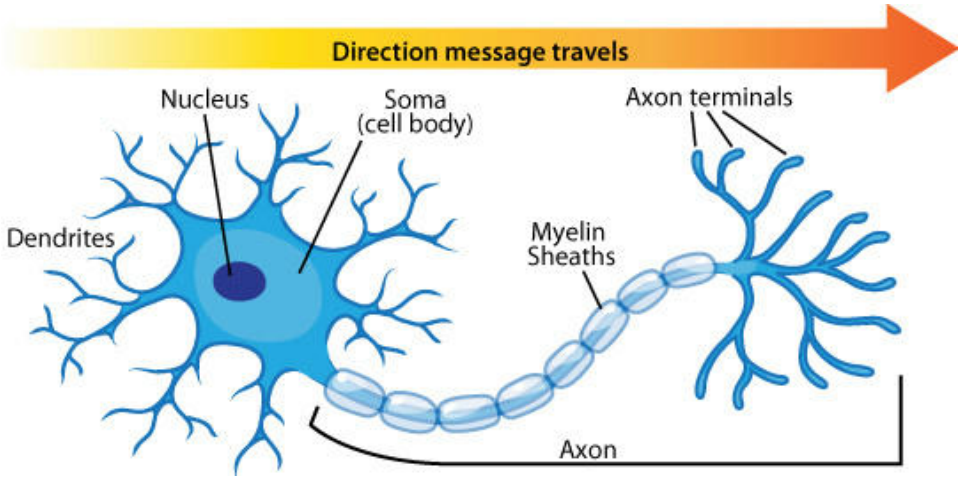

Neuron has a structure of dendrites with synaptic weights

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

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

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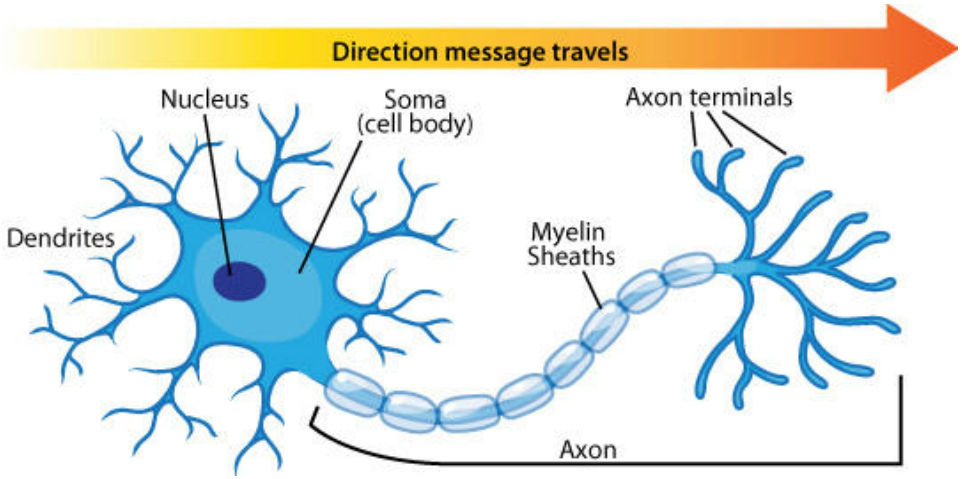

Each incoming dendrite has some voltage potential

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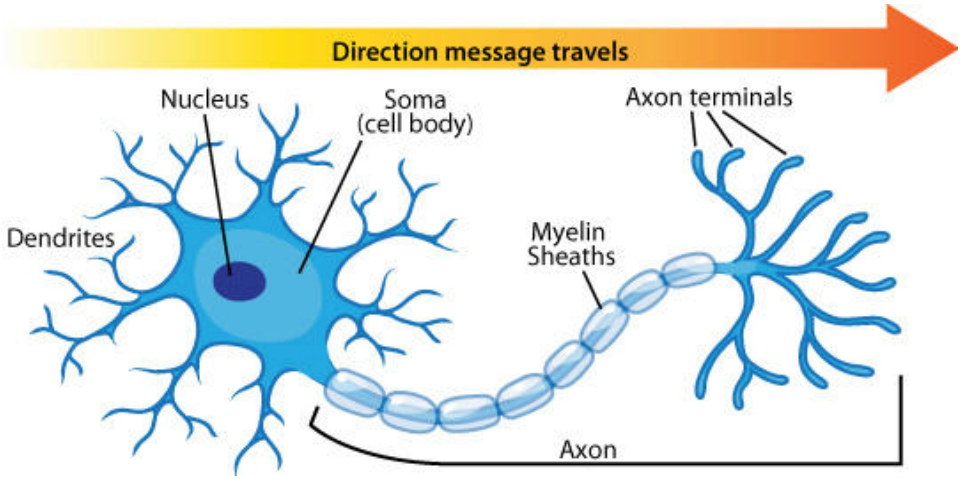

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$$f\left(\begin{bmatrix} x_1 \\ \vdots \\ x_{d_x} \end{bmatrix}, \begin{bmatrix} \theta_1 \\ \vdots \\ \theta_{d_x} \end{bmatrix}\right)$$

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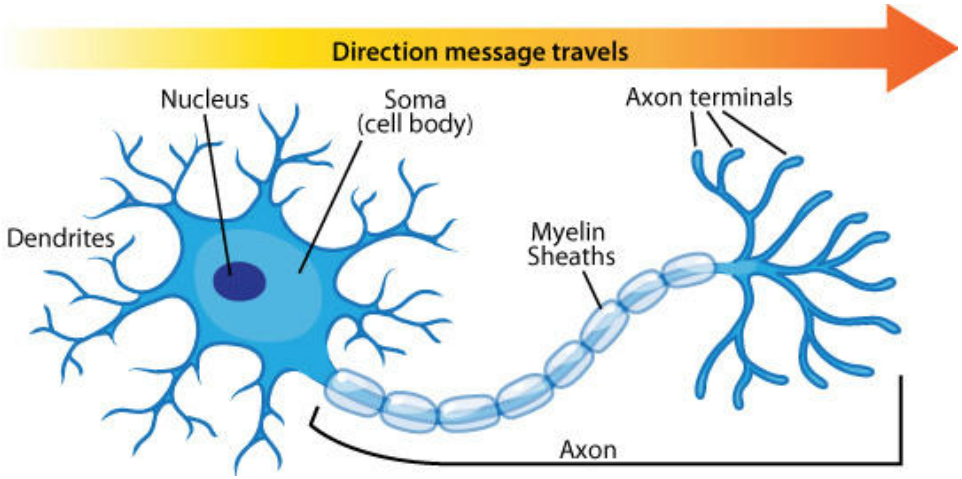

Voltage potentials sum together to give us the voltage in the cell body

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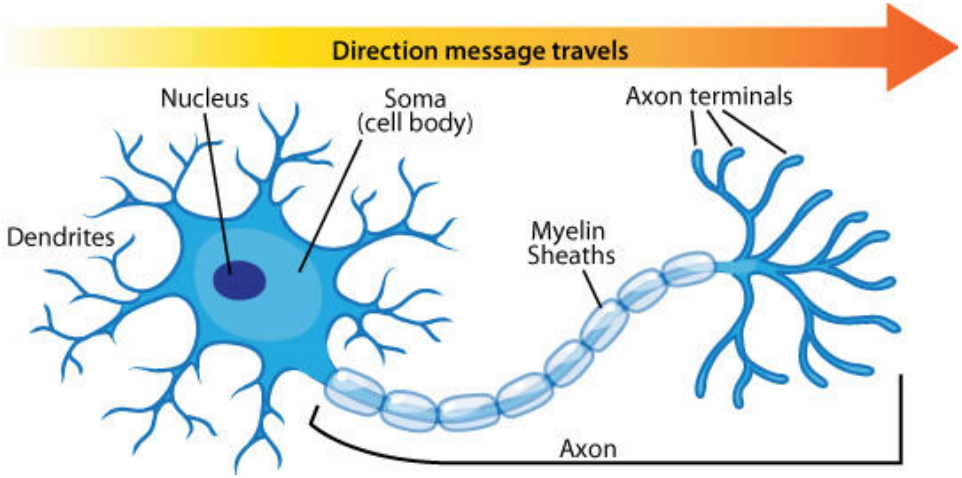

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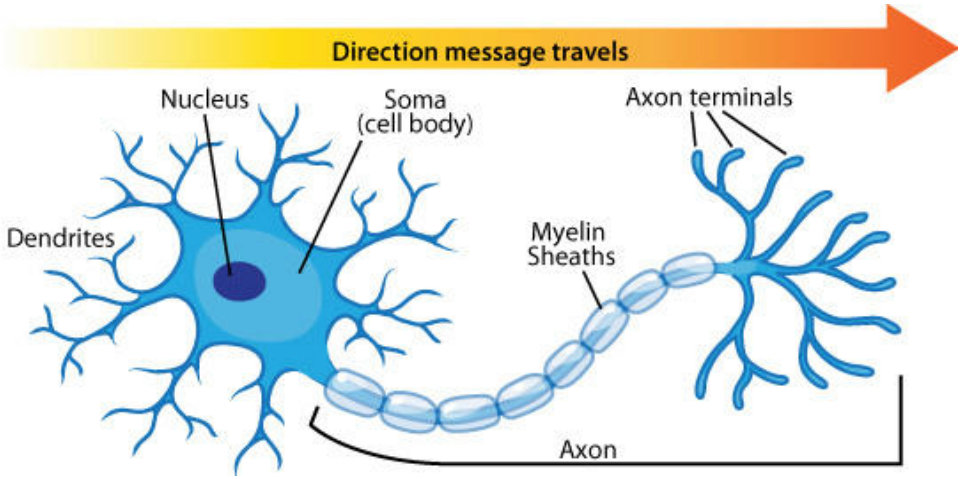

The axon fires only if the voltage is over a threshold

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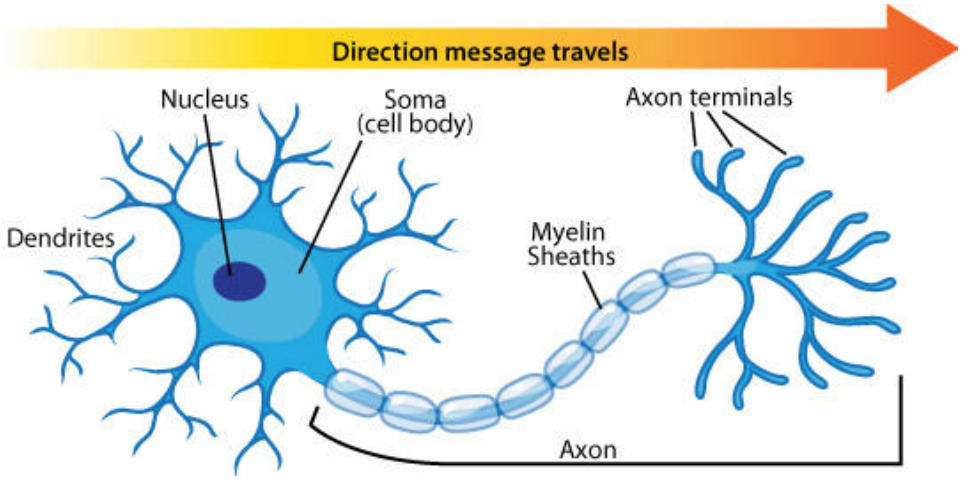

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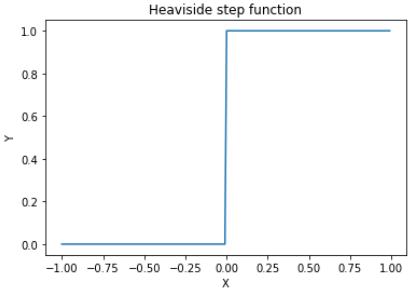

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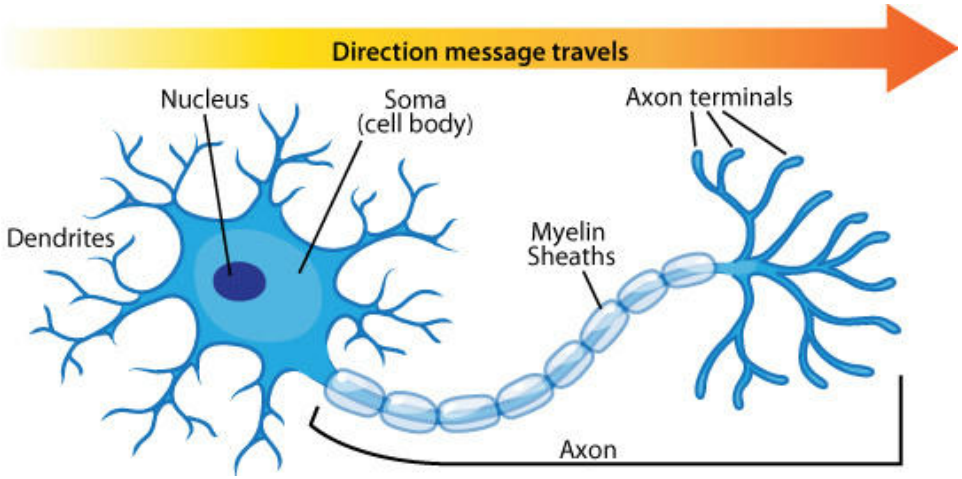

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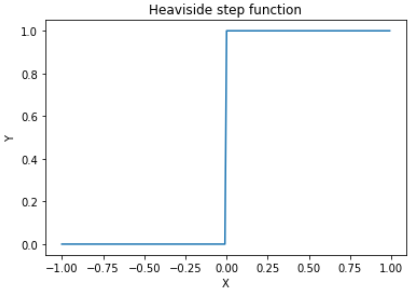
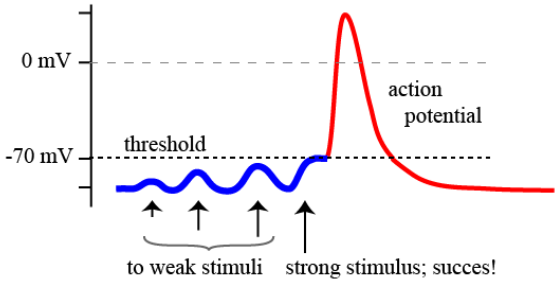
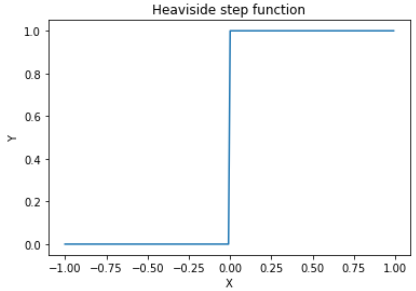


$$f\left(\begin{bmatrix} x_1 \\ \vdots \\ x_n \end{bmatrix}, \begin{bmatrix} \theta_1 \\ \vdots \\ \theta_n \end{bmatrix}\right) = \sigma\left(\sum_{j=1}^{d_x} \theta_j x_j\right)$$

Maybe we want to vary the activation threshold





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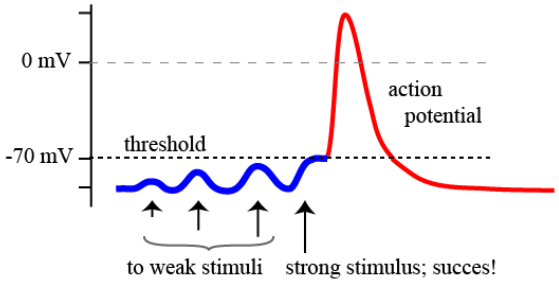

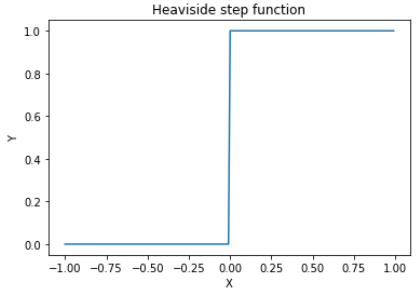

$$f\left(\begin{bmatrix}1\\x_1\\\vdots\\x_{d_x}\end{bmatrix},\begin{bmatrix}\theta_0\\\theta_1\\\vdots\\\theta_{d_x}\end{bmatrix}\right)=\sigma\left(\theta_0+\sum_{j=1}^{d_x}\theta_j x_j\right)=\sigma\left(\sum_{j=0}^{d_x}\theta_j x_j\right)$$

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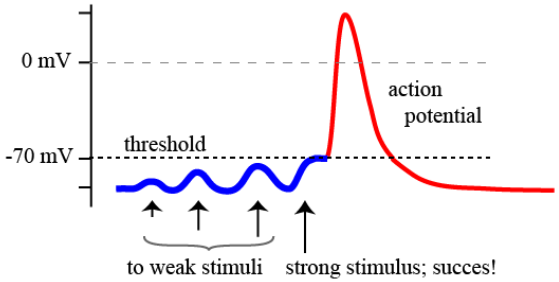

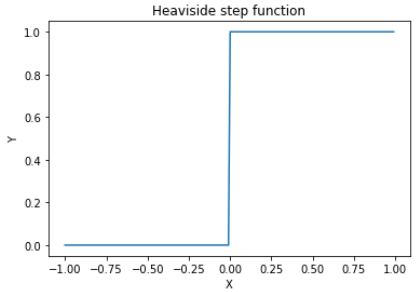

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$$\overline{\boldsymbol{x}}=\begin{bmatrix}1\\\boldsymbol{x}\end{bmatrix},\quad f(\boldsymbol{x},\boldsymbol{\theta})=\sigma(\boldsymbol{\theta}^\top\overline{\boldsymbol{x}})$$

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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!

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

We model a neuron using a linear model and activation function

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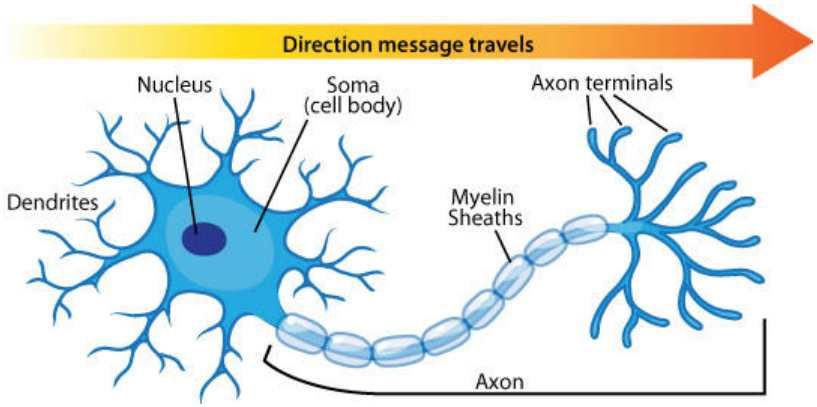

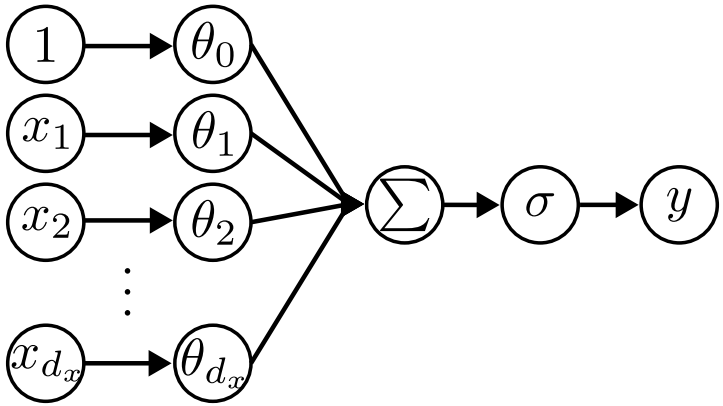

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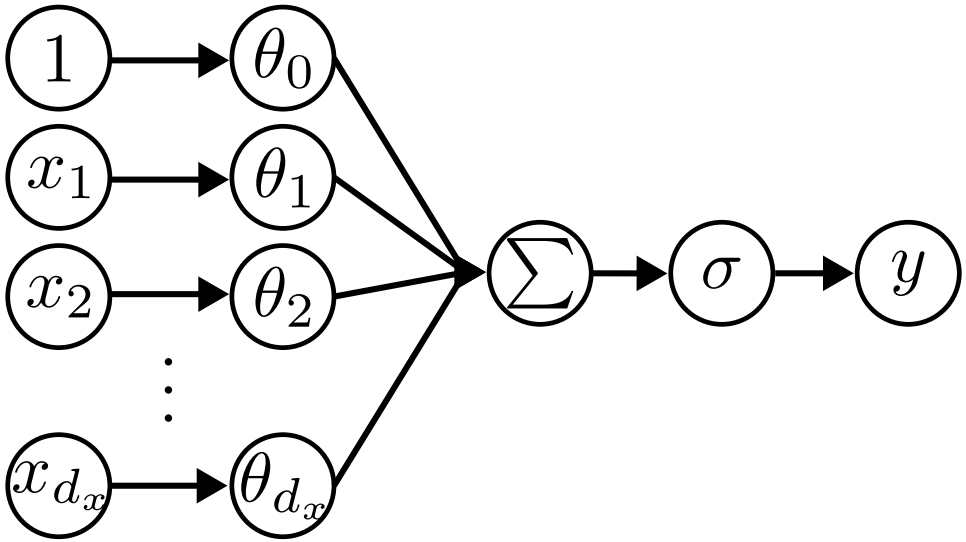
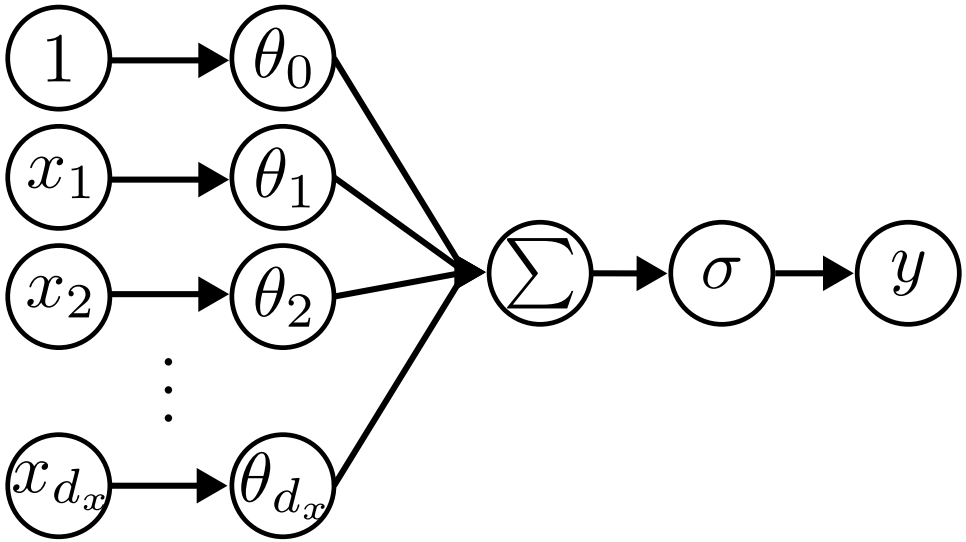
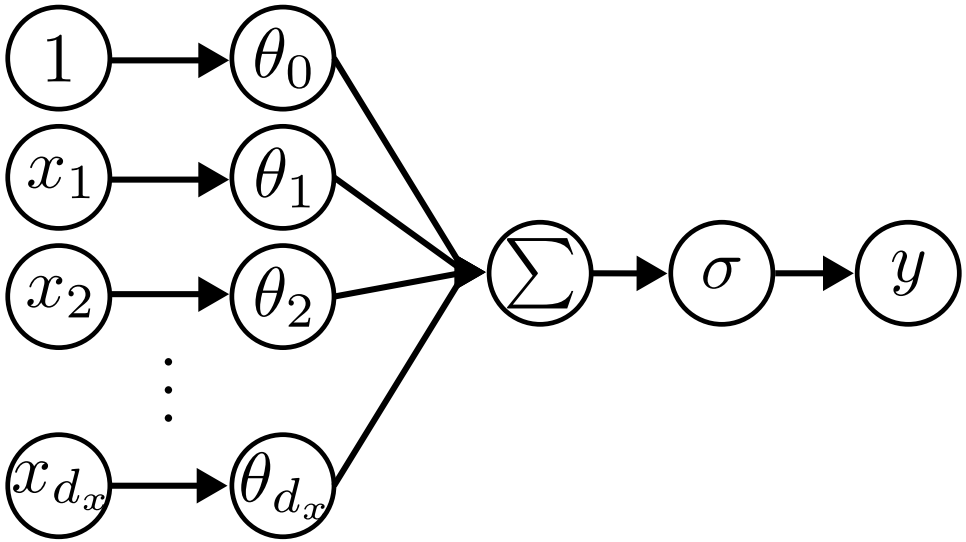
$$f\left(\boldsymbol{x}, \begin{bmatrix} b \\ \boldsymbol{w} \end{bmatrix}\right) = b + \boldsymbol{w}^\top \boldsymbol{x}$$

Relax


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

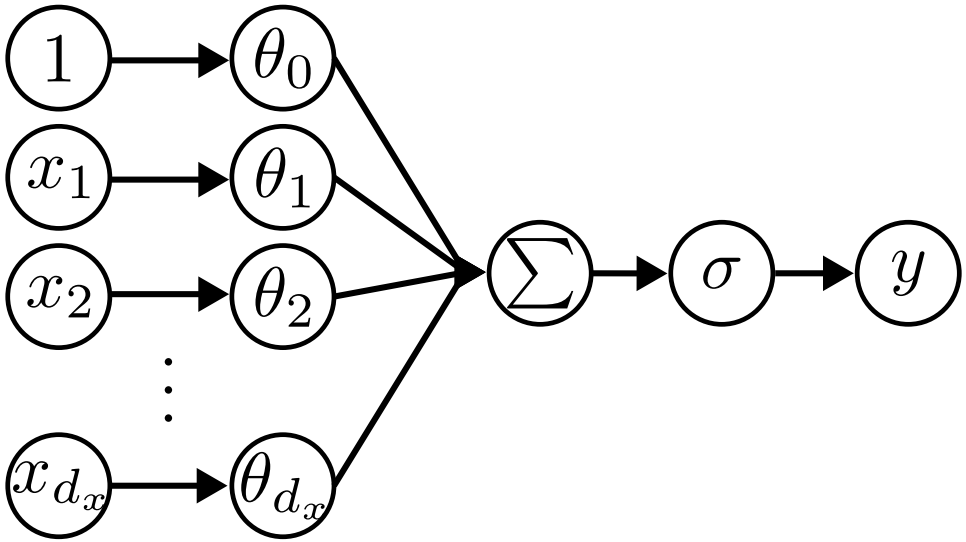


In machine learning, we represent functions



In machine learning, we represent functions

What kinds of functions can our neuron represent?



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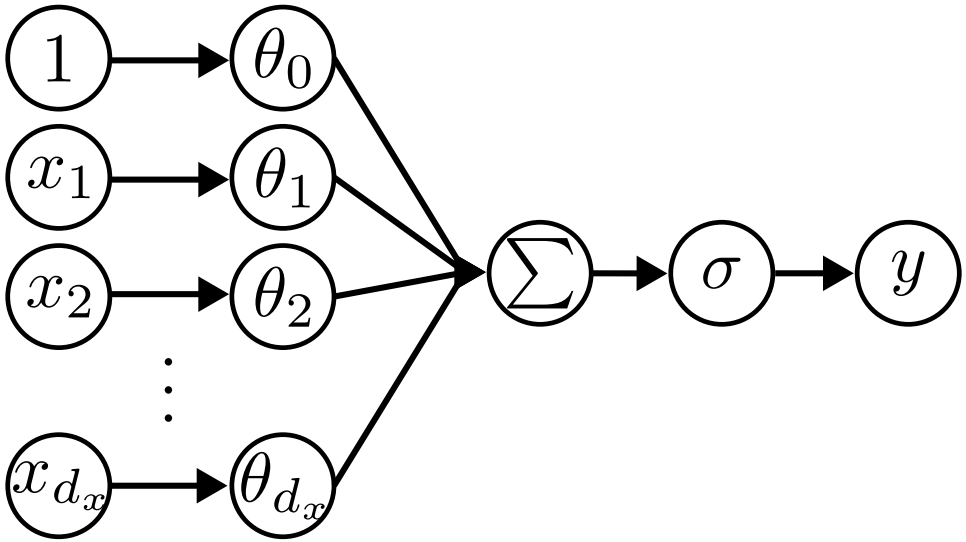
Let us consider some **boolean** functions



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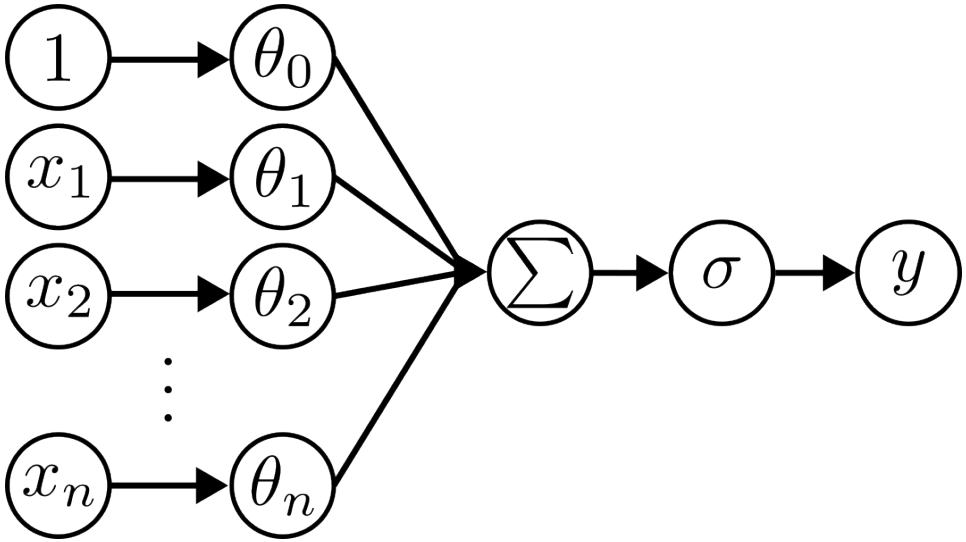
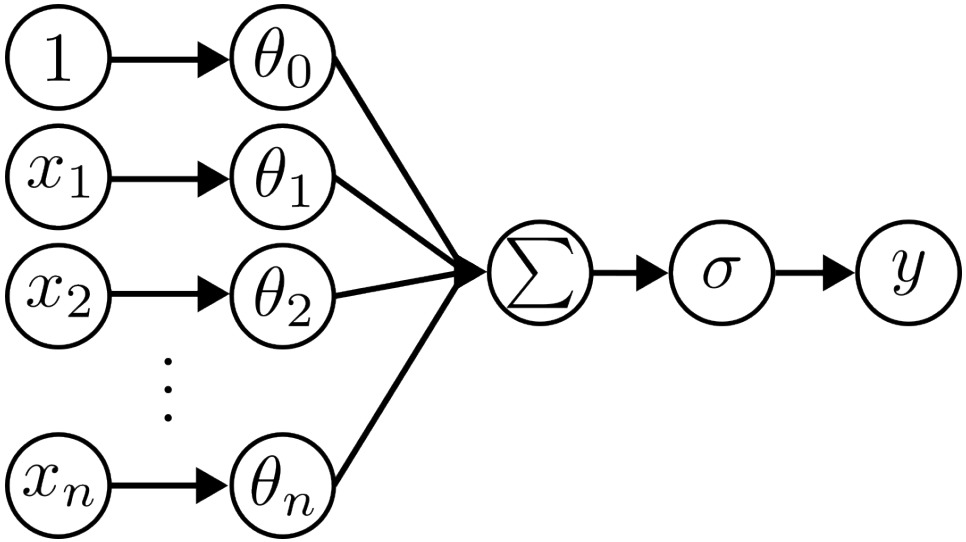
Let us start with a logical AND function

Review: Activation function (Heaviside step function)





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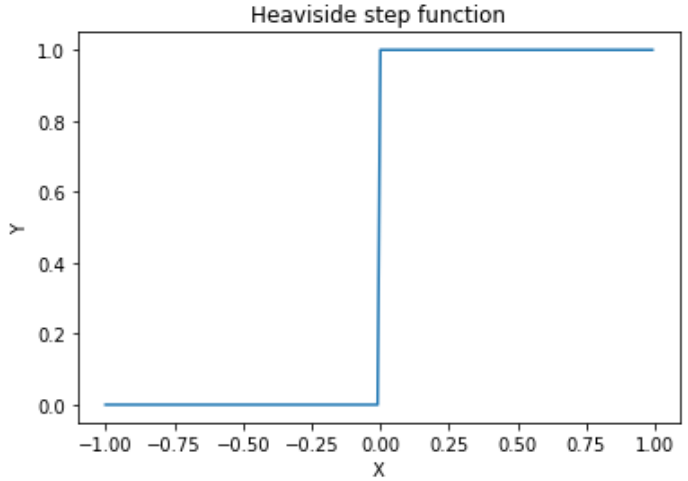

$$\sigma(x) = H(x) = \begin{cases} 1 \text{ if } x > 0 \\ 0 \text{ if } x \leq 0 \end{cases}$$

Implement AND using an artificial neuron

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$$f\left([x_1 \;\; x_2]^\top, [\theta_0 \;\; \theta_1 \;\; \theta_2]^\top\right) = \sigma(\theta_0 1 + \theta_1 x_1 + \theta_2 x_2)$$

Implement AND using an artificial neuron

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$$\boldsymbol{\theta} = [\theta_0 \;\; \theta_1 \;\; \theta_2]^\top = [-1 \;\; 1 \;\; 1]^\top$$

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

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Implement OR using an artificial neuron

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$$\boldsymbol{\theta} = [\theta_0 \;\; \theta_1 \;\; \theta_2]^\top = [0 \;\; 1 \;\; 1]^\top$$

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

Implement XOR 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	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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$$f\left(\begin{bmatrix} x_1 & x_2 \end{bmatrix}^\top, \begin{bmatrix} \theta_0 & \theta_1 & \theta_2 \end{bmatrix}^\top\right) = \sigma(1\theta_0 + x_1\theta_1 + x_2\theta_2)$$

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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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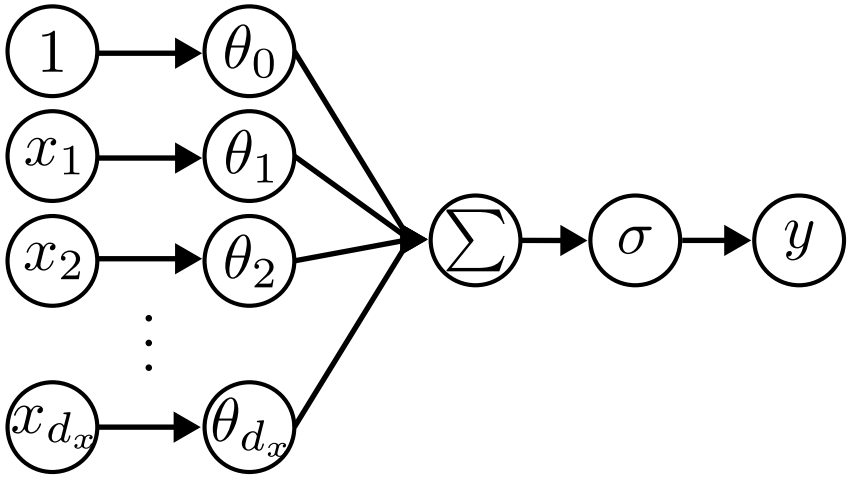
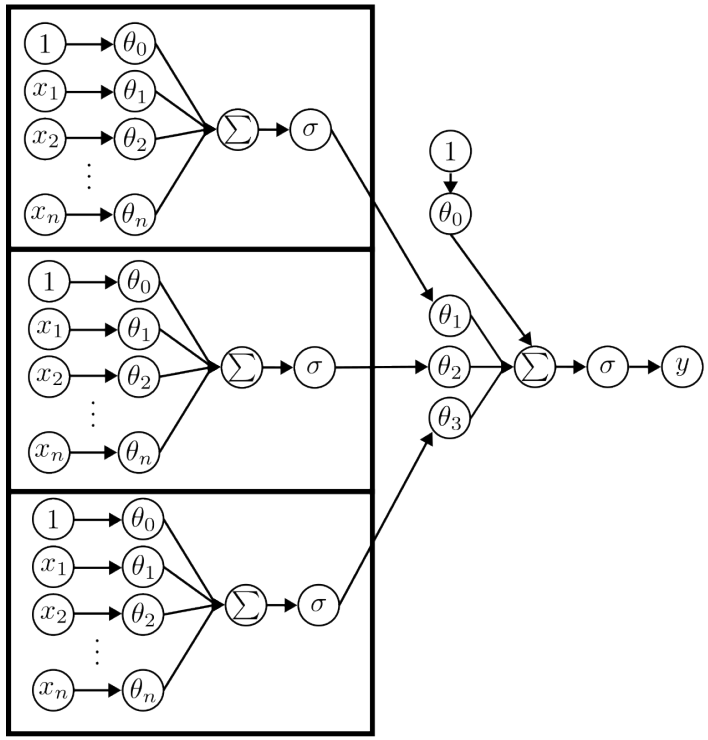
Computer: Artificial neurons $\rightarrow$ Artificial neural network

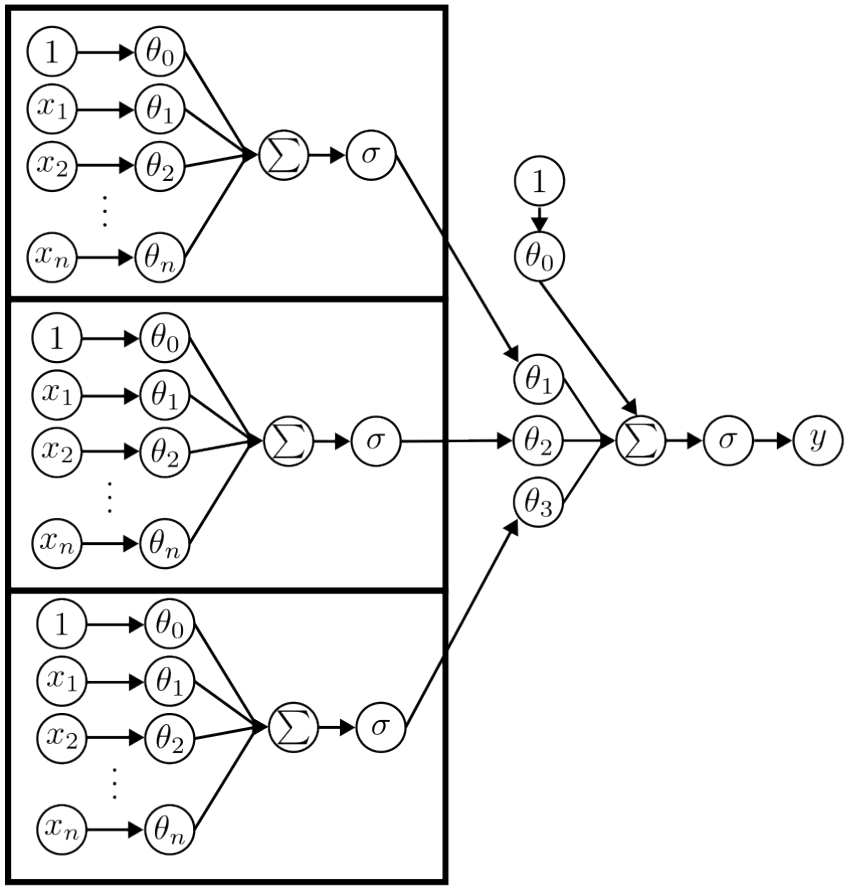
Connect artificial neurons into a network



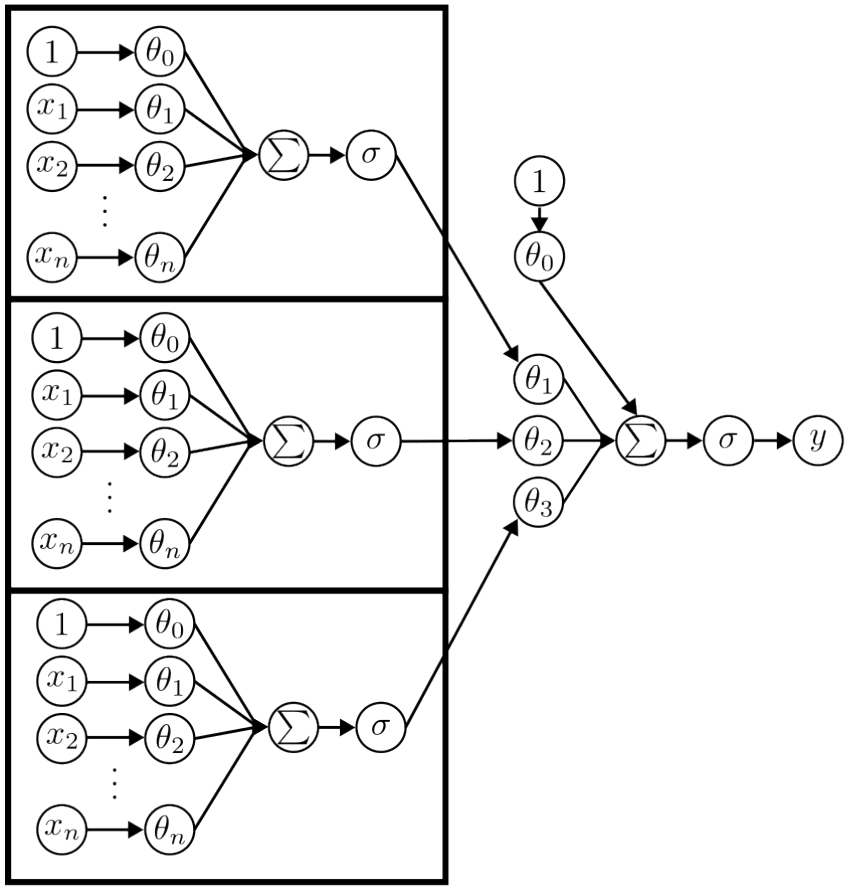
Neuron



Neural Network



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



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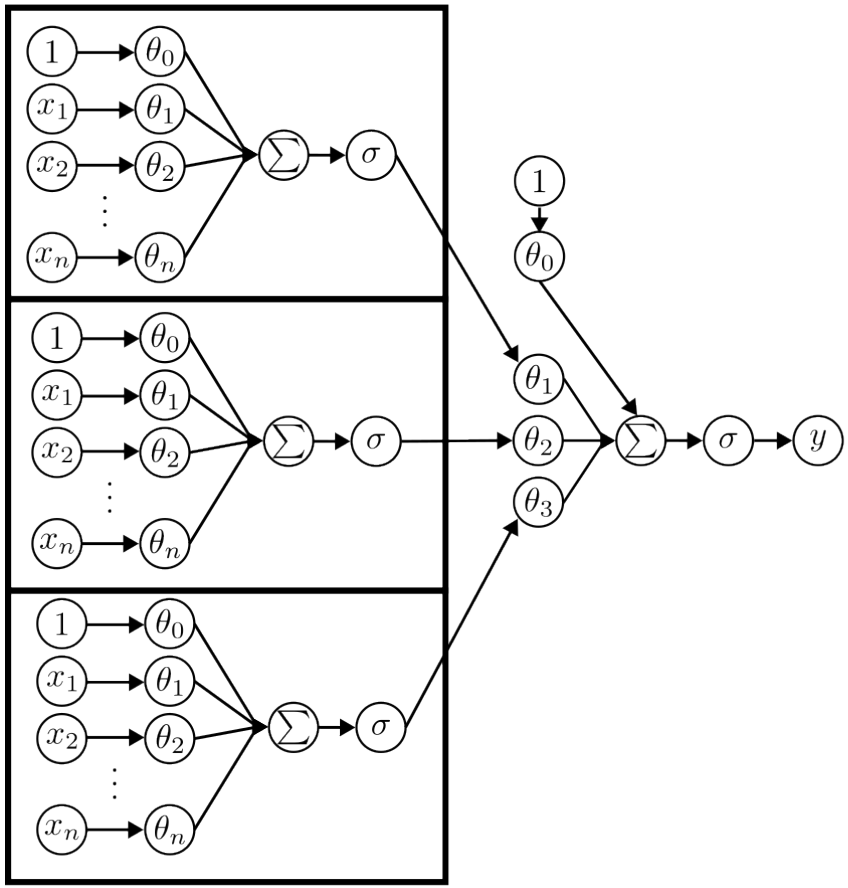

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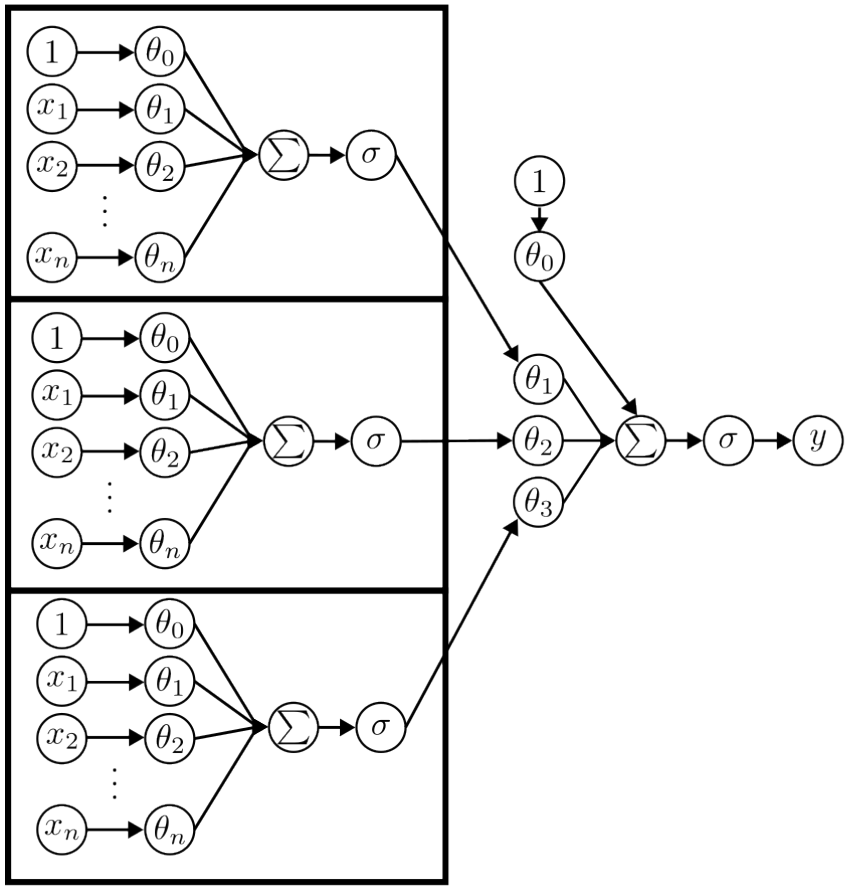

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Let us try to implement XOR using a wide and deep neural network

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

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d_y neurons (wide):

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

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

For a single neuron:

$$f\left(\begin{bmatrix} x_1 \\ \vdots \\ x_{d_x} \end{bmatrix}, \begin{bmatrix} \theta_0 \\ \theta_1 \\ \vdots \\ \theta_{d_x} \end{bmatrix}\right) = \sigma\left(\sum_{i=0}^{d_x} \theta_i \overline{x}_i\right)$$

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$$f(\boldsymbol{x}, \boldsymbol{\theta}) = \sigma(b + \boldsymbol{w}^\top \boldsymbol{x})$$

For a wide network:

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

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$$\boldsymbol{\theta} = [\boldsymbol{\theta}_1 \;\; \boldsymbol{\theta}_2 \;\; \ldots \;\; \boldsymbol{\theta}_\ell]^\top = [\boldsymbol{\varphi} \;\; \boldsymbol{\psi} \;\; \ldots \;\; \boldsymbol{\xi}]^\top$$

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

Written another way

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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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Proof Sketch: Approximate a continuous function $g : \mathbb{R} \mapsto \mathbb{R}$ using a linear combination of Heaviside functions

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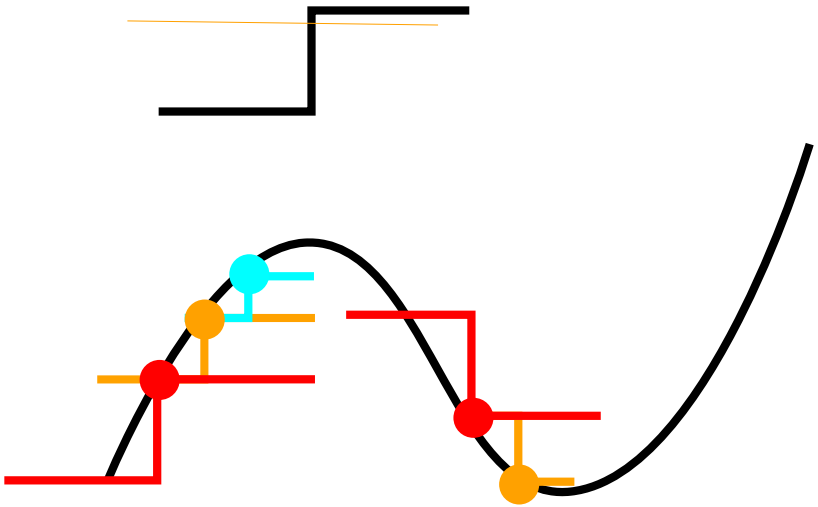

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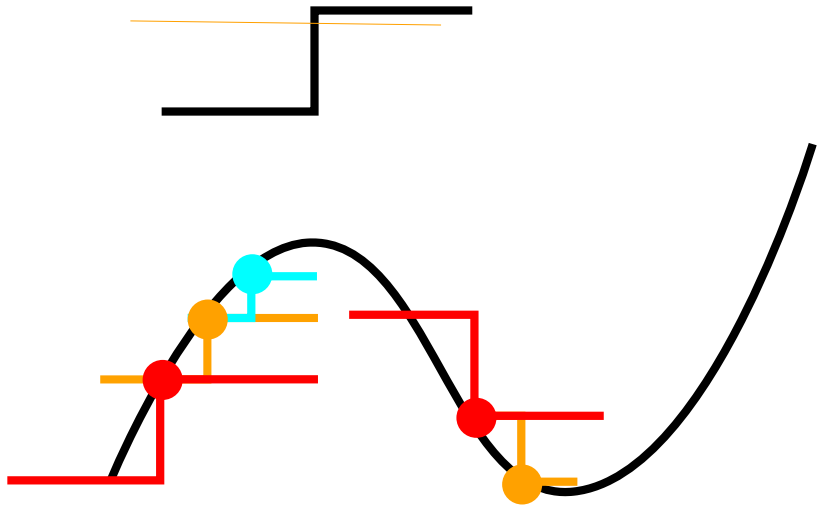

$$\exists\left(\boldsymbol{\theta} \in \mathbb{R}^{1\times d_h}, \boldsymbol{\varphi} \in \mathbb{R}^{(d_h+1)\times d_1}\right) \text{ such that } \lim_{(d_h+1)\mapsto\infty}\left[\boldsymbol{\varphi}^\top \sigma\left(\overline{\boldsymbol{\theta}^\top \overline{x}}\right)\right]$$

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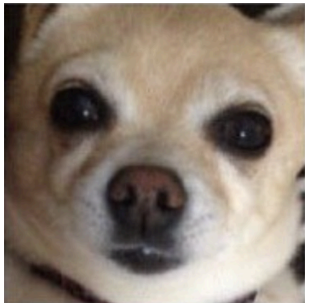
Task: predict how many ♥ a photo gets on social media



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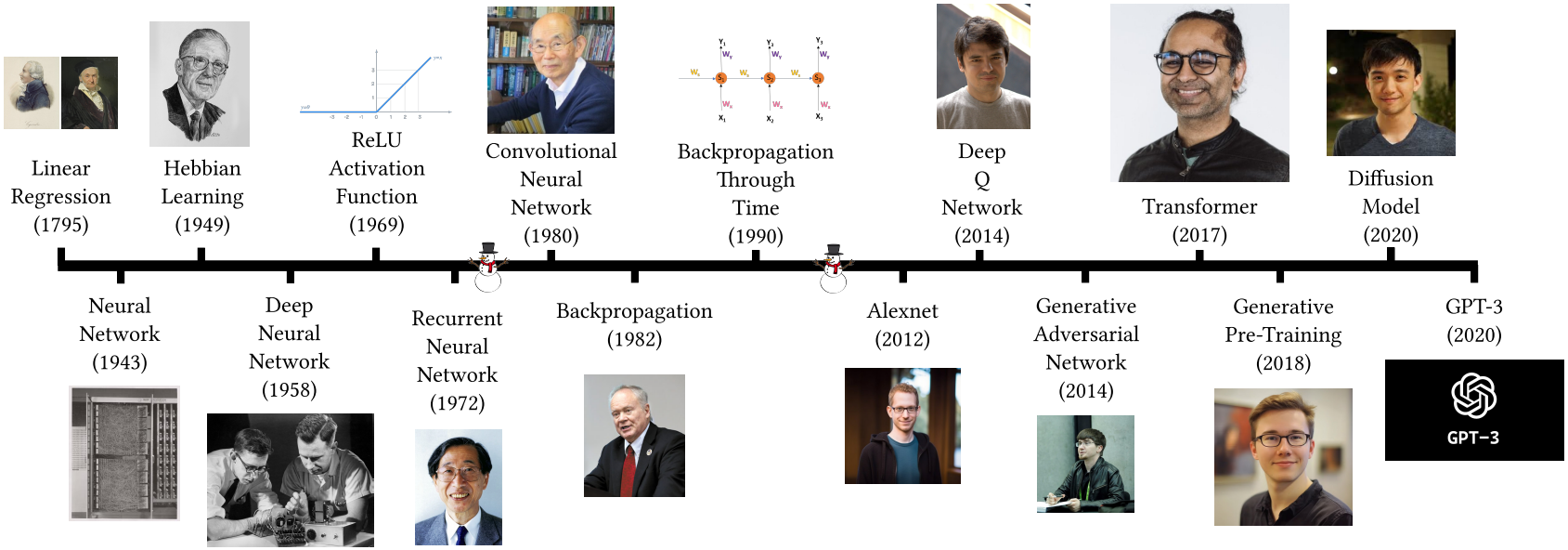

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I will explain them again very simply

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

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

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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