Neural Networks

CISC 7026: Introduction to Deep Learning

University of Macau

1. Review
2. Multivariate linear regression
3. Limitations of linear regression
4. History of neural networks
5. Biological neurons
6. Artificial neurons
7. Perceptron
8. Multilayer Perceptron

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- 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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Goal: Given someone's education, predict how long they will live

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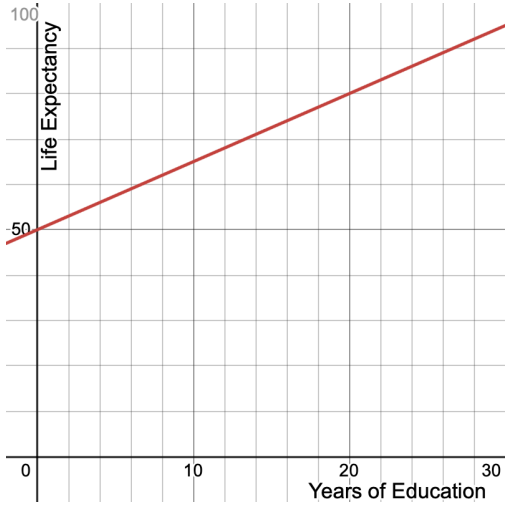
$$f(x, \boldsymbol{\theta}) = f\left(x, \begin{bmatrix} \theta_1 \\ \theta_0 \end{bmatrix}\right) = \theta_1 x + \theta_0$$



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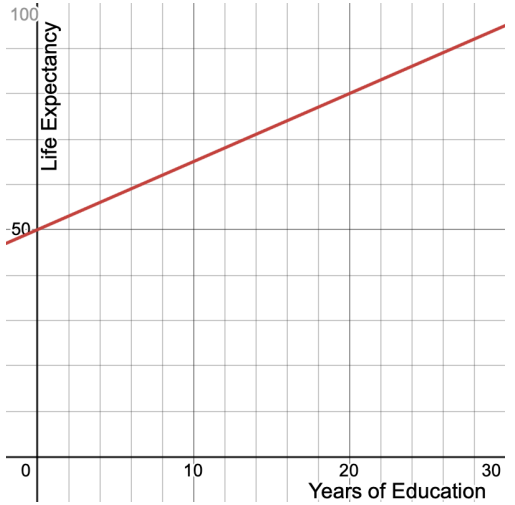

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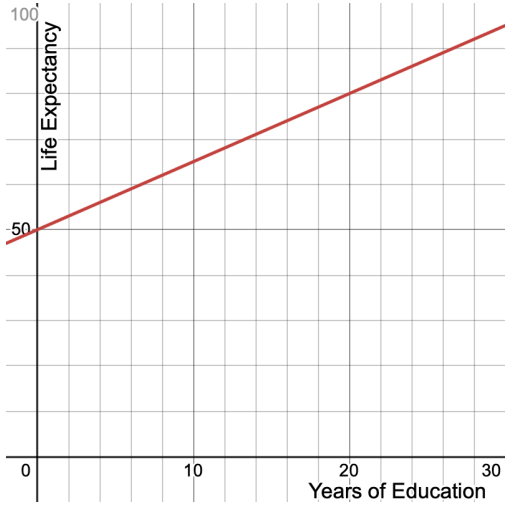

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$$\text{error}(f(x, \boldsymbol{\theta}), y) = (f(x, \boldsymbol{\theta}) - y)^2$$

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We wrote the loss function for a single datapoint x_i, y_i using the square error

$$\mathcal{L}(x_i, y_i, \boldsymbol{\theta}) = \text{error}(f(x_i, \boldsymbol{\theta}), y_i) = (f(x_i, \boldsymbol{\theta}) - y_i)^2$$

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$$\mathcal{L}(\boldsymbol{x}, \boldsymbol{y}, \boldsymbol{\theta}) = \sum_{i=1}^{n} \text{error}(f(x_i, \boldsymbol{\theta}), y_i) = \sum_{i=1}^{n} (f(x_i, \boldsymbol{\theta}) - y_i)^2$$

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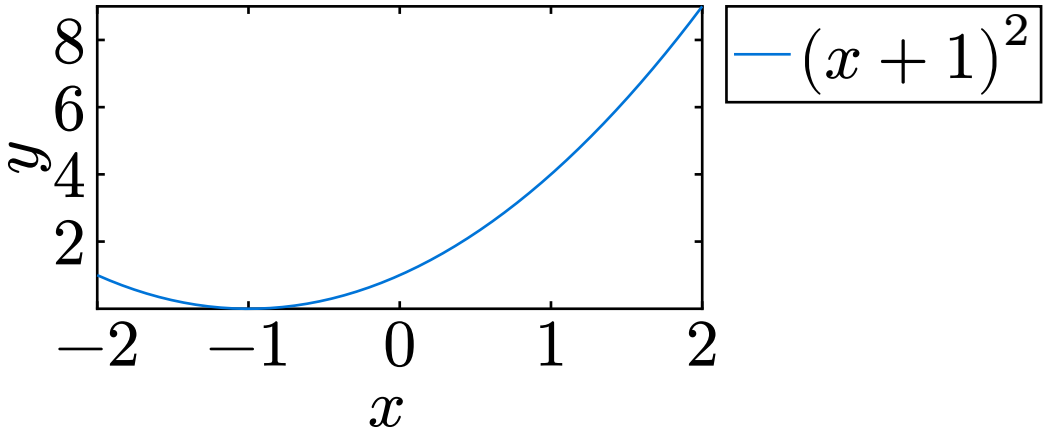

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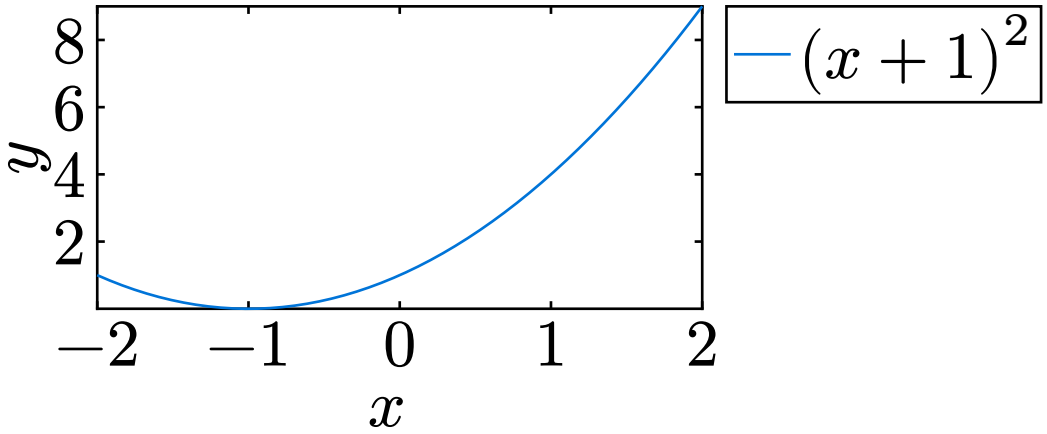

$$\arg\min_x f(x) = -1$$

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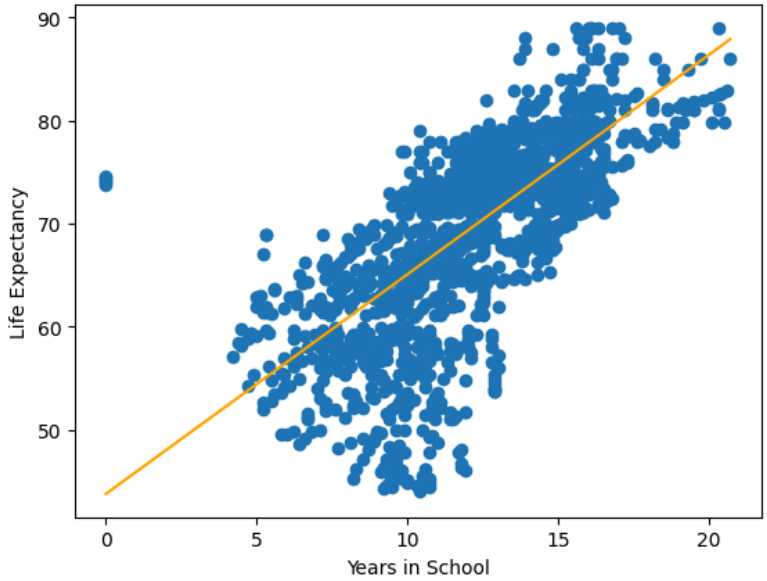

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$$\boldsymbol{X}_D = \begin{bmatrix} x_1 & 1 \\ x_2 & 1 \\ \vdots & \vdots \\ x_n & 1 \end{bmatrix} \Rightarrow \boldsymbol{X}_D = \begin{bmatrix} \log(1+x_1) & 1 \\ \log(1+x_2) & 1 \\ \vdots & \vdots \\ \log(1+x_n) & 1 \end{bmatrix}$$

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

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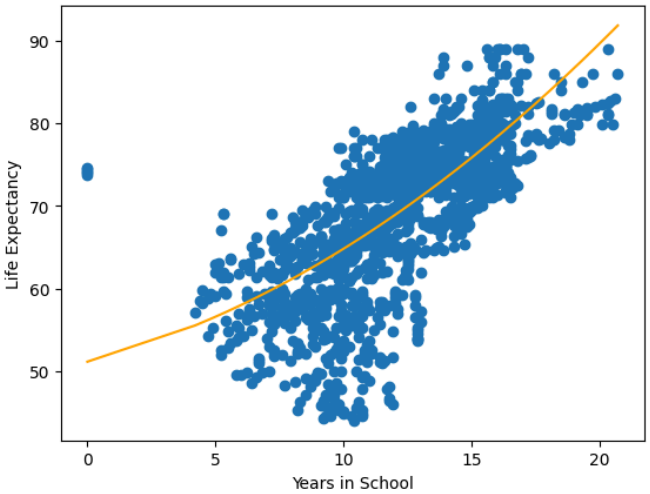
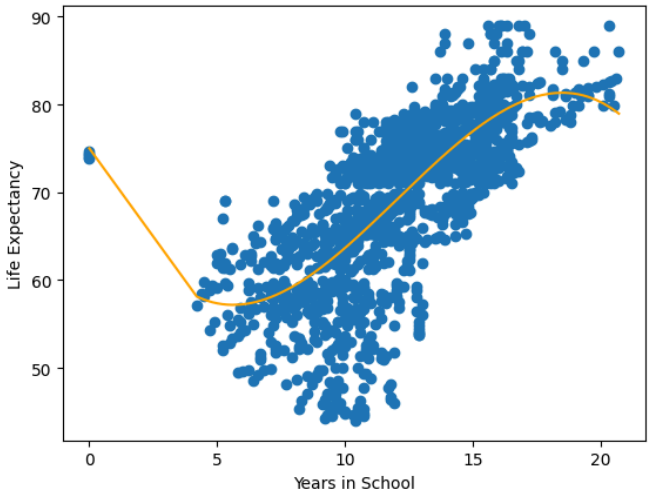
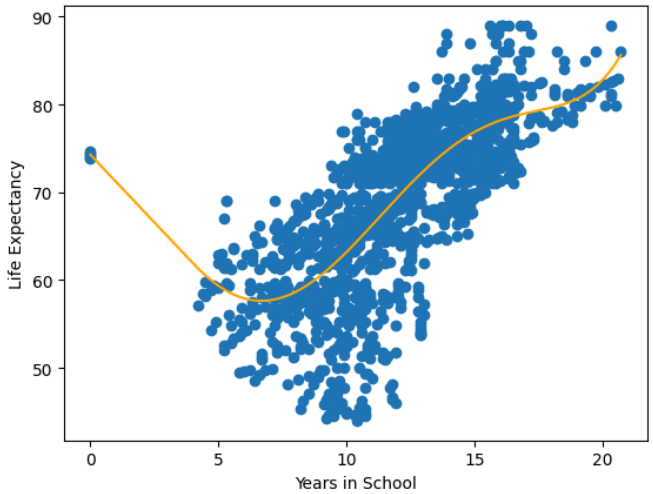


$m = 2$



$m = 3$



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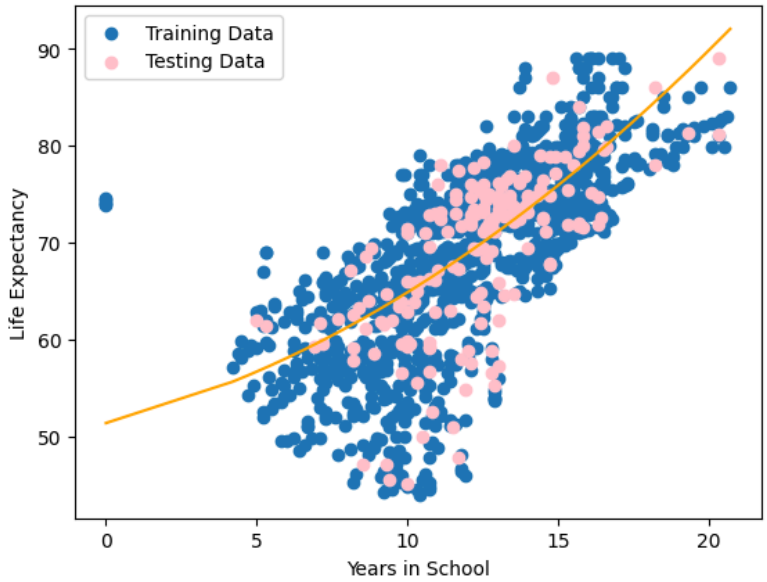

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We can solve these problems using linear regression too

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Issues with very complex problems

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

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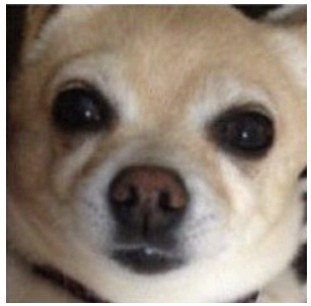

$$X \in \mathbb{Z}_{+}^{256 \times 256}$$

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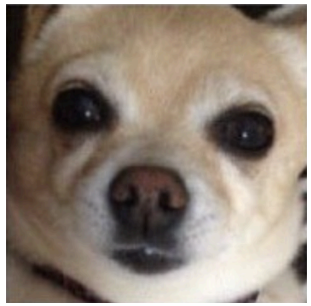

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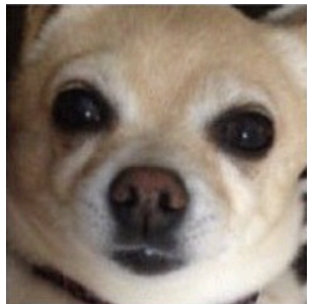
This image contains 65536 pixels, so x has 65536 dimensions



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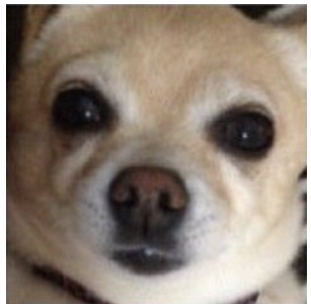

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What does the design matrix look like for an m-degree polynomial of this image?

$$\boldsymbol{X}_D = \begin{bmatrix} x_1^m & x_1^{m-1} & \dots & x_1^1 & 1 \\ x_2^m & x_2^{m-1} & \dots & x_2^1 & 1 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ x_n^m & x_n^{m-1} & \dots & x_n^1 & 1 \\ x_1^{n-1}x_2 & x^{n-2}x_2^2 & \dots & 0 & 1 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ x_1x_2\dots x_n & 0 & \dots & 0 & 1 \end{bmatrix}$$

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Question: How big is the matrix for 65,536 pixels and $m = 3$?

Answer: $65,536^3 \approx 10^{14}$ parameters

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Polynomial regression scales poorly to high dimensional data

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1. **Poor scalability**
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$$\theta_m \lim_{x\to\infty} x^m$$ Rewrite

$$\theta_m \lim_{x\to\infty} x^m = \infty$$ If $\theta_m > 0$

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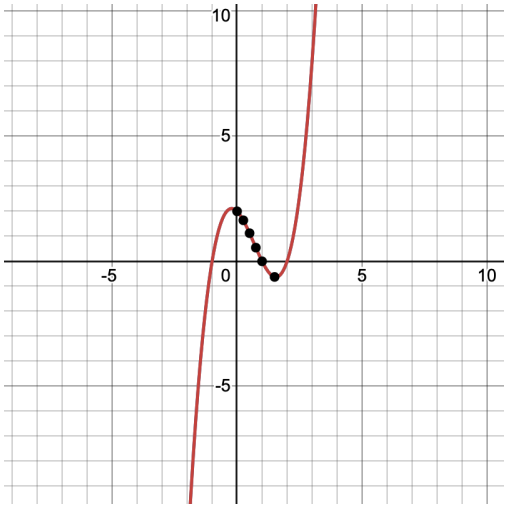

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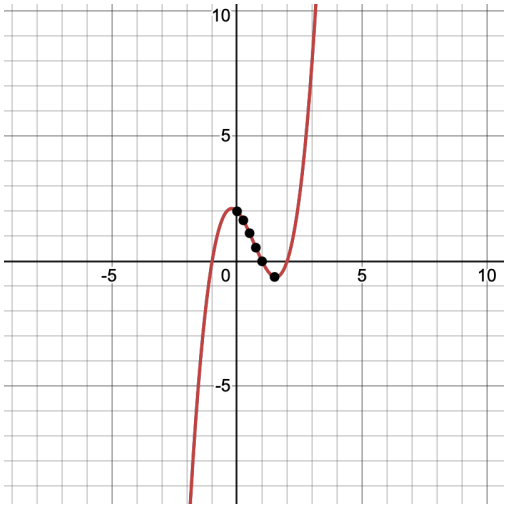

Remember, to predict new data we want our functions to generalize

Linear regression has issues

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Can we improve upon linear regression?

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Yes, with neural networks

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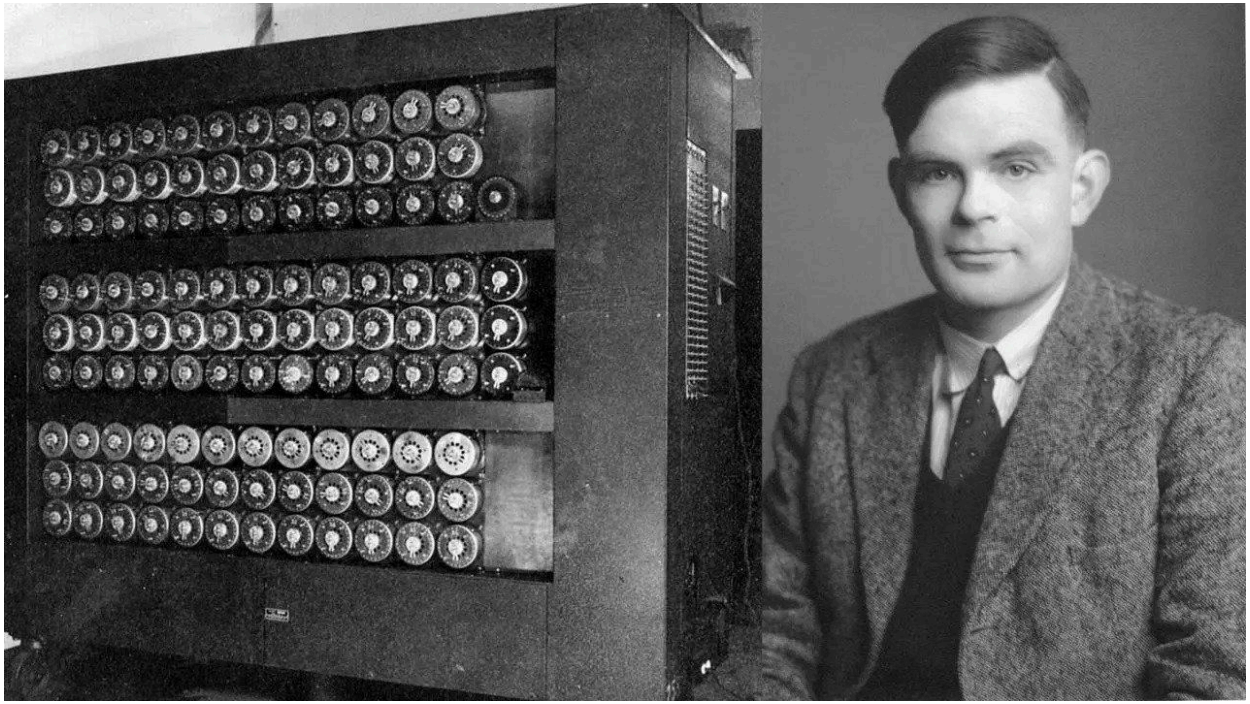
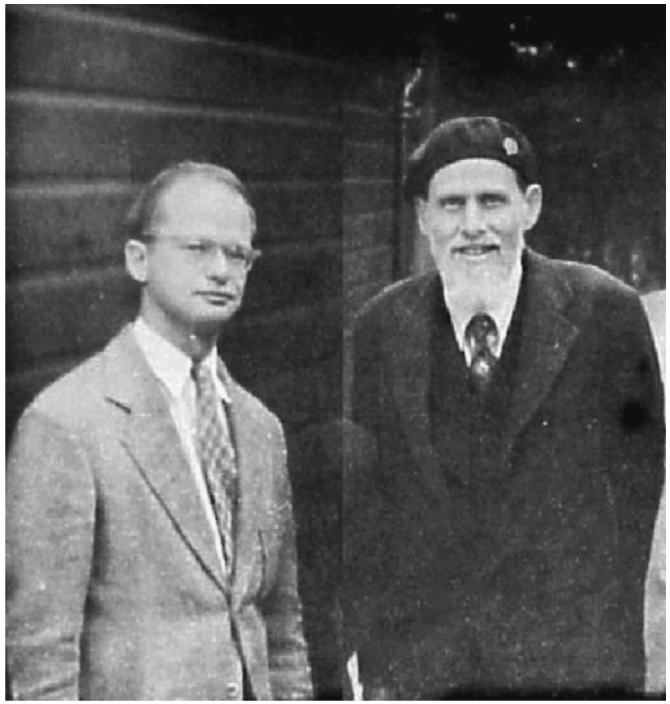


Meanwhile, a neuroscientist and mathematician (McCullough and Pitts) were trying to understand the human brain



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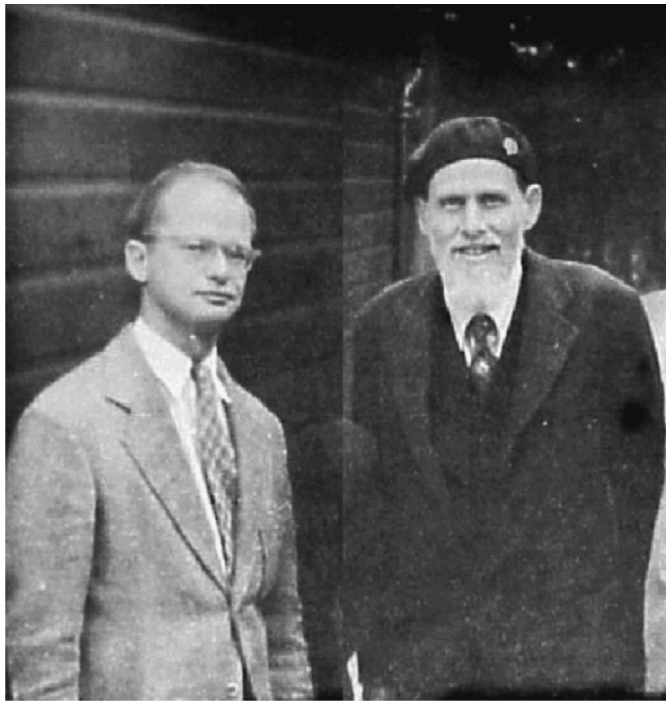
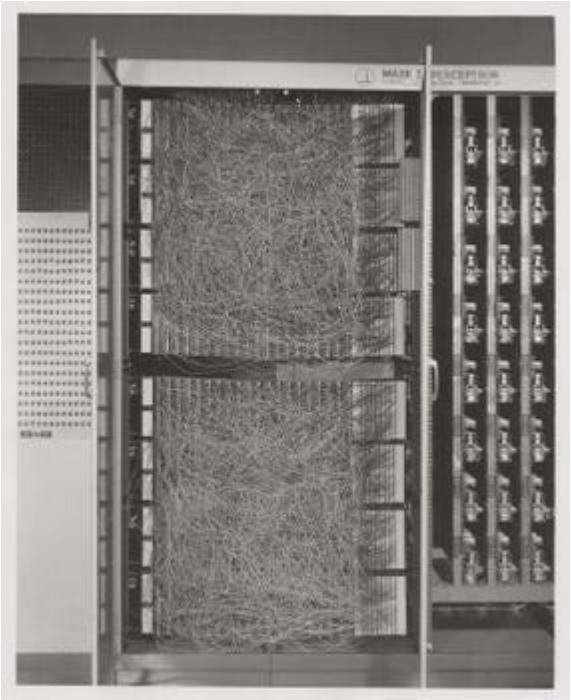


They designed the theory for the first neural network

A few years later, Rosenblatt implemented this neural network using a new invention – the computer



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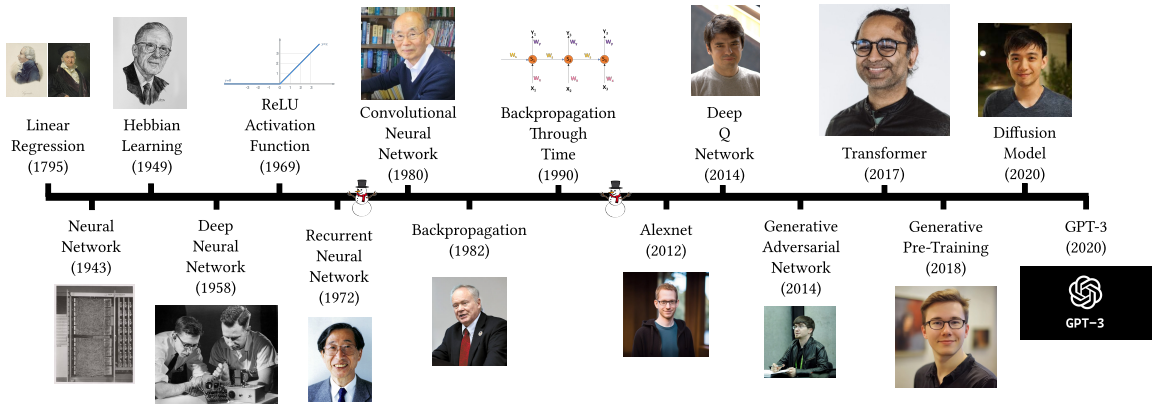

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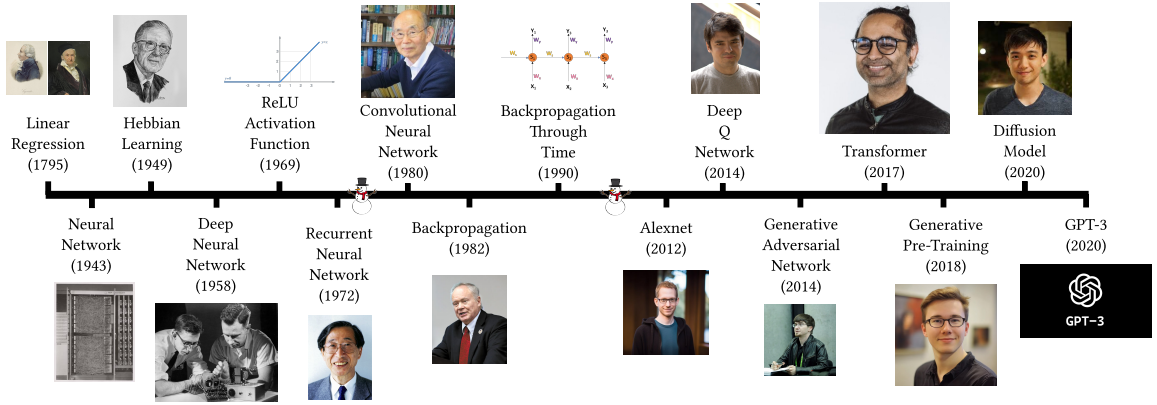

Around 2012, these improvements culminated in neural networks that perform like humans

So what is a neural network?

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It is a function, inspired by how the brain works

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

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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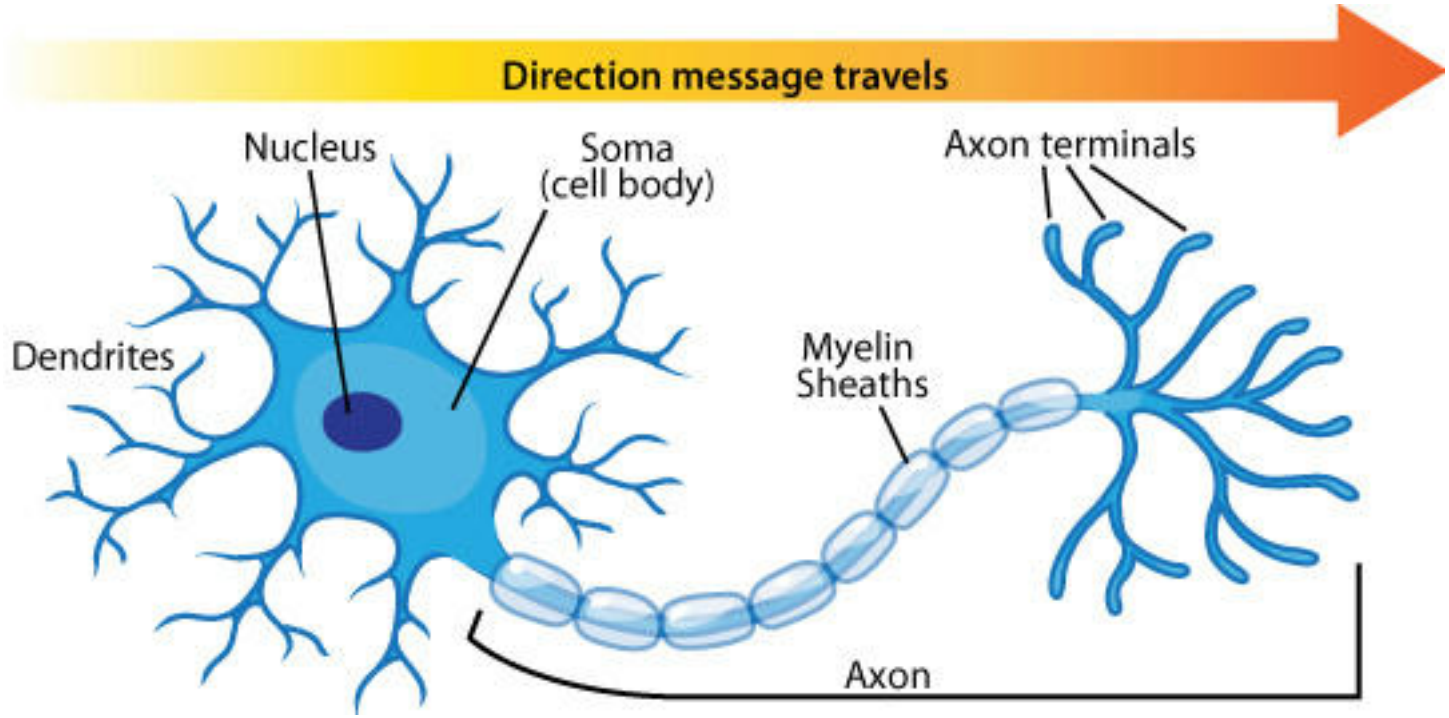
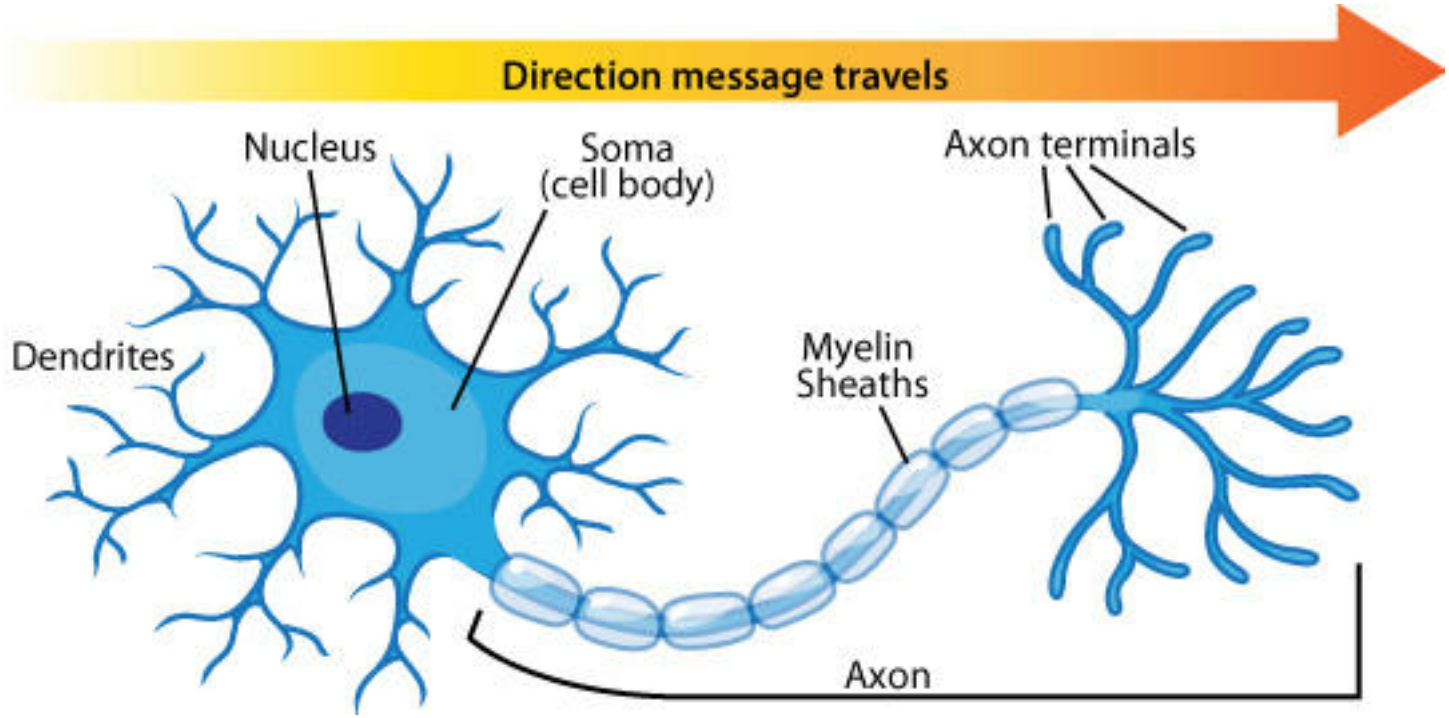
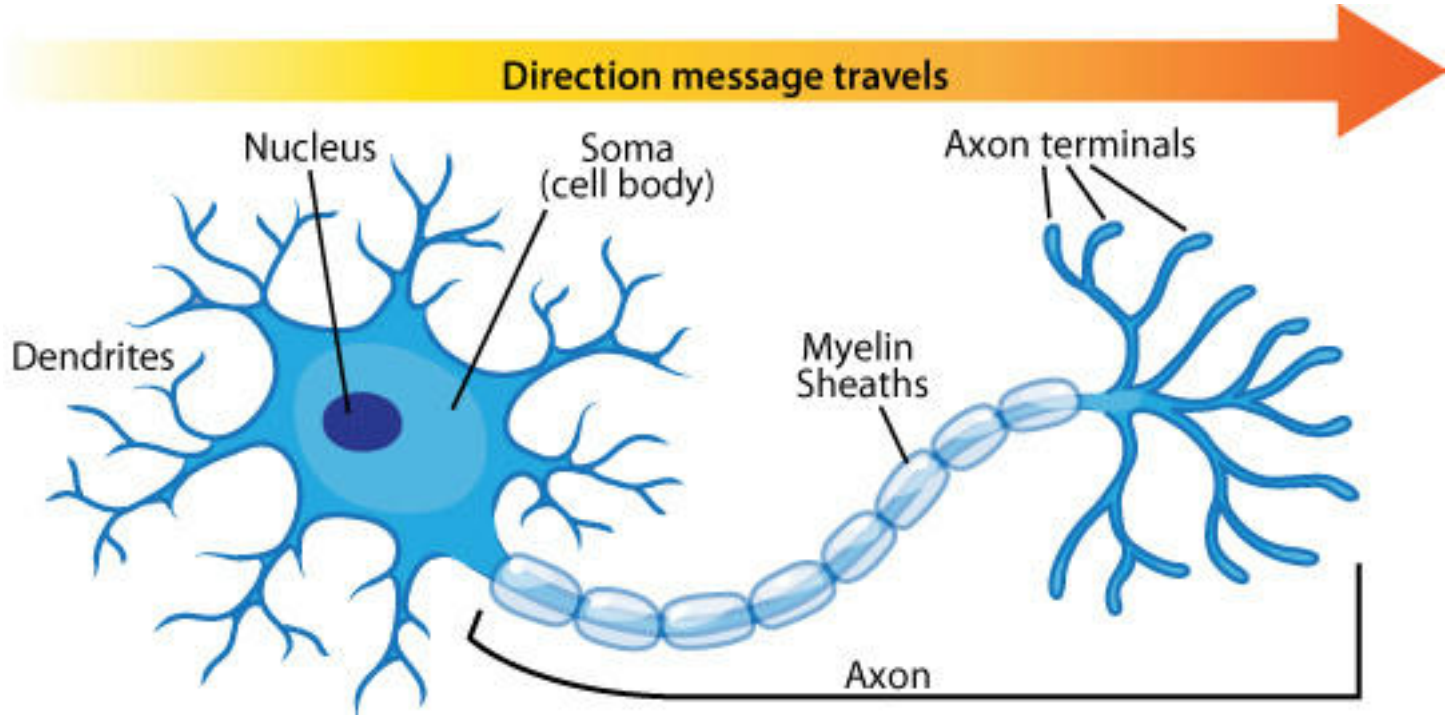


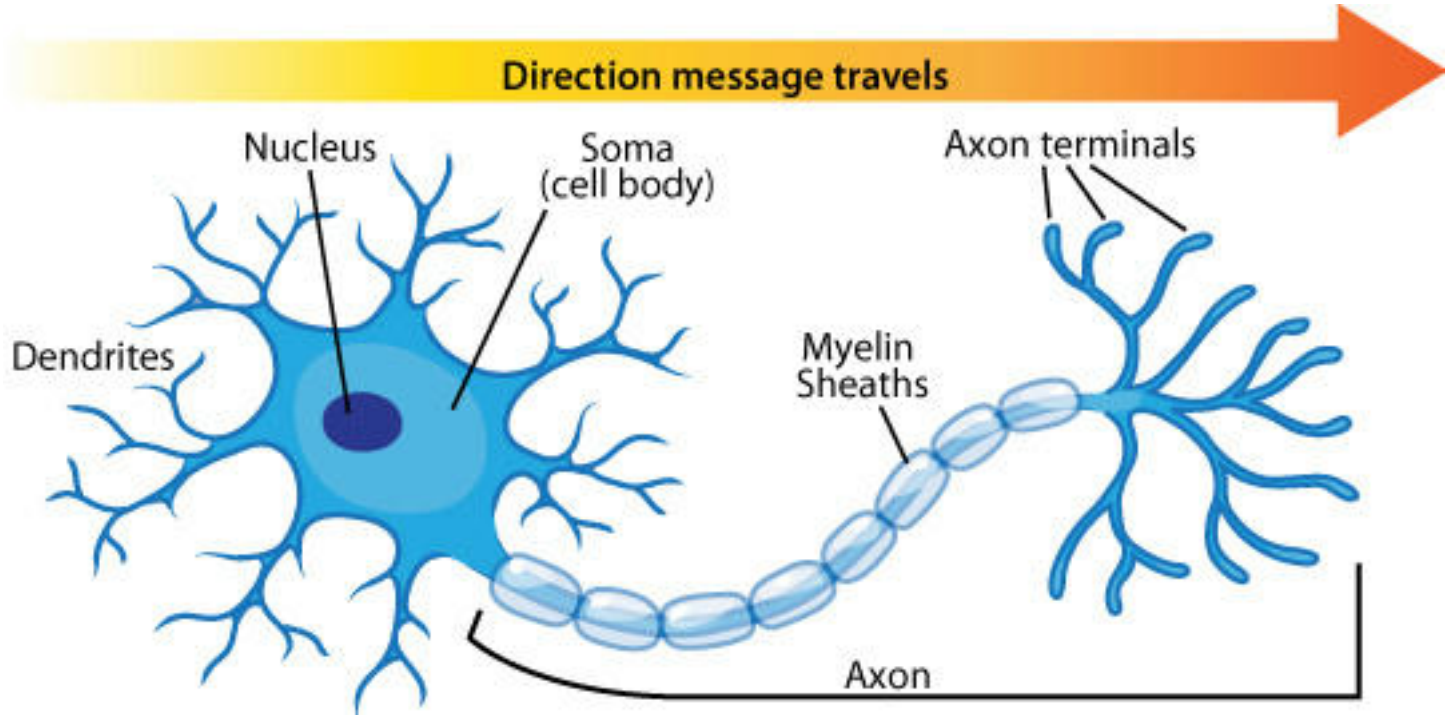
A simplified neuron consists of many parts



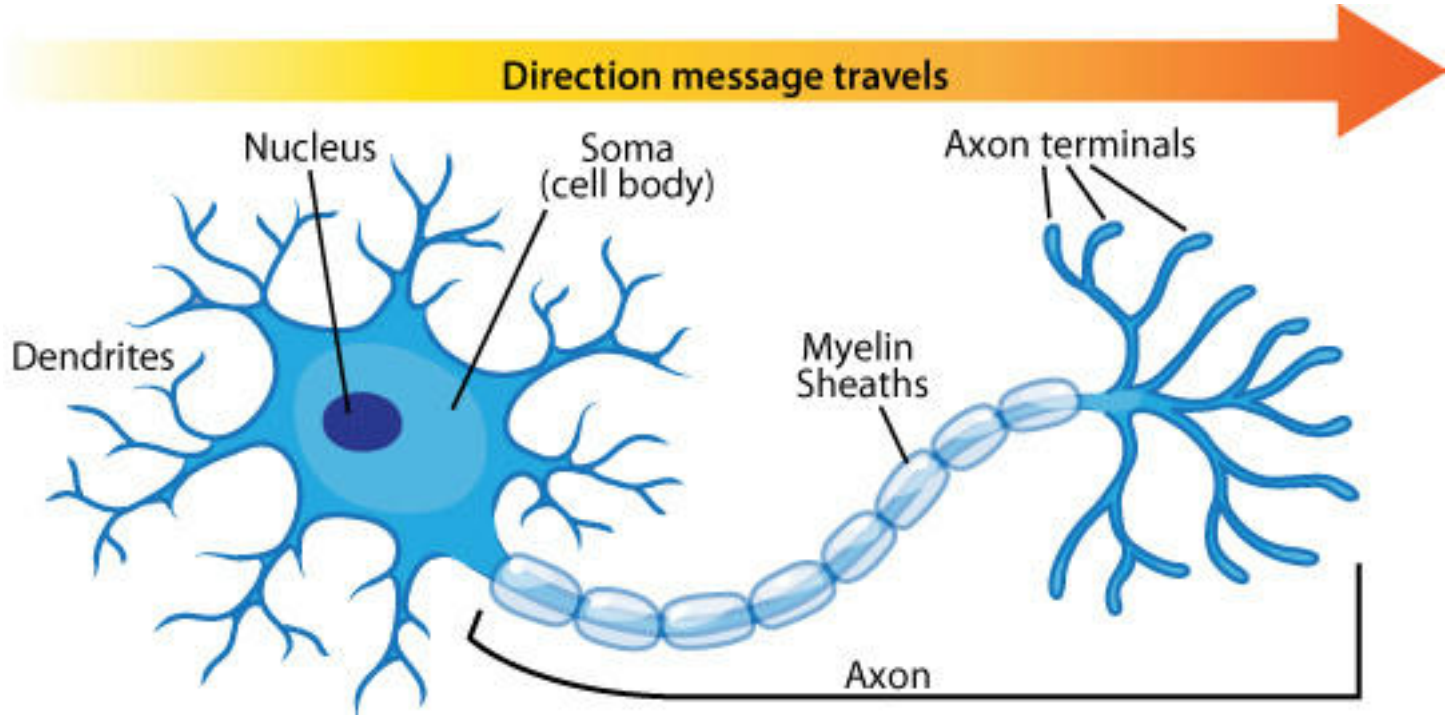
Neurons send and process messages from other neurons



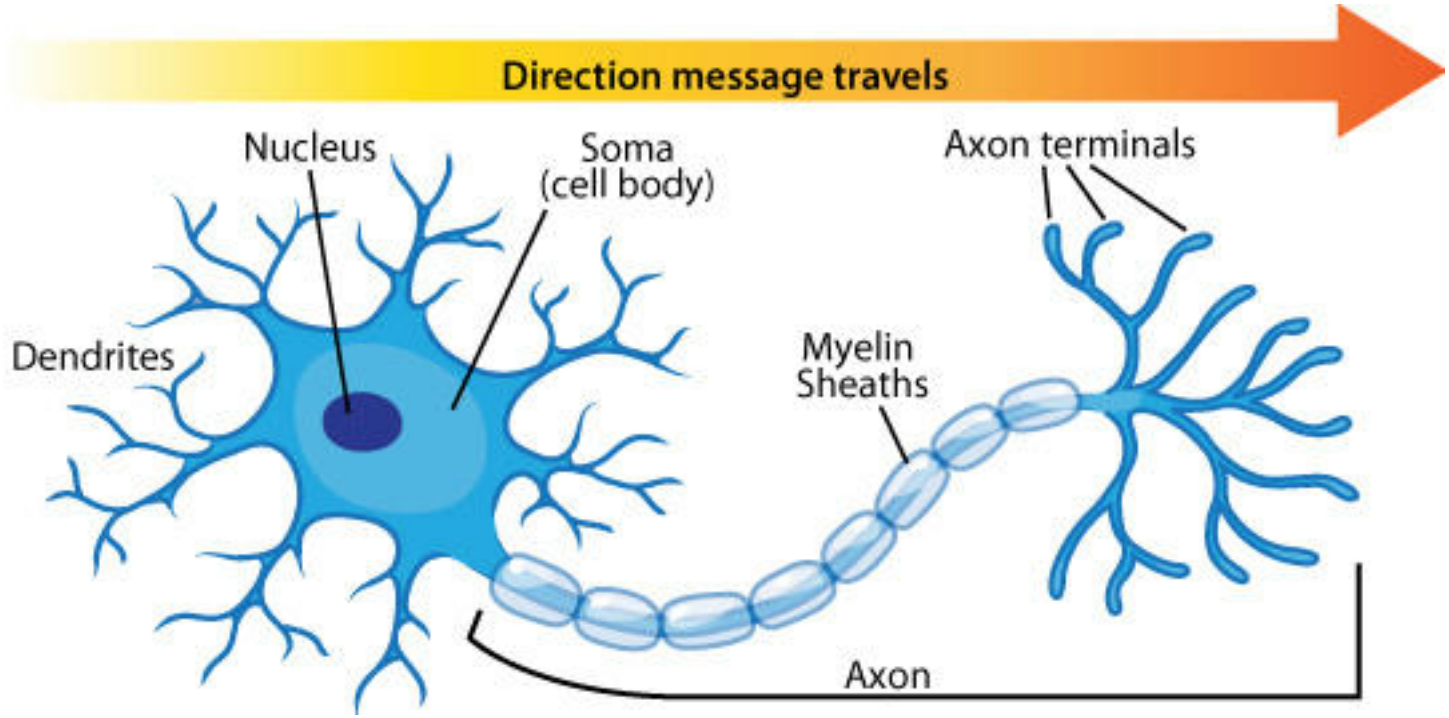
Incoming electrical signals travel along dendrites



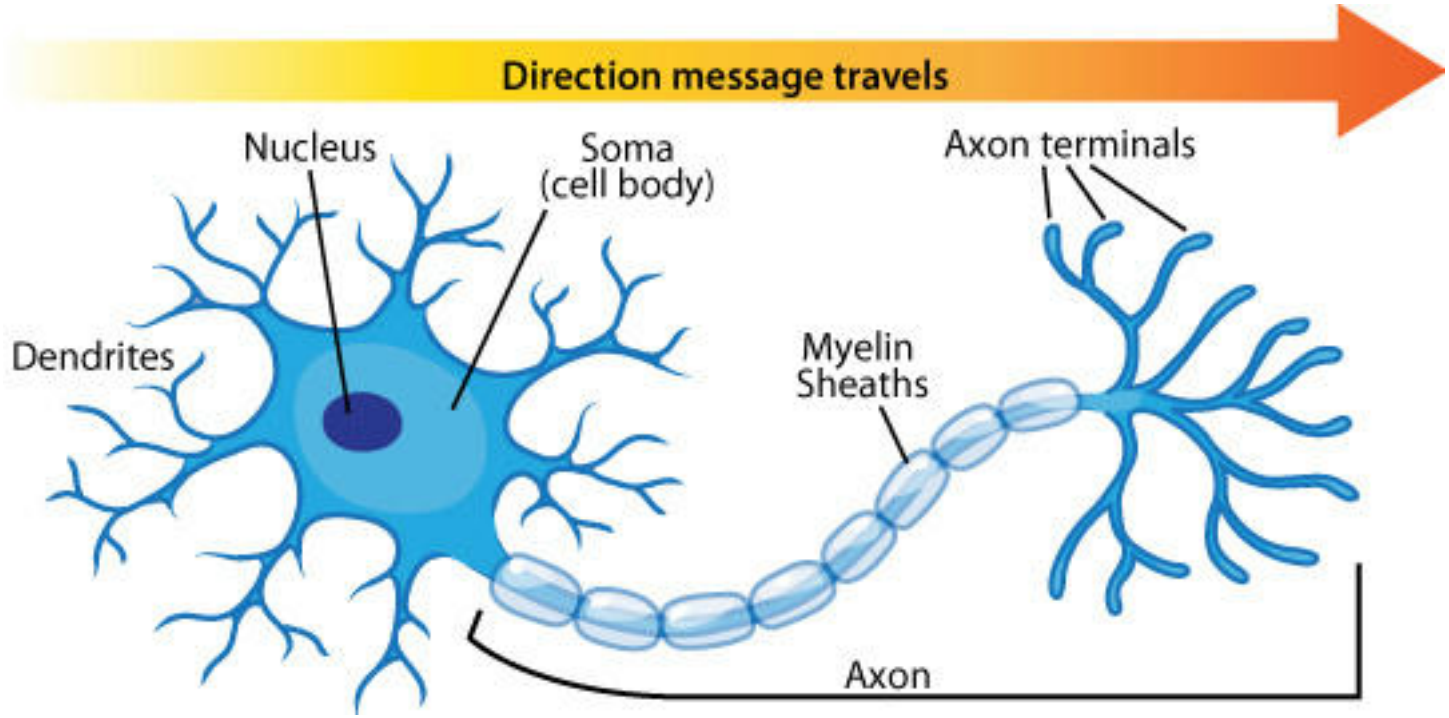
Dendrites are not all equal! Different dendrites have different diameters and structures



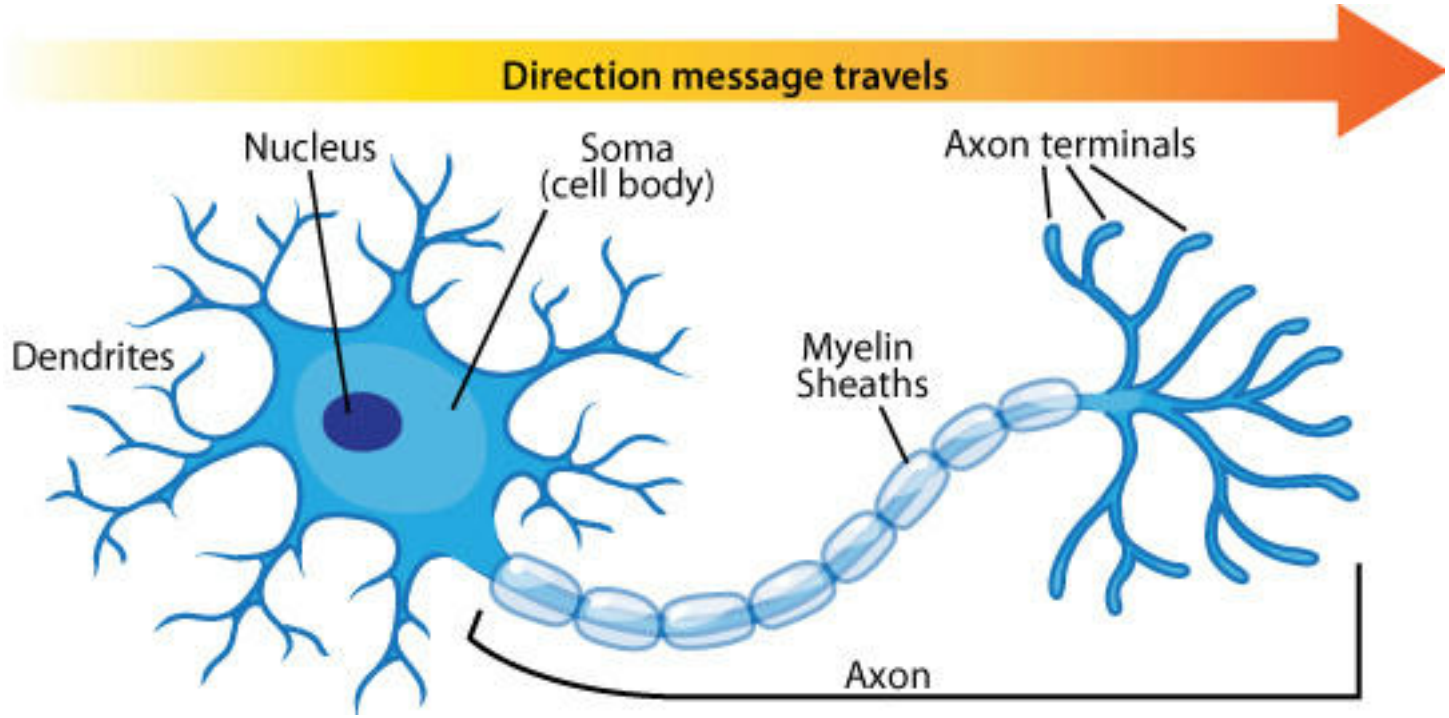
The axon outputs an electrical signal to other neurons



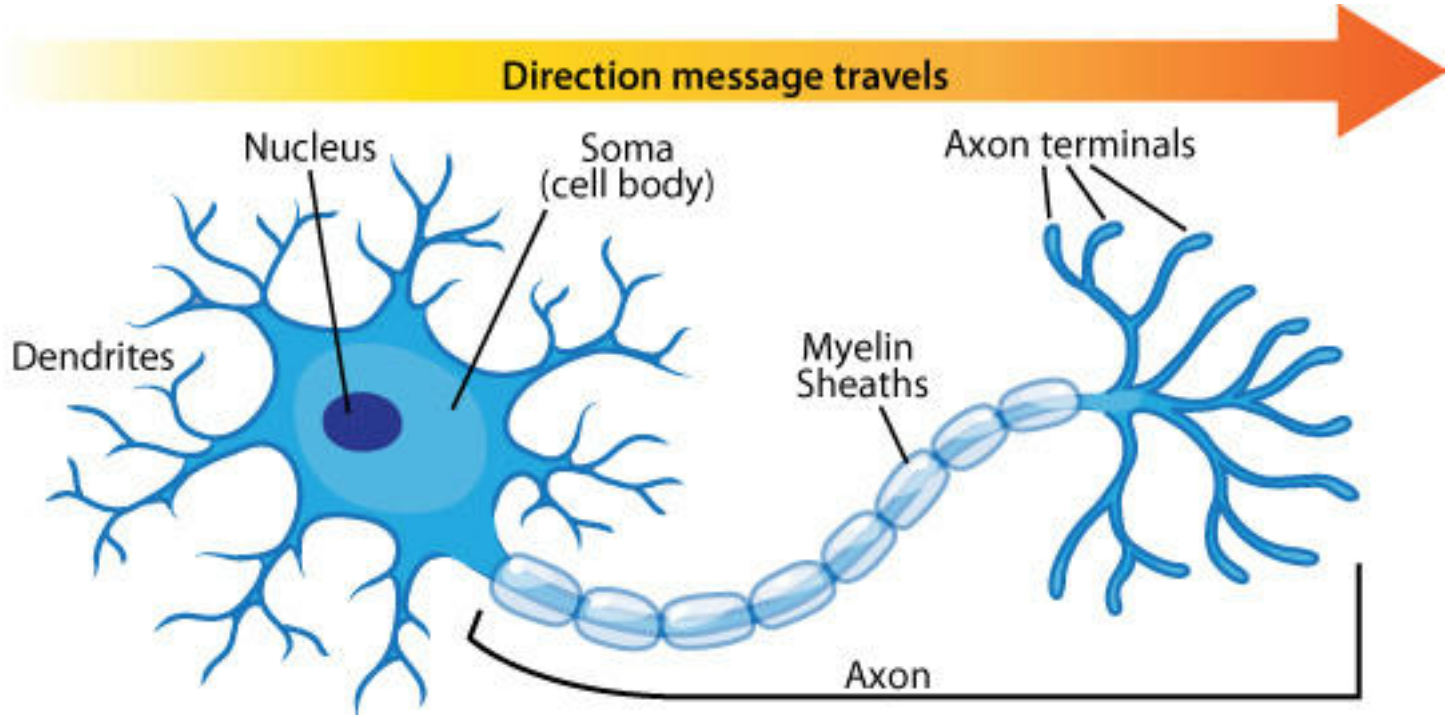
The axon terminals will connect to dendrites of other neurons



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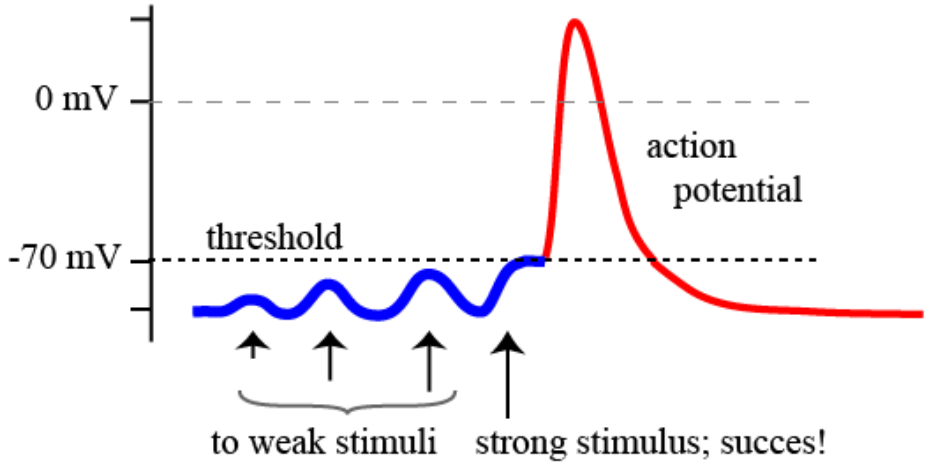
Incoming impulses (via dendrites) change the electric potential of the neuron



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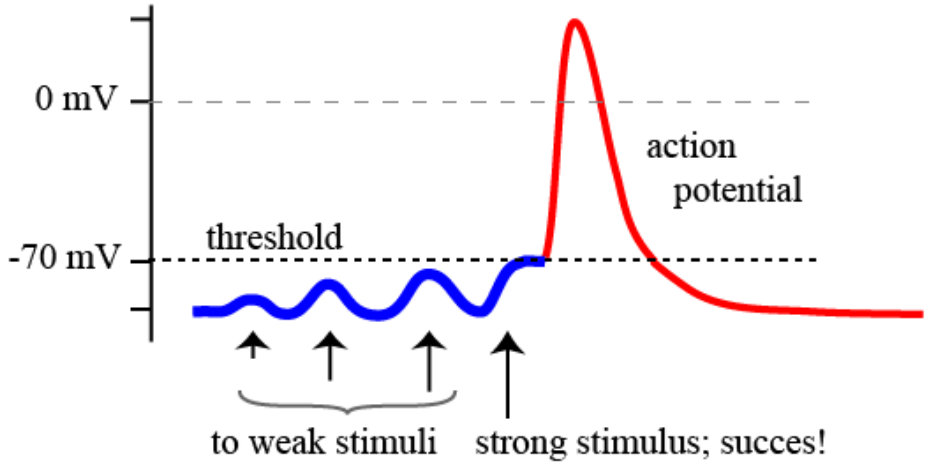

Recall that in a parallel circuit, we can sum voltages together

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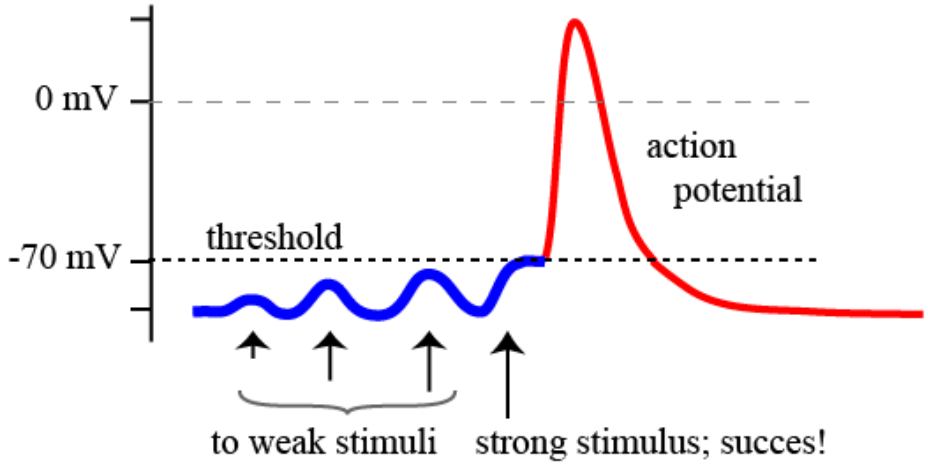
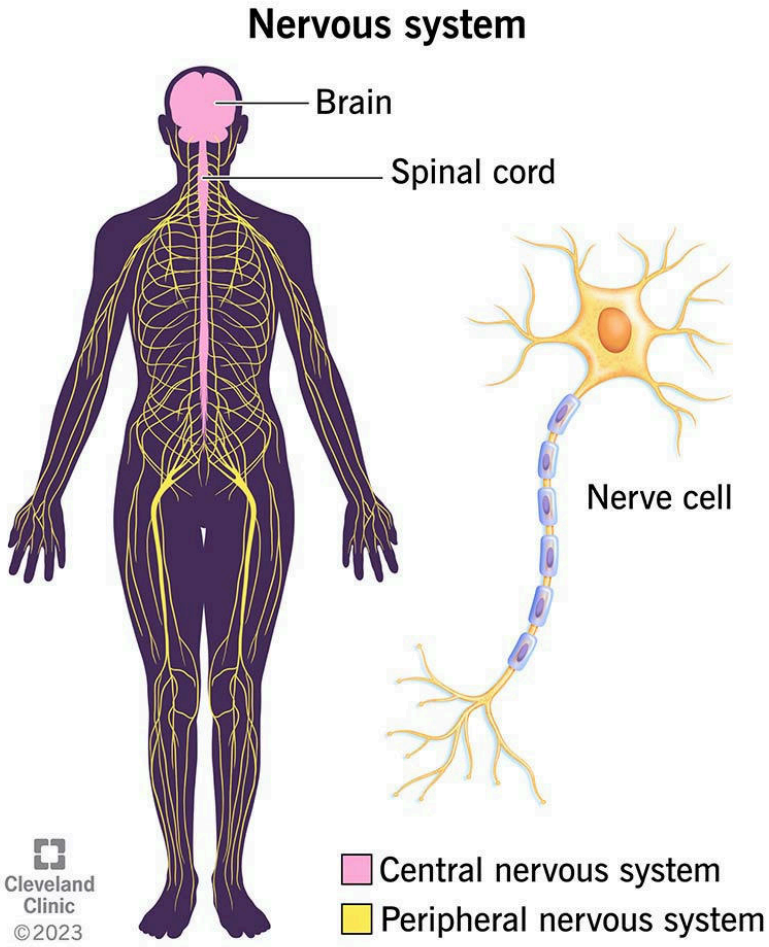


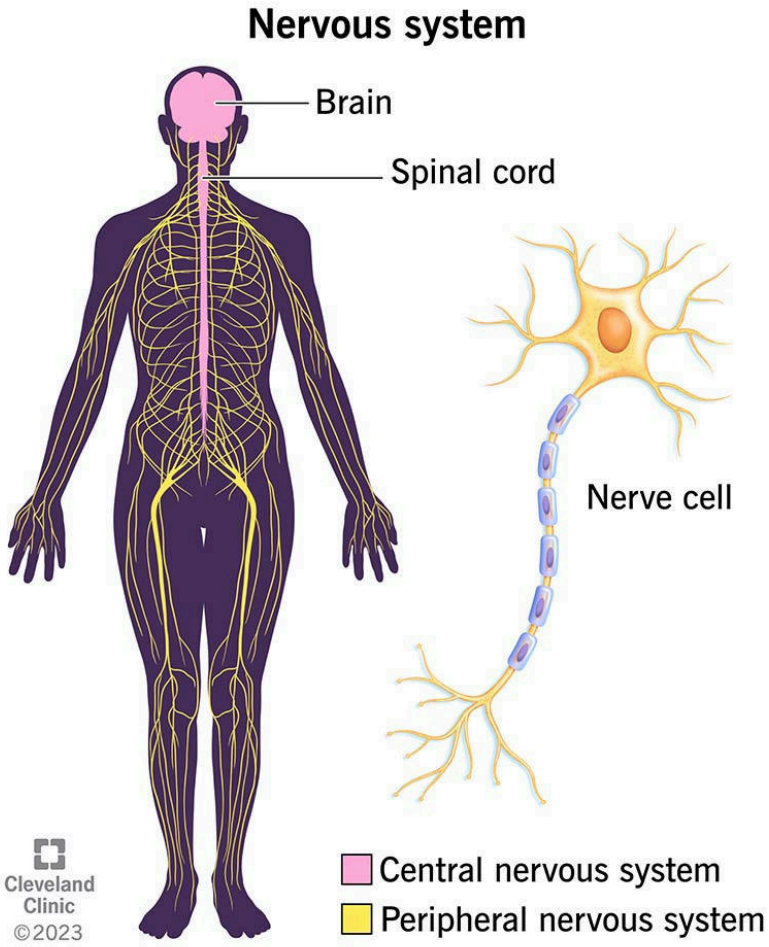
Recall that in a parallel circuit, we can sum voltages together

Many active dendrites will add together and trigger an impulse

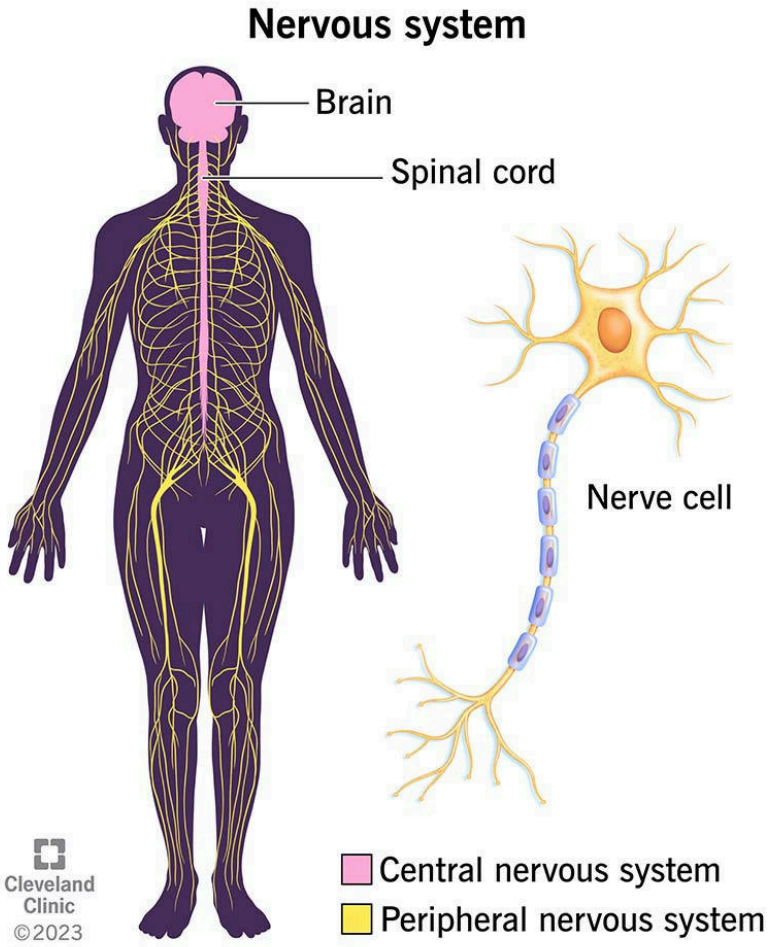
Pain triggers initial nerve impulse, starts a chain reaction into the brain



When the signal reaches the brain, we will think



After thinking, we will take action



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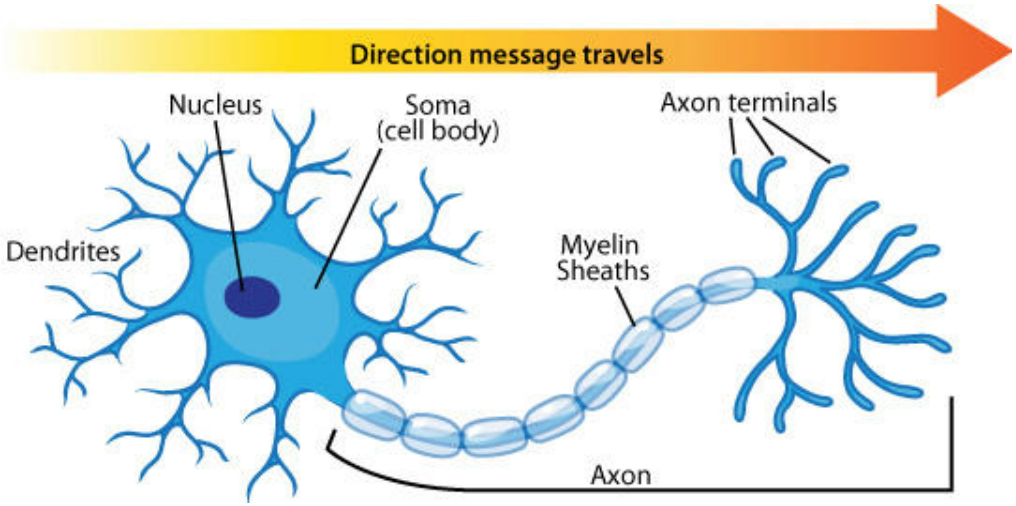
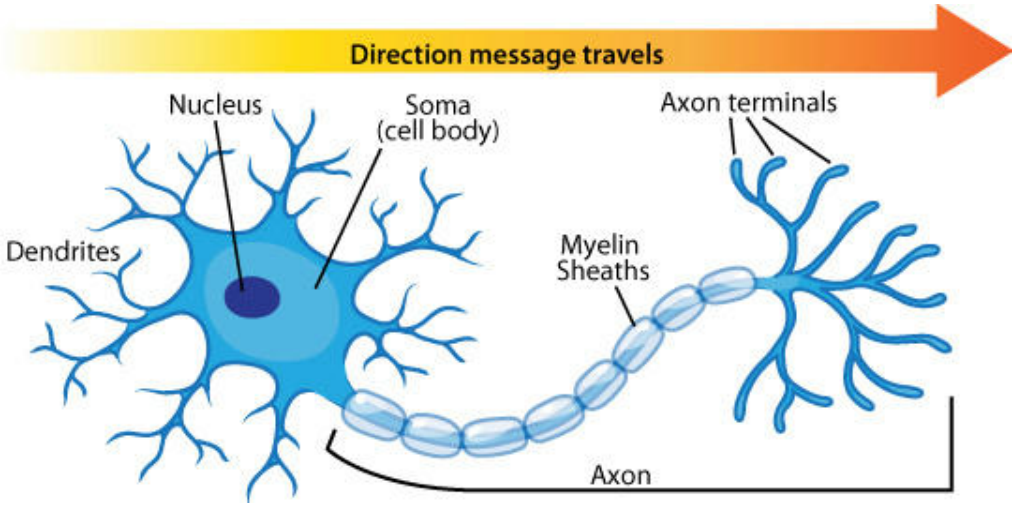
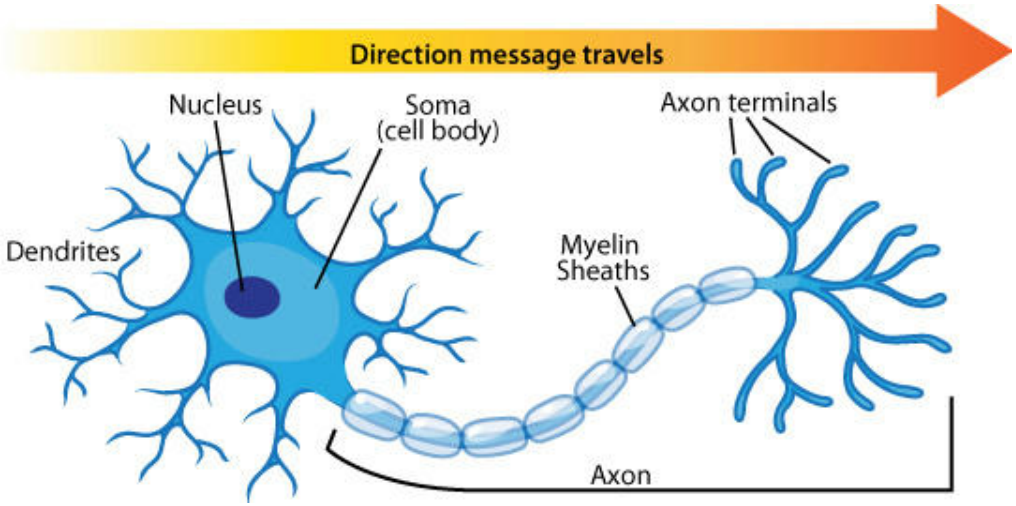

Direction message travels
Nucleus
Soma
(cell body)
Axon terminals
Dendrites
Myelin
Sheaths
Axon



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



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Answer:

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

Let us implement an artifical neuron as a function

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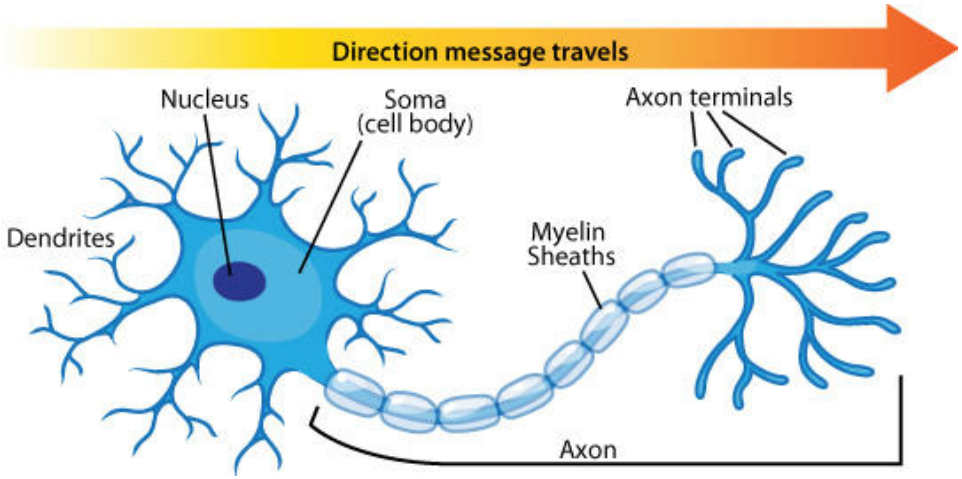

Neuron has a structure of dendrites

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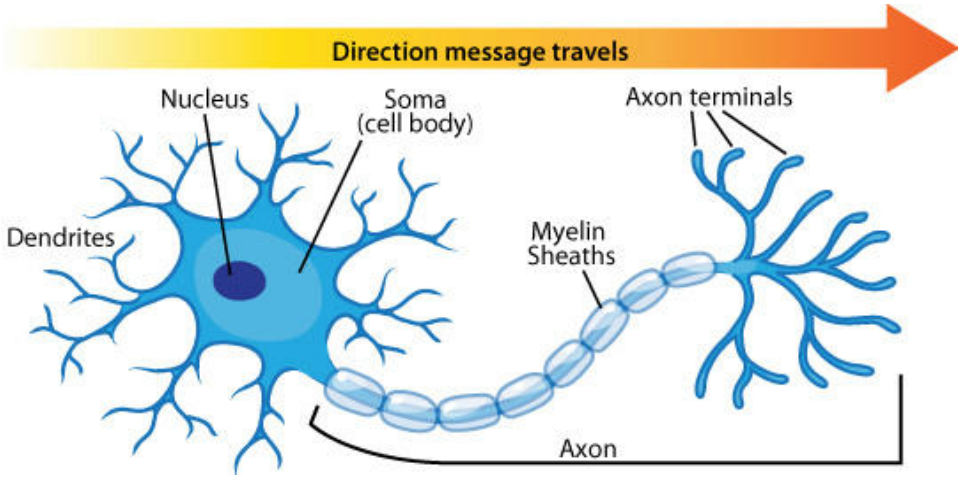

Neuron has a structure of dendrites

$$f\left(\begin{bmatrix}\theta_1\\ \theta_2\\ \vdots\\ \theta_n\end{bmatrix}\right) = f\left(\begin{bmatrix}0.5\\ 3.1\\ \vdots\\ 2.0\end{bmatrix}\right)$$

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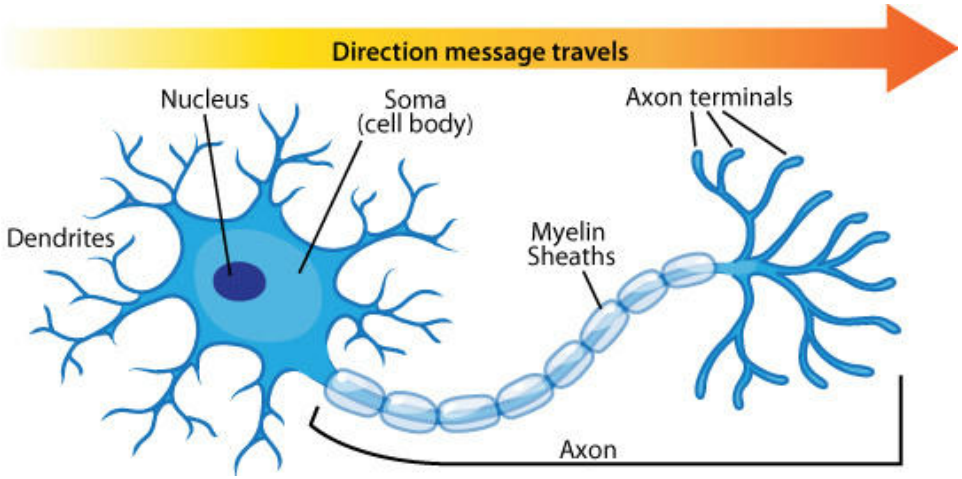

Each incoming dendrite has some voltage potential

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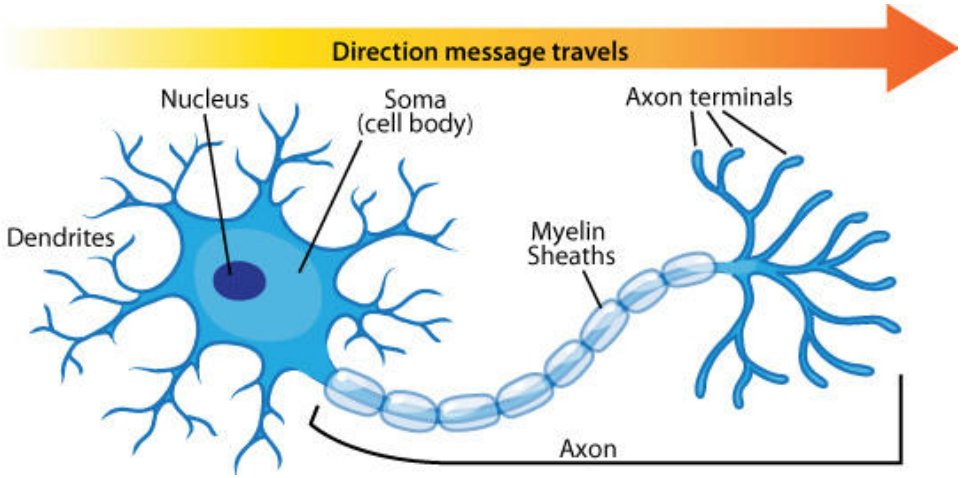
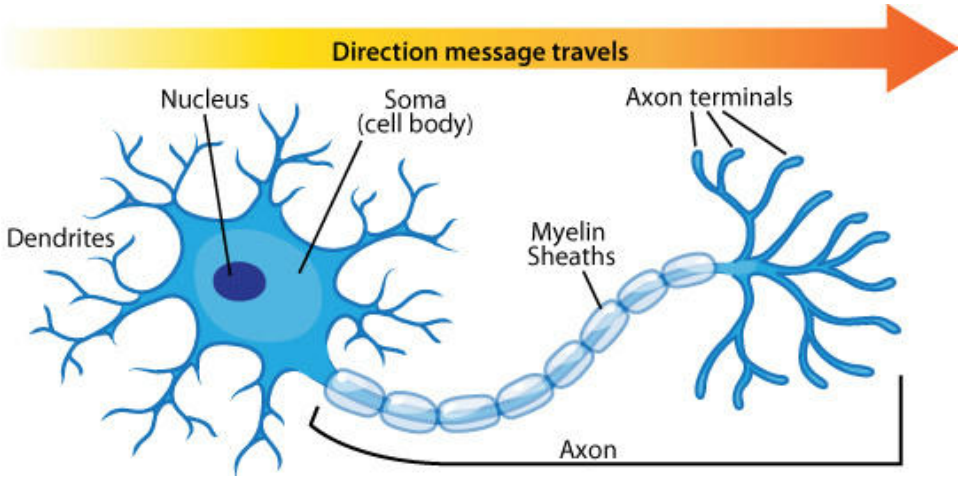


Each incoming dendrite has some voltage potential

$$f\left(\begin{bmatrix} x_i\langle 1\rangle \\ \vdots \\ x_i\langle n\rangle \end{bmatrix}, \begin{bmatrix} \theta_1 \\ \vdots \\ \theta_n \end{bmatrix}\right)$$

$$\boldsymbol{x}_i = \begin{bmatrix} x_i\langle 1\rangle \\ \vdots \\ x_i\langle n\rangle \end{bmatrix} = \begin{bmatrix} 0.5 \\ \vdots \\ -0.3 \end{bmatrix}$$

Let us implement an artifical neuron as a function



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

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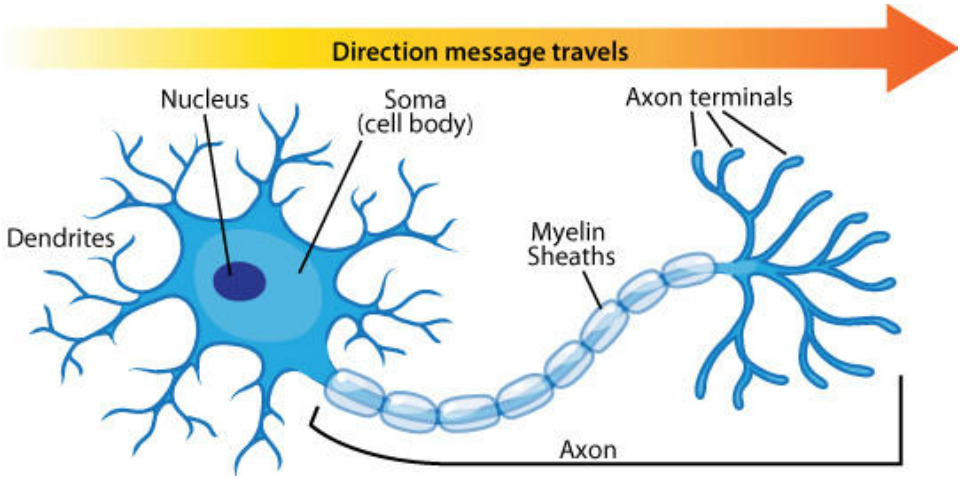

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$$f\left(\begin{bmatrix} x_i\langle 1\rangle \\ \vdots \\ x_i\langle n\rangle \end{bmatrix}, \begin{bmatrix} \theta_1 \\ \vdots \\ \theta_n \end{bmatrix}\right) = \sum_{j=1}^{n} x_i\langle j\rangle \theta_j$$

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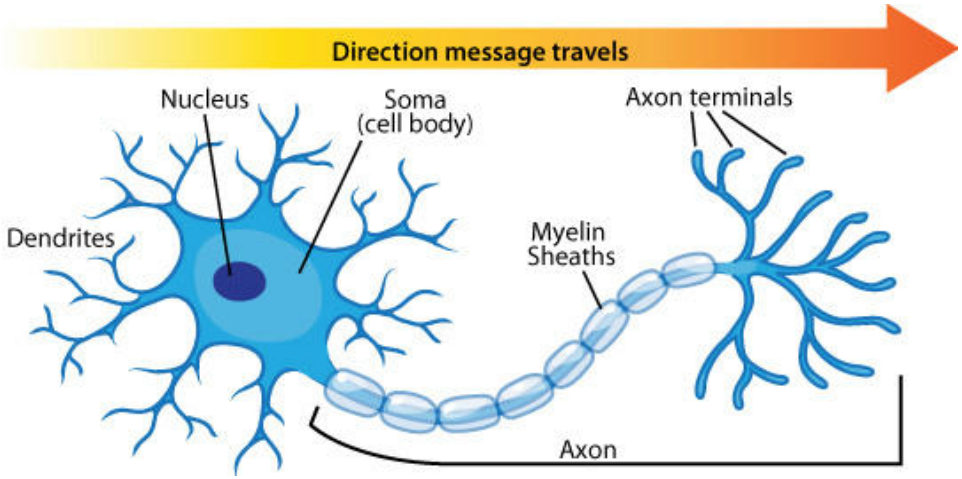

The axon fires only if the voltage is over a threshold

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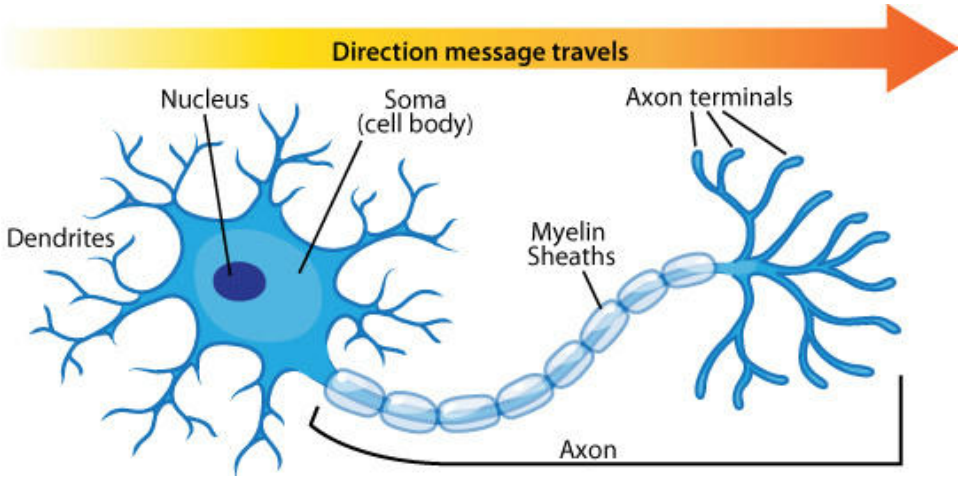

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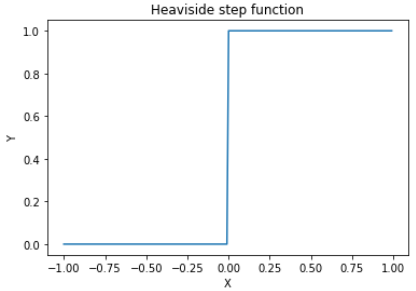
$$\sigma(x) =$$



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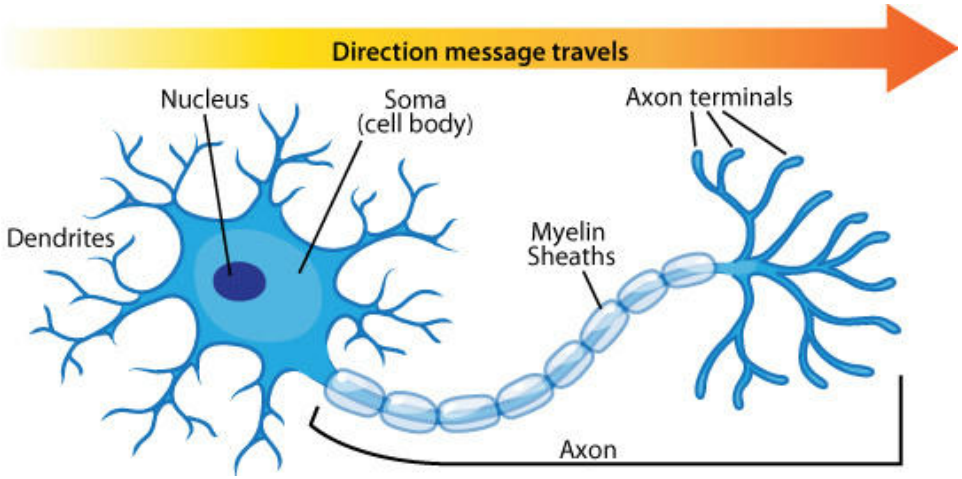

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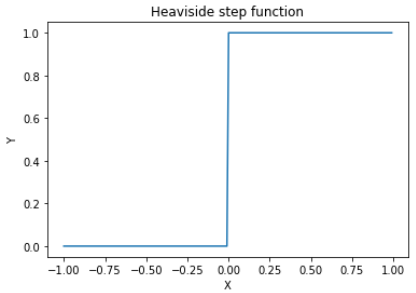

$$f\left(\begin{bmatrix} x_1 \\ \vdots \\ x_n \end{bmatrix}, \begin{bmatrix} \theta_1 \\ \vdots \\ \theta_n \end{bmatrix}\right) = \sigma\left(\sum_{j=1}^{n} x_i \langle j \rangle \theta_j\right)$$

This is almost the artificial neuron!

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Let us write this out for clarity

$$f(\boldsymbol{x}, \boldsymbol{\theta}) = \sigma(x\langle n \rangle \theta_n + x\langle n-1 \rangle \theta_{n-1} + ... + x\langle 1 \rangle \theta_1)$$

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Question: Does this look familiar to anyone?

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Question: Does this look familiar to anyone?

Answer: This is a multivariate linear model!

$$f(\boldsymbol{x}, \boldsymbol{\theta}) = \sigma\left(\sum_{i=1}^{n} x_i \theta_i\right)$$

Artificial neuron

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$$f(\boldsymbol{x}, \boldsymbol{\theta}) = \theta_0 + \theta_1 x_1 + \theta_2 x_2 + \ldots + \theta_n x_n$$

Linear model

$$f(\boldsymbol{x}, \boldsymbol{\theta}) = \sigma\left(\sum_{i=1}^{n} x_i \theta_i\right)$$ Artificial neuron

$$f(\boldsymbol{x}, \boldsymbol{\theta}) = \theta_0 + \theta_1 x_1 + \theta_2 x_2 + \ldots + \theta_n x_n$$ Linear model

It is the linear model with an activation function!

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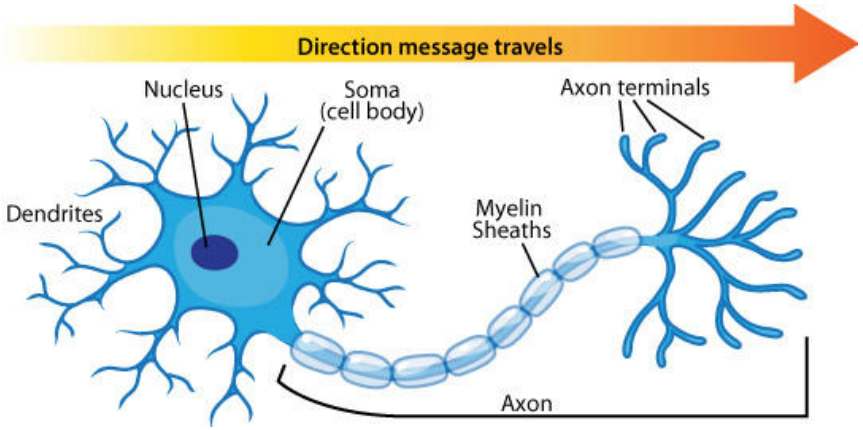

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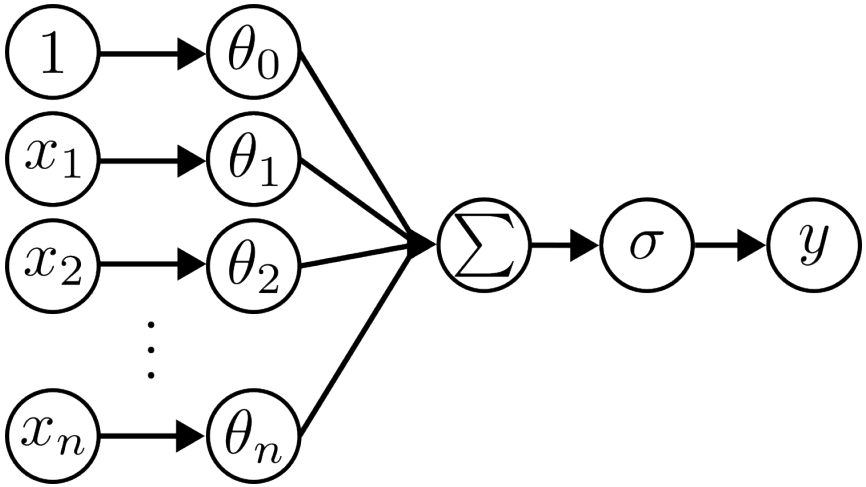

We can also write a neuron in terms of a dot product

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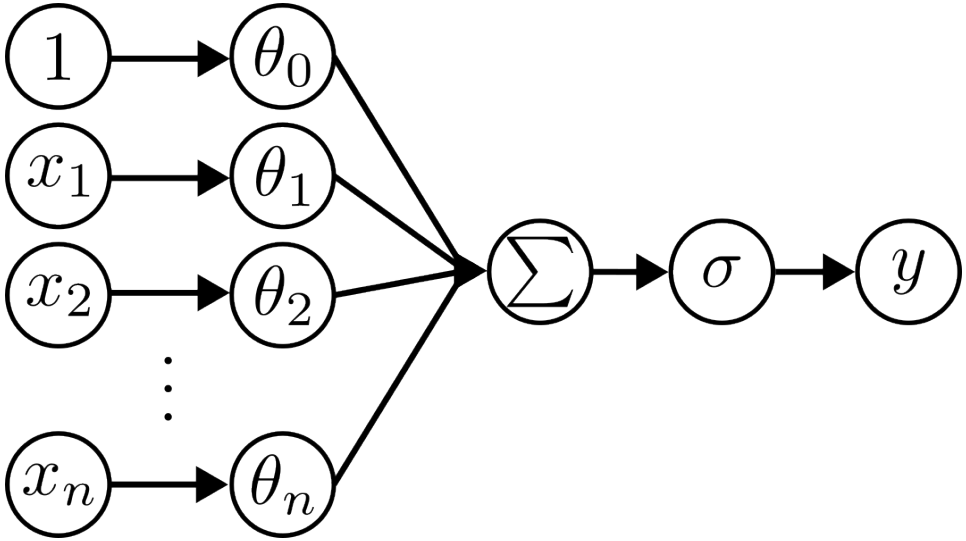
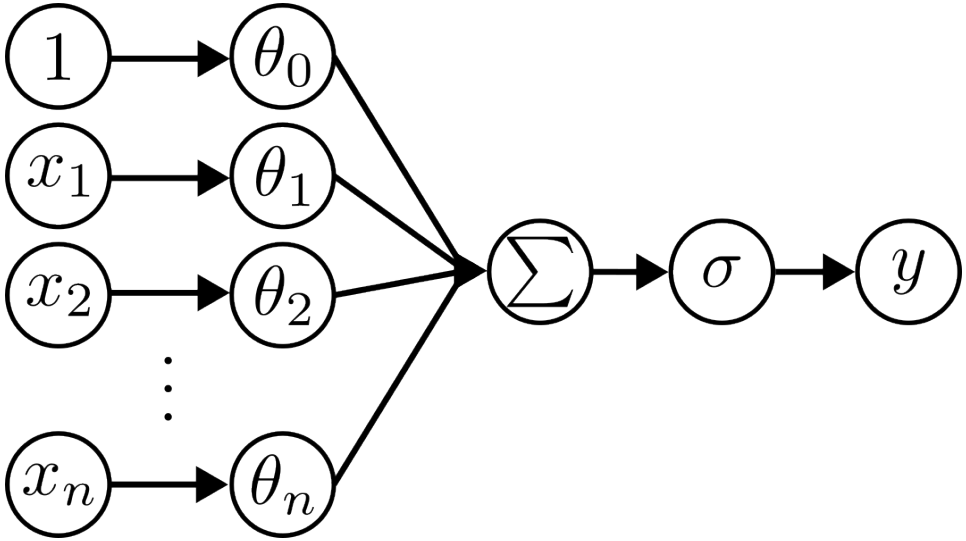
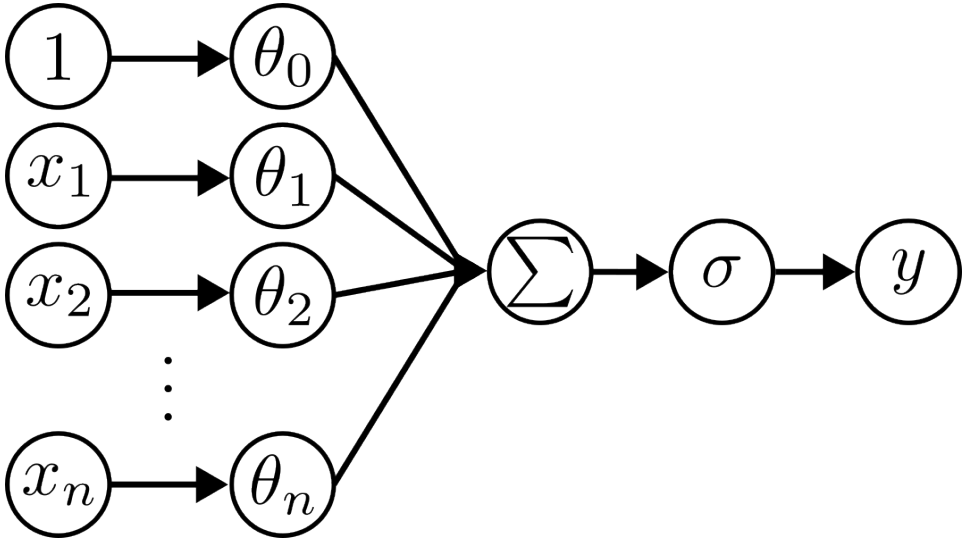
$$b = \theta_0, \boldsymbol{w} = \boldsymbol{\theta}_{1:n}$$

Relax


1
θ_0
x_1
θ_1
x_2
θ_2
x_n
θ_n
$\sum$
σ
y

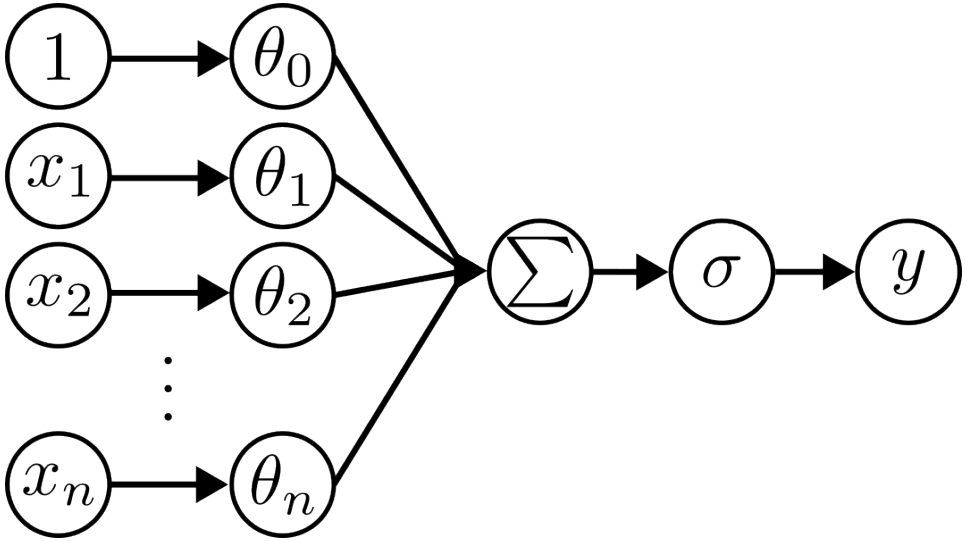


Recall that in machine learning we deal with functions



Recall that in machine learning we deal with functions

What kinds of functions can our neuron represent?



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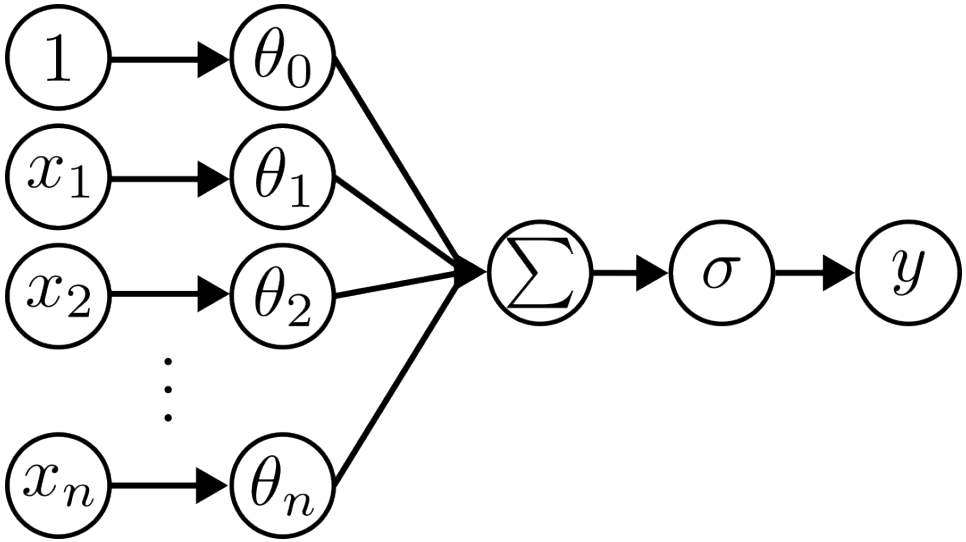
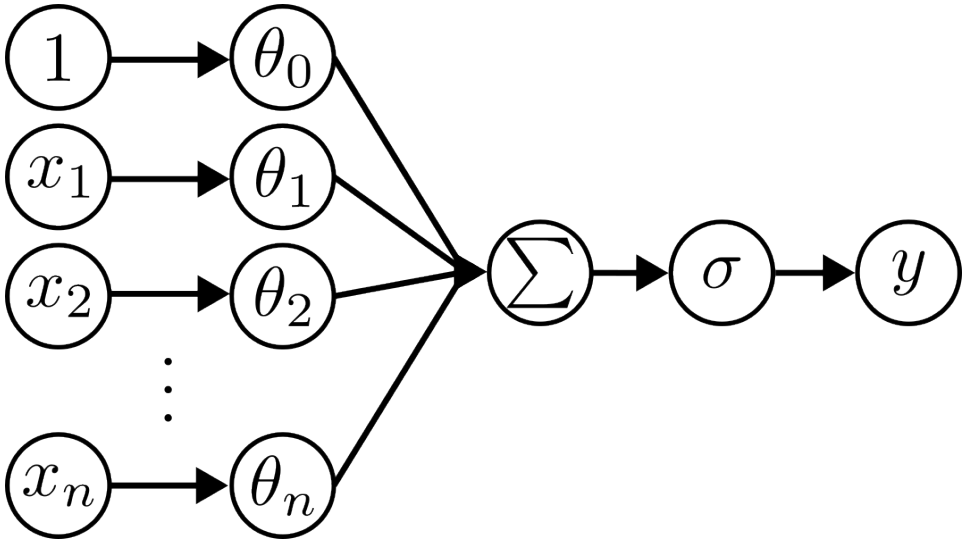
Let us start with a logical AND function

Recall the activation function (Heaviside step)





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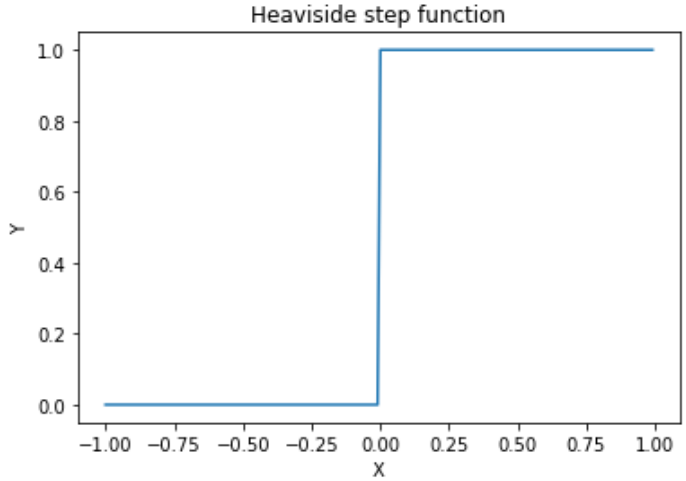

$$H(x) = \begin{cases} 1 \text{ if } x > 0 \\ 0 \text{ if } x \leq 0 \end{cases}$$

Implement AND using an artificial neuron

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$$f(x_1, x_2, \boldsymbol{\theta}) = H(\theta_0 + x_1\theta_1 + x_2\theta_2)$$

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

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0	0	0	$H(0 + 1 \cdot 0 + 1 \cdot 0) = H(0)$	0
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1	0	1	$H(0 + 1 \cdot 0 + 1 \cdot 1) = H(1)$	1
1	1	1	$H(1 + 1 \cdot 1 + 1 \cdot 1) = H(2)$	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		

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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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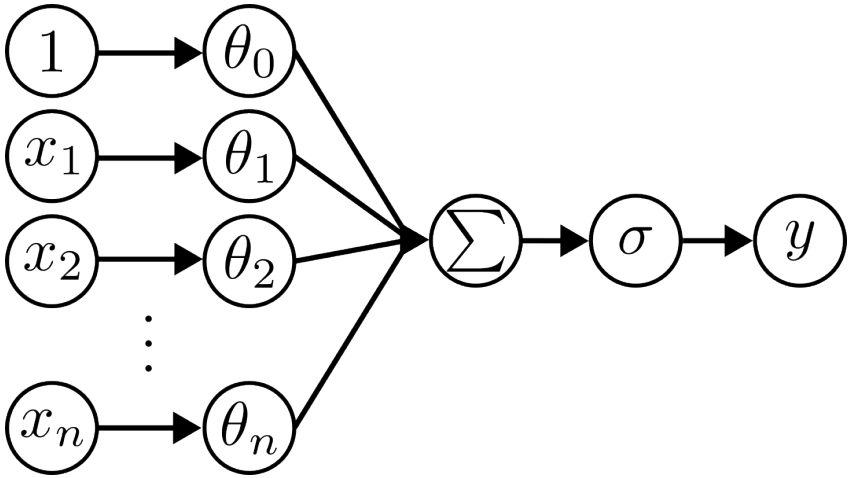
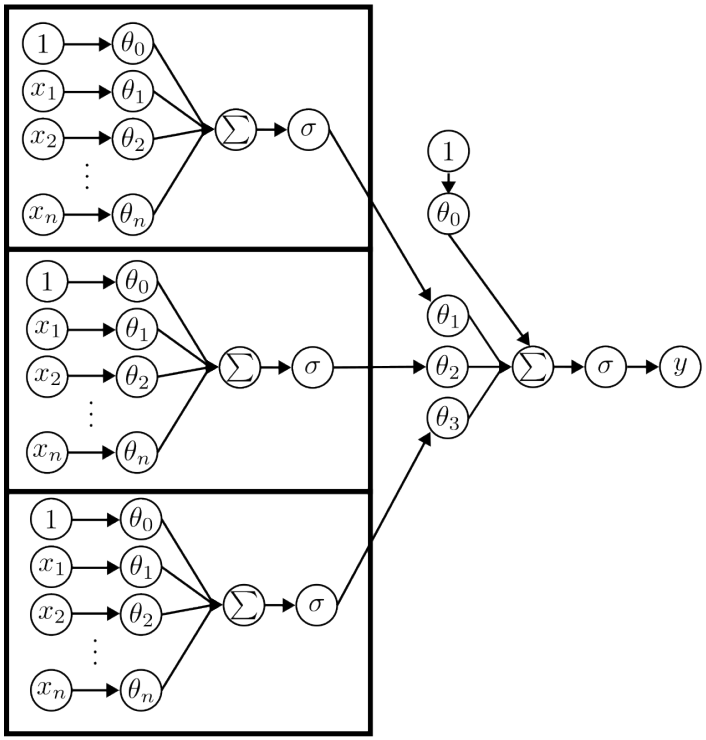
Computer: Artificial neurons $\rightarrow$ Artificial neural network

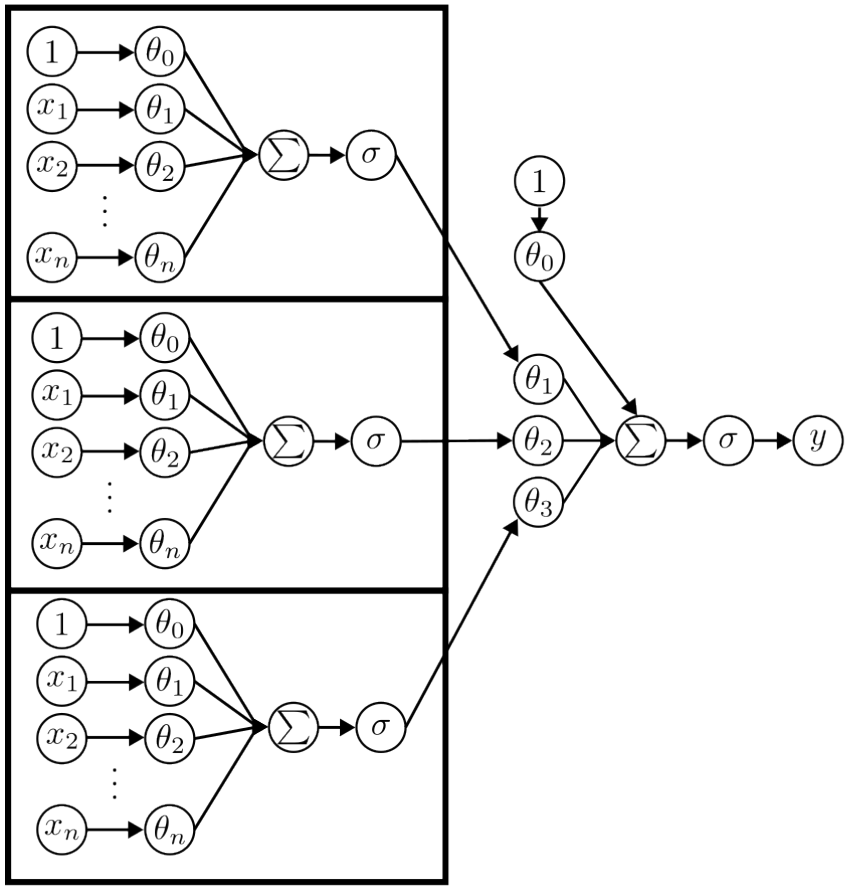
Connect artificial neurons into a network



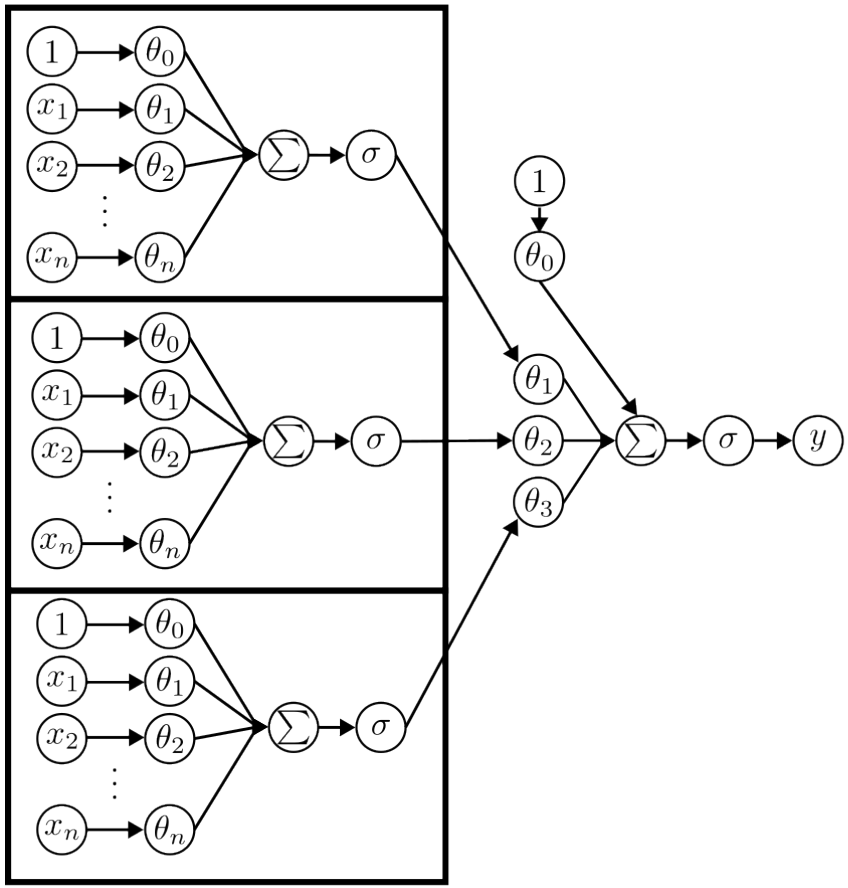
Neuron



Neural Network

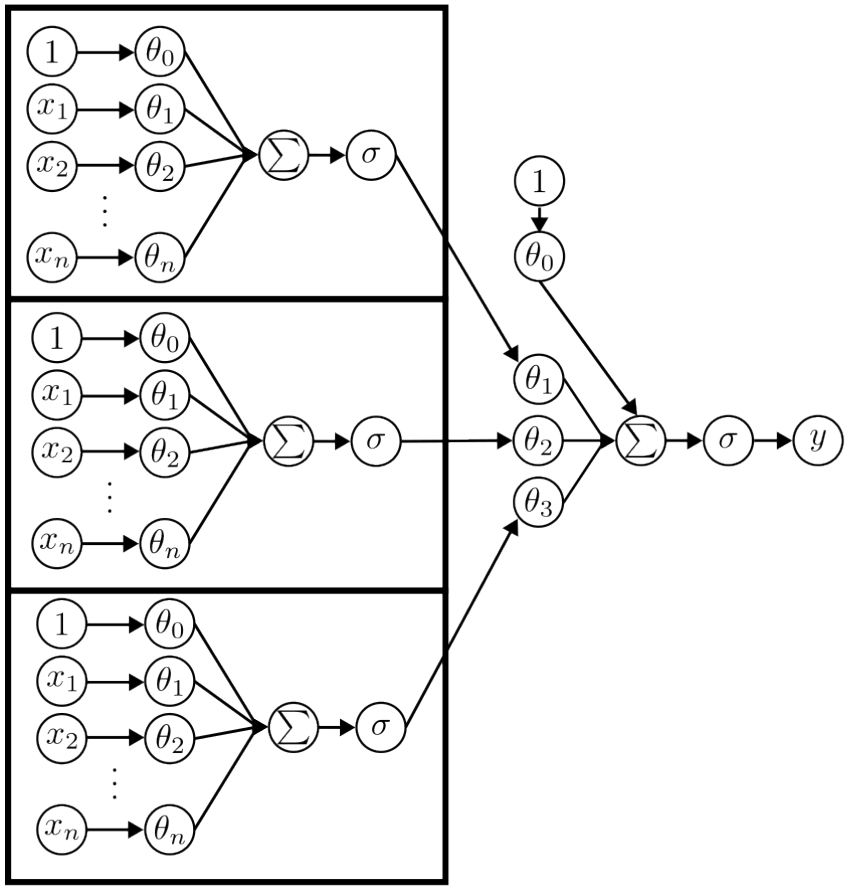


Adding neurons in **parallel** creates a **wide** neural network



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

Adding neurons in **series** creates a **deep** neural network



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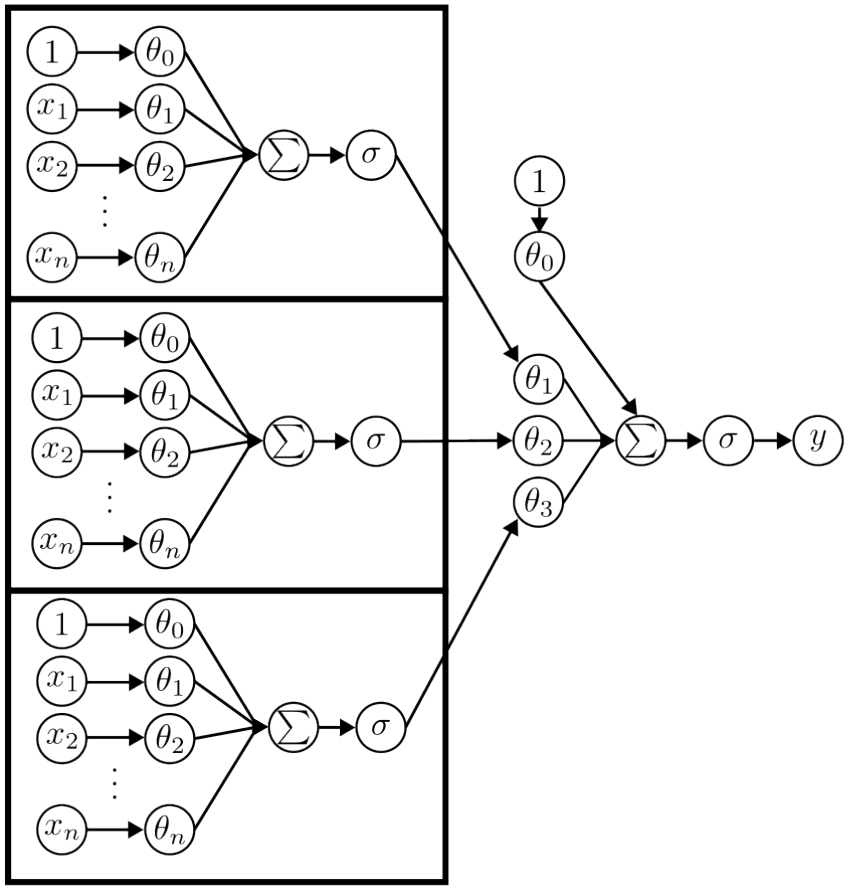
Today's powerful neural networks are both **wide** and **deep**



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

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

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Each row in the output corresponds to the output of a single neuron

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This is very confusing to write, but we can rewrite it as matrix multiplication

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

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$$f : \mathbb{R}^n, \boldsymbol{\theta} \mapsto \mathbb{R}$$

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Multiple neurons (deep):

$$f : \mathbb{R}^n, \boldsymbol{\theta}, \boldsymbol{\psi}, ..., \boldsymbol{\rho} \mapsto \mathbb{R}^m$$

A single neuron

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A composition of neurons with parameters $\boldsymbol{\theta}, \boldsymbol{\psi}, \boldsymbol{\rho}$

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$$f_\ell(\ldots f_2(f_1(\boldsymbol{x}, \boldsymbol{\theta}_1), \boldsymbol{\psi}) \ldots)$$

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$$\boldsymbol{z}_1 = f_1(\boldsymbol{x}, \boldsymbol{\theta}) = \boldsymbol{\theta}_{\cdot,0} + \boldsymbol{\theta}_{\cdot,1:n}\boldsymbol{x}$$

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Implement XOR using a deep and wide neural network

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$$
\begin{aligned}
f(x_1, x_2, \boldsymbol{\theta}) = H\big(&\theta_{3,0} \\
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\end{aligned}
$$

$$
\boldsymbol{\theta} = \begin{bmatrix} \theta_{1,0} & \theta_{1,1} & \theta_{1,2} \\ \theta_{2,0} & \theta_{2,1} & \theta_{2,2} \\ \theta_{3,0} & \theta_{3,1} & \theta_{3,2} \end{bmatrix} = \begin{bmatrix} -0.5 & 1 & 1 \\ -1.5 & 1 & 1 \\ -0.5 & 1 & -2 \end{bmatrix}
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$$

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

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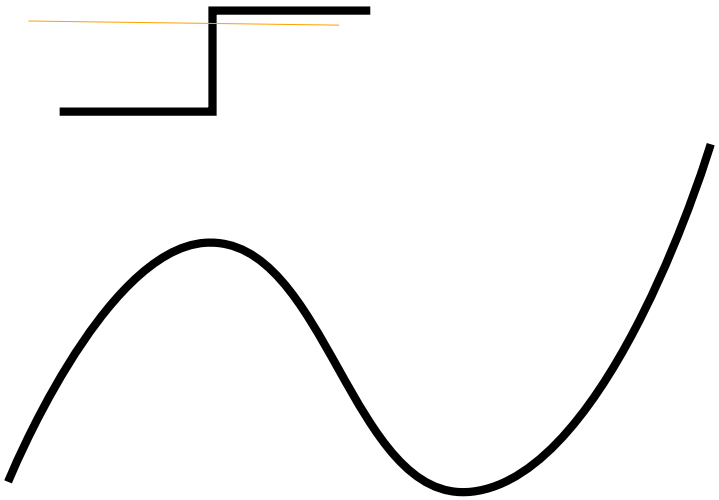

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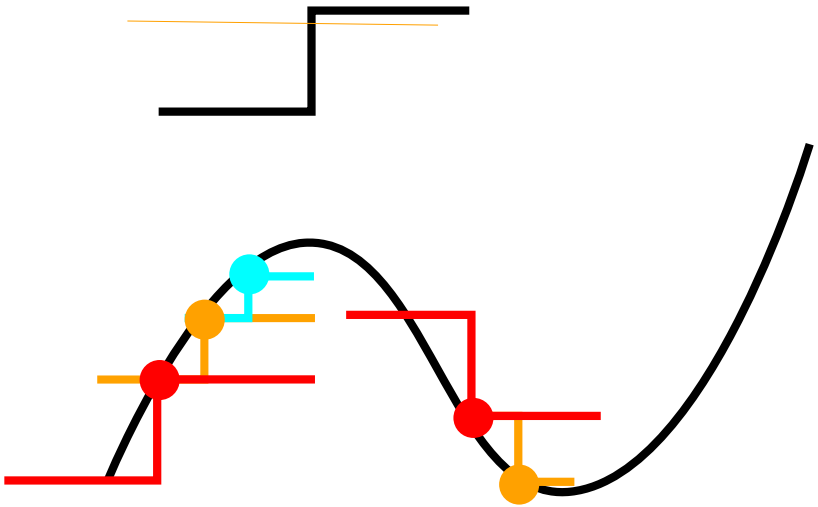

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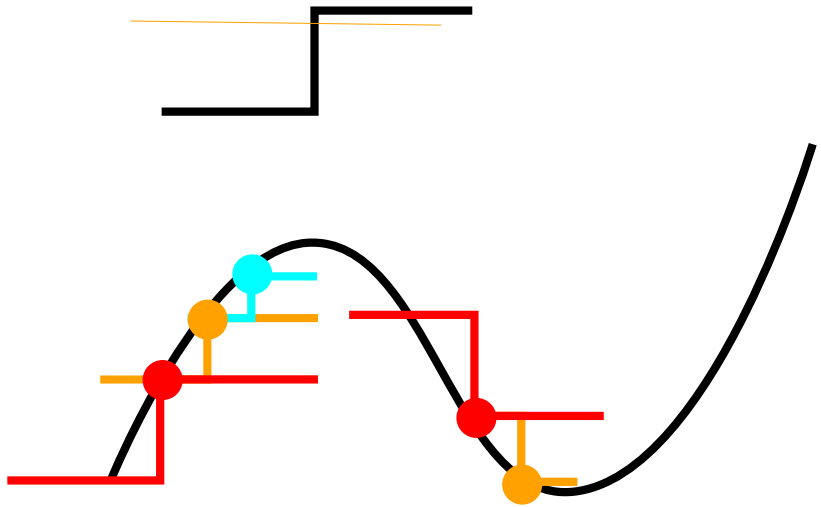

$$\text{Roughly, } \exists \boldsymbol{\theta} \Rightarrow \lim_{n \mapsto \infty} \left[\theta_{2,0} + \theta_{2,1} \sum_{j=1}^{n} \sigma\left(\theta_{1,0} + \theta_{1,j} x\right) \right] = g(x); \quad \forall g$$

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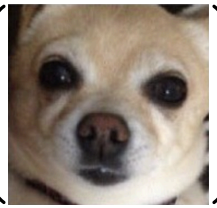
$g\left(\right.$  $\left.\right) = \text{Dog}$ $\quad$ $g\left(\right.$  $\left.\right) = \text{Muffin}$

Very powerful finding! The basis of deep learning.

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Relax

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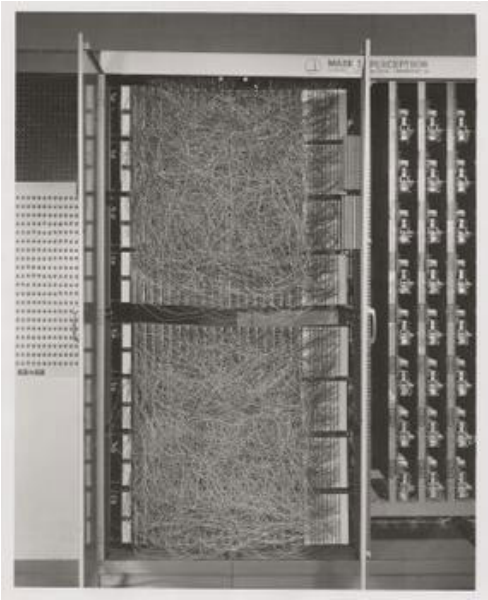
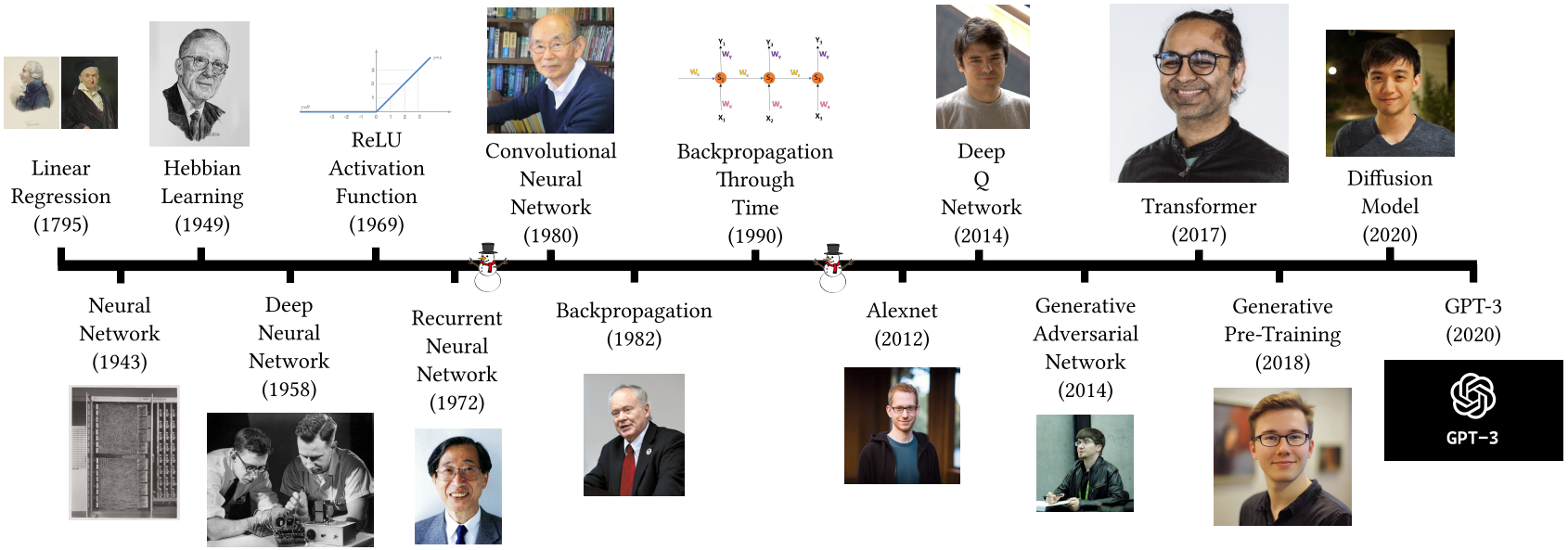
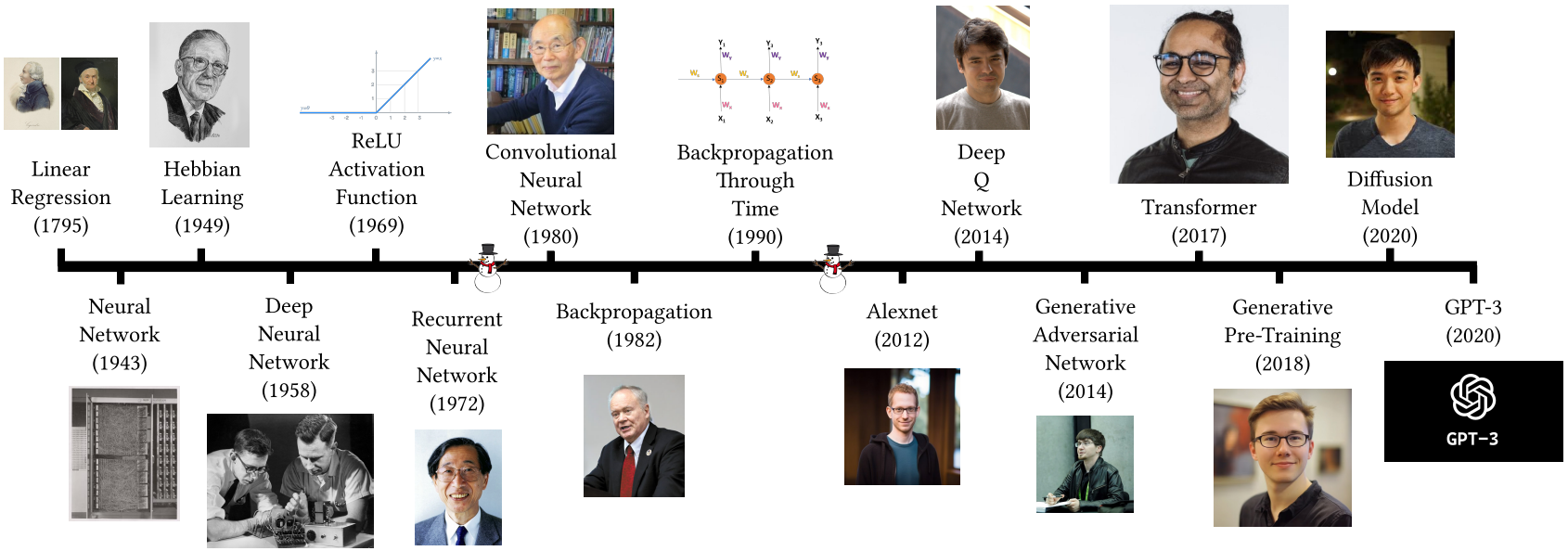


20×20 grid of pixels to process images


Linear Regression (1795)
Hebbian Learning (1949)
ReLU Activation Function (1969)
Convolutional Neural Network (1980)
Backpropagation Through Time (1990)
Deep Q Network (2014)
Transformer (2017)
Diffusion Model (2020)
Neural Network (1943)
Deep Neural Network (1958)
Recurrent Neural Network (1972)
Backpropagation (1982)
Alexnet (2012)
Generative Adversarial Network (2014)
Generative Pre-Training (2018)
GPT-3 (2020)
GPT-3



Question: If the deep neural network was invented in 1958, why did it take 70 years for us to care about deep learning?

Answer: Deep learning requires very deep and wide networks

1. Hardware advances enabled very deep and wide networks

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When the network is deep, we call it a Multi-Layer Perceptron (MLP)

We often use the term “layers”, when referring to a specific depth of the neural network

- Four-layer MLP means a neural network with a depth of four
- Corresponds to four parameter matrices in $\boldsymbol{\theta}$

Let us construct deep and wide neural networks in `torch` and `jax`

Here are the equations for one neural network layer

$$f(\boldsymbol{x}, \boldsymbol{\theta}) = \sigma\left(\boldsymbol{\theta}_{\cdot,0} + \boldsymbol{\theta}_{\cdot,1:n}\boldsymbol{x}\right) \quad \text{or} \quad f(\boldsymbol{x}, (\boldsymbol{b}, \boldsymbol{W})) = \sigma(\boldsymbol{b} + \boldsymbol{W}\boldsymbol{x})$$

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Let us do this in colab! https://colab.research.google.com/drive/1bLtf3QY-yROIif_EoQSU1WS7svd0q8j7?usp=sharing