Neural Networks

CISC 7026: Introduction to Deep Learning

University of Macau

Notation Change

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

1. Review
2. Multivariate linear regression
3. Limitations of linear regression
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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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Approach: Learn the parameters θ such that

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

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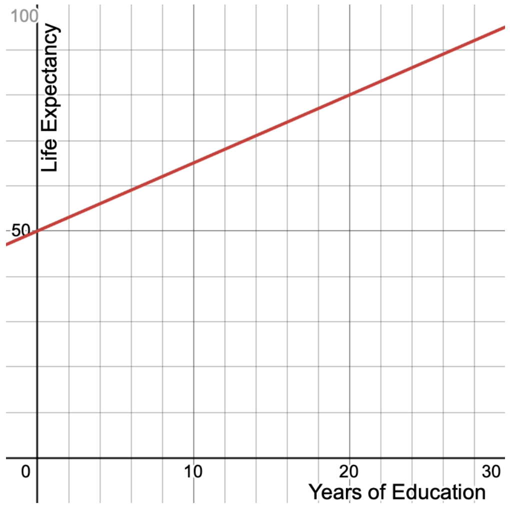
$$f(x, \boldsymbol{\theta}) = f\left(x, \begin{bmatrix} \theta_1 \\ \theta_0 \end{bmatrix}\right) = \theta_1 x + \theta_0$$



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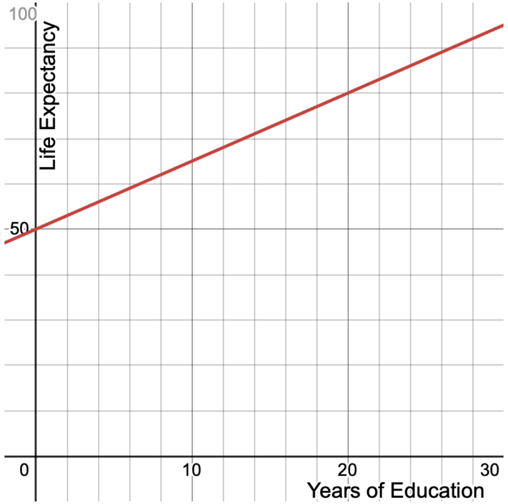

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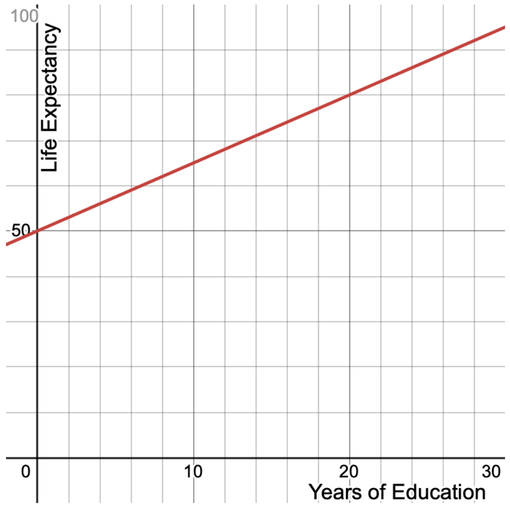

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$$\text{error}(f(x, \boldsymbol{\theta}), y) = (f(x, \boldsymbol{\theta}) - y)^2$$

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

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

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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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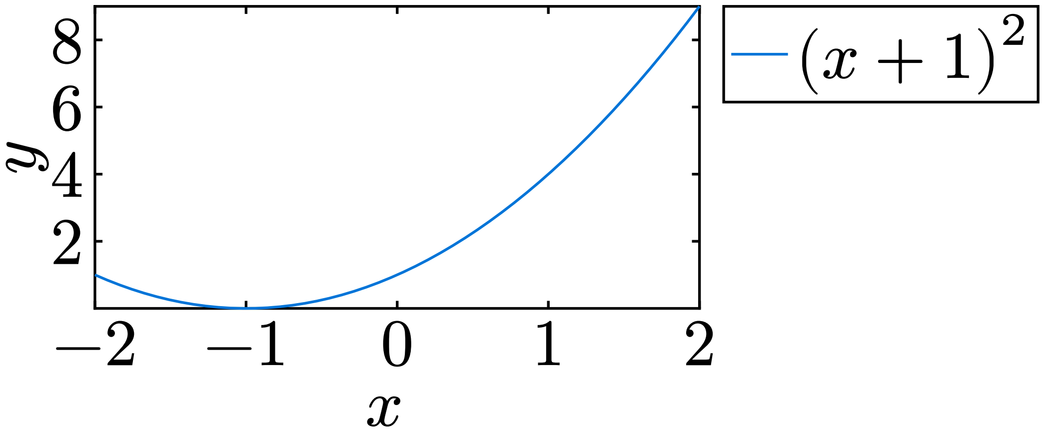

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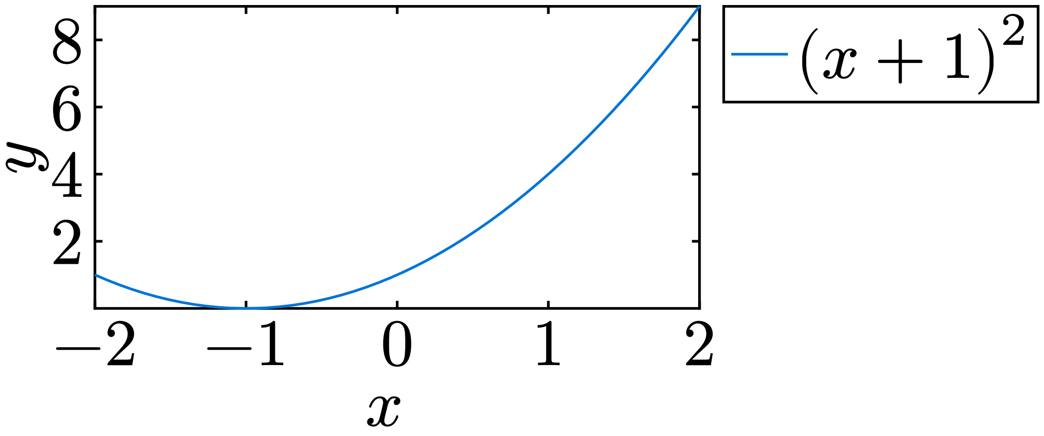

$$\arg\min_x f(x) = -1$$

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

$$= \underset{\boldsymbol{\theta}}{\arg\min} \sum_{i=1}^{n} \Big(f\big(x_{[i]}, \boldsymbol{\theta}\big) - y_{[i]}\Big)^2$$

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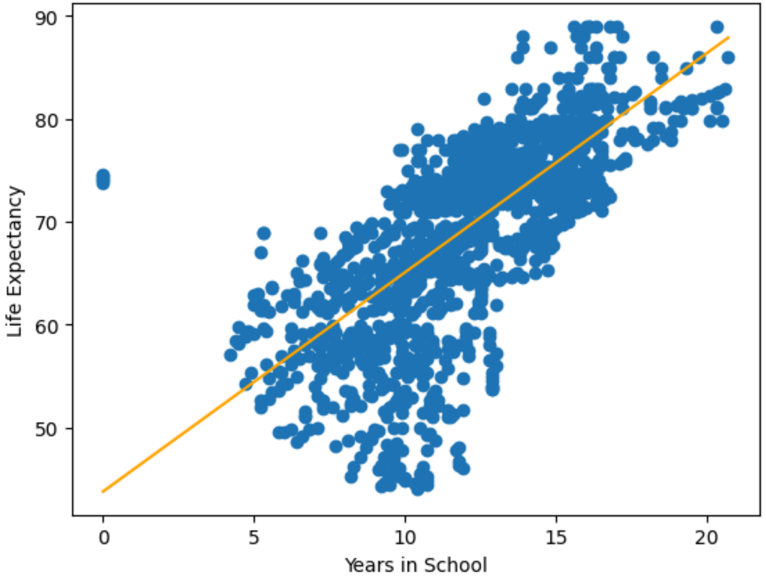

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$$\boldsymbol{X}_D = \begin{bmatrix} x_{[1]} & 1 \\ x_{[2]} & 1 \\ \vdots & \vdots \\ x_{[n]} & 1 \end{bmatrix} \Rightarrow \boldsymbol{X}_D = \begin{bmatrix} \log\left(1 + x_{[1]}\right) & 1 \\ \log\left(1 + x_{[2]}\right) & 1 \\ \vdots & \vdots \\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

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

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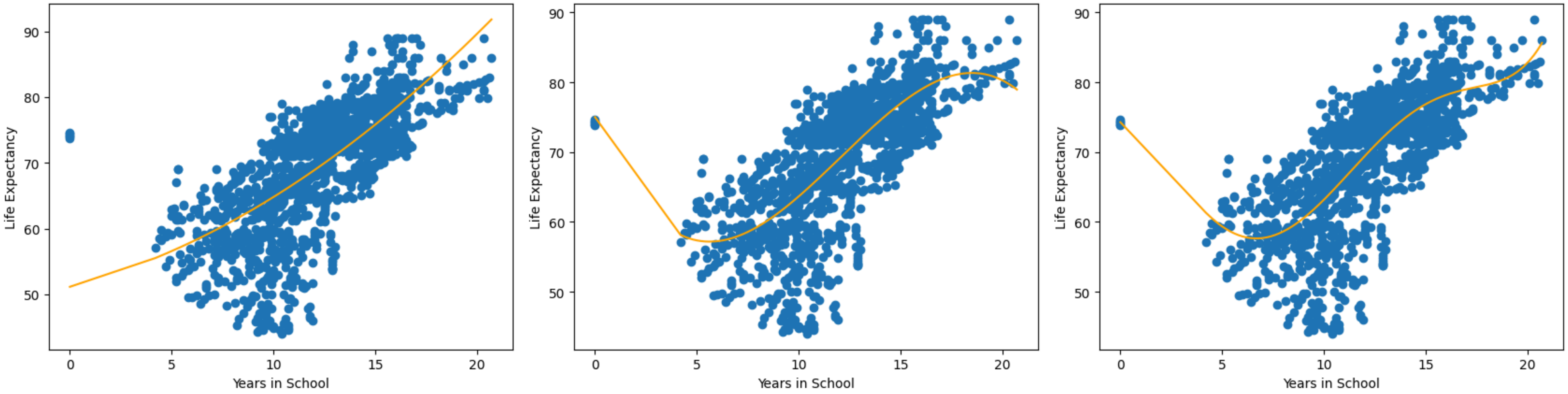

$m = 2$ $m = 3$ $m = 5$

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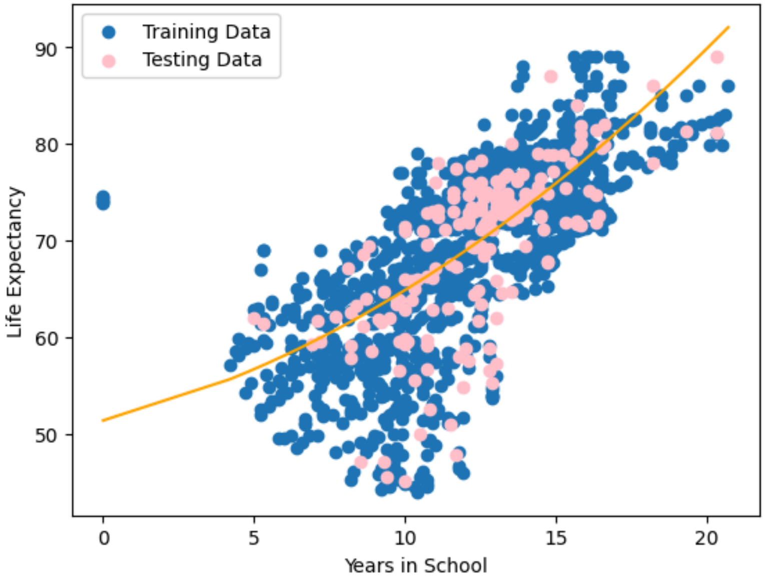

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We can solve these problems using linear regression too

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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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Issues with very complex problems

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2. Polynomials do not generalize well

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One-dimensional polynomial functions

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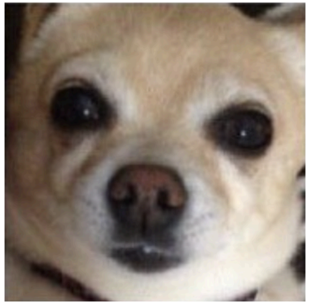

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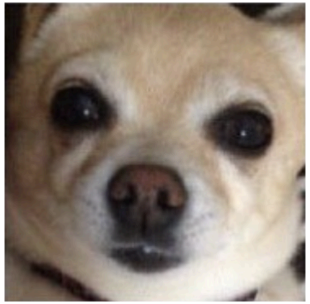

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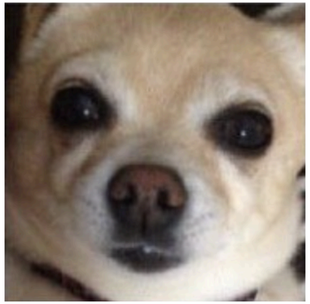

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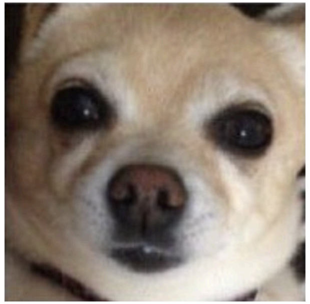

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$$
\boldsymbol{X}_D = \begin{bmatrix}
x^m_{[1],d_x} & \cdots & x^m_{[1],1} & \cdots & x^{m-1}_{[1],d_x} & \cdots & x^{m-1}_{[1],1} & \cdots & \cdots & 1 \\
\vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\
x^m_{[n],d_x} & \cdots & x^m_{[n],1} & \cdots & x^{m-1}_{[n],d_x} & \cdots & x^{m-1}_{[n],1} & \cdots & \cdots & 1 \\
x^m_{[1],d_x} & x^{m-1}_{[1],d_x} x_{[1],d_x-1} & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & 1 \\
\vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots
\end{bmatrix}
$$

Question: How many rows in this matrix?

$$\boldsymbol{X}_D = \begin{bmatrix} x_{[1], d_x}^m & \dots & x_{[1], 1}^m & \dots & x_{[1], d_x}^{m-1} & \dots & x_{[1], 1}^{m-1} & \dots & \dots & 1 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ x_{[n], d_x}^m & \dots & x_{[n], 1}^m & \dots & x_{[n], d_x}^{m-1} & \dots & x_{[n], 1}^{m-1} & \dots & \dots & 1 \\ x_{[1], d_x}^m & x_{[1], d_x}^{m-1} x_{[1], d_x - 1} & \dots & \dots & \dots & \dots & \dots & \dots & \dots & 1 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \end{bmatrix}$$

Question: How many rows 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: $(d_x)^m + 1 = 65536^{20} + 1 \approx 10^{96}$

To find $\boldsymbol{\theta}$, we must invert $\boldsymbol{X}_D^\top \boldsymbol{X}_D$

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We cannot predict how many ♥
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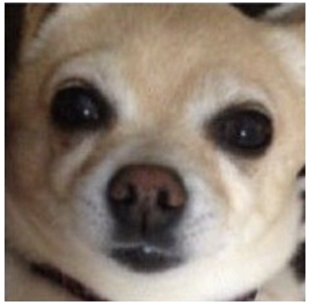

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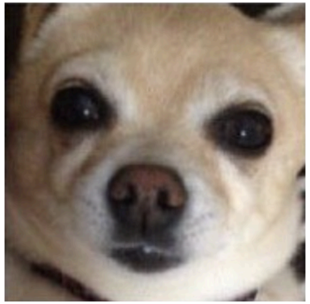

Polynomial regression does not scale to large inputs

Issues with very complex problems

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

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Equation of a polynomial

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Factor out x^m

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Evaluate right limit

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Rewrite

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

If $\theta_m > 0$

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

Rewrite

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If $\theta_m > 0$

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

If $\theta_m < 0$

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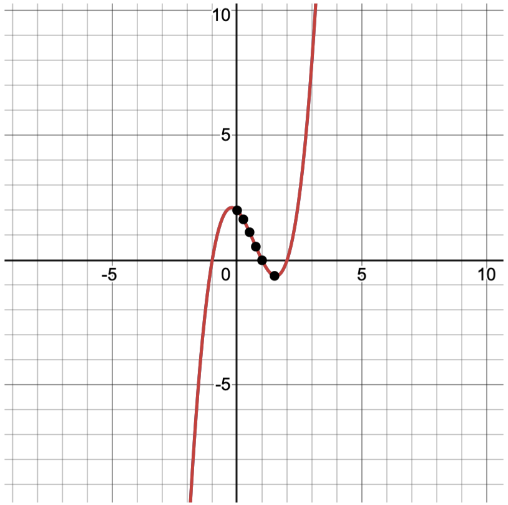

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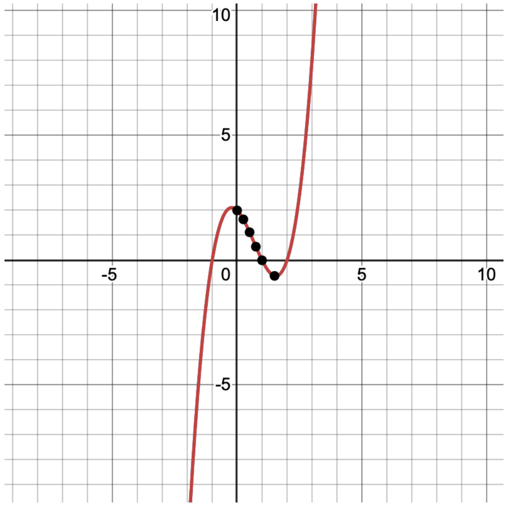

Remember, to predict new data we want our functions to generalize

Linear regression has issues

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1. Poor scalability
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Can we improve upon linear regression?

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Yes, with neural networks

In 1939-1945, there was a World War

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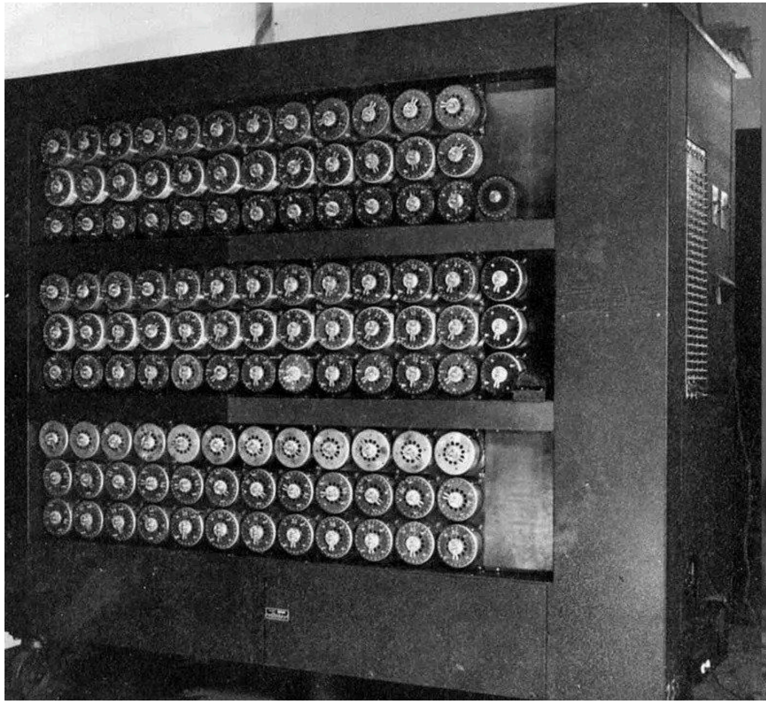
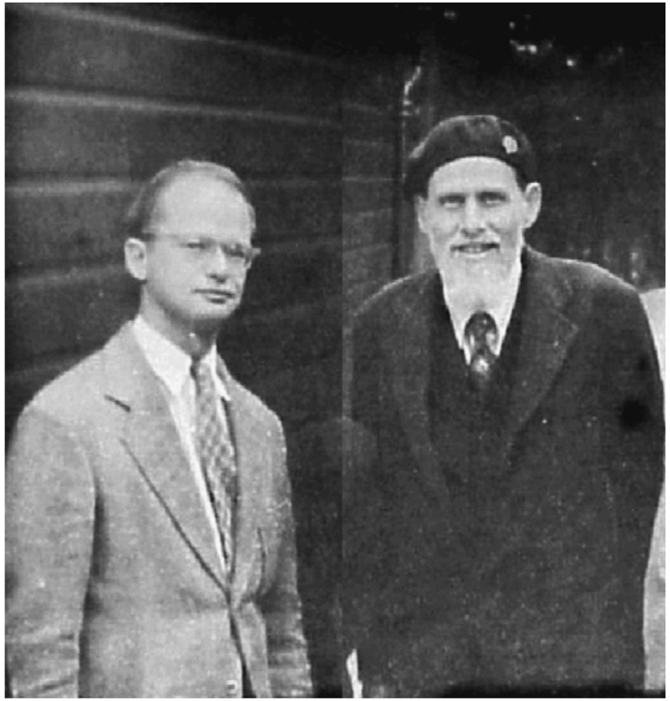
 

Meanwhile, a neuroscientist and mathematician (McCullough and Pitts) were trying to understand the human brain



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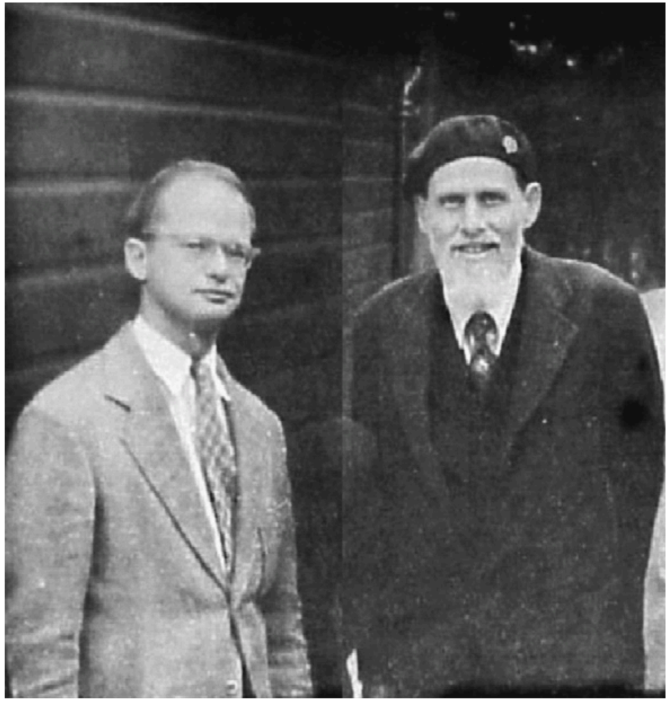
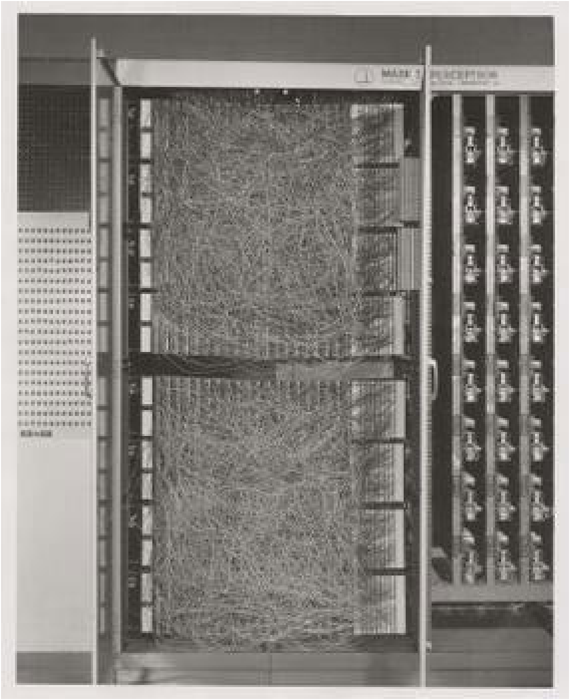


They designed the theory for the first neural network

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



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

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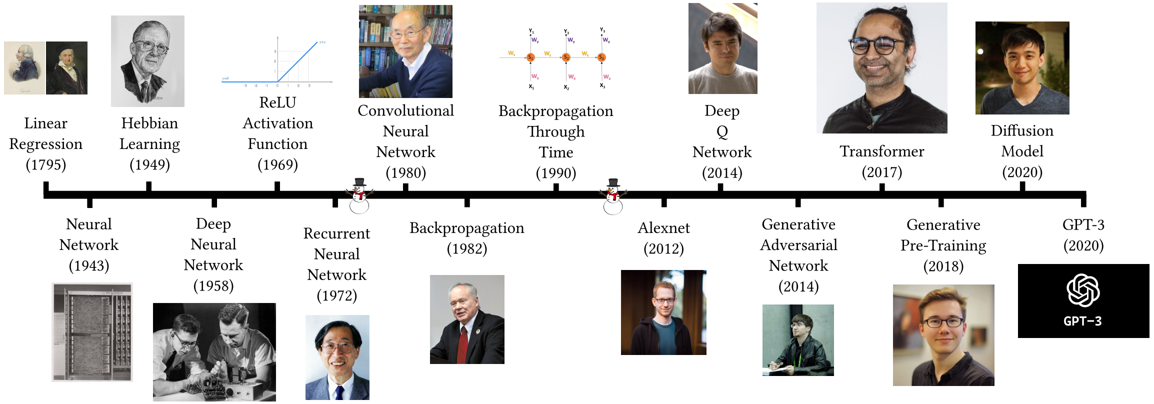
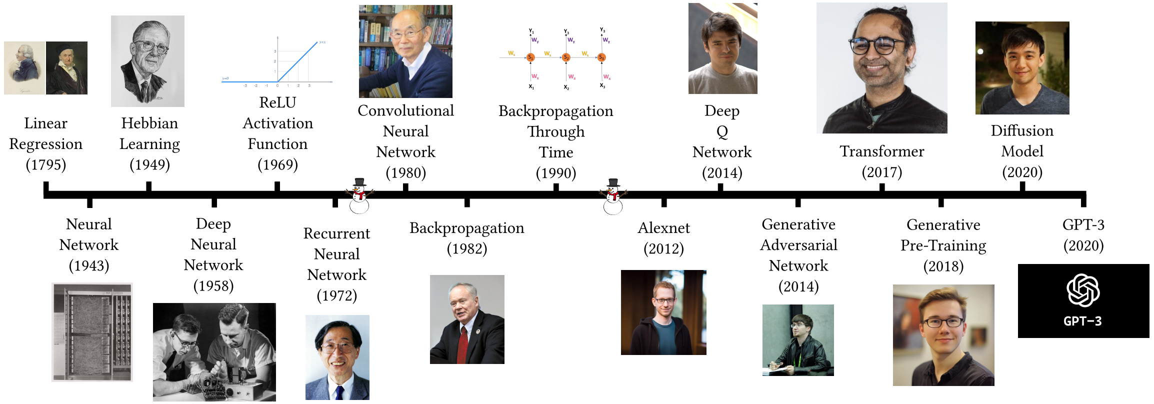


Through advances in theory and hardware, neural networks became slightly better



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

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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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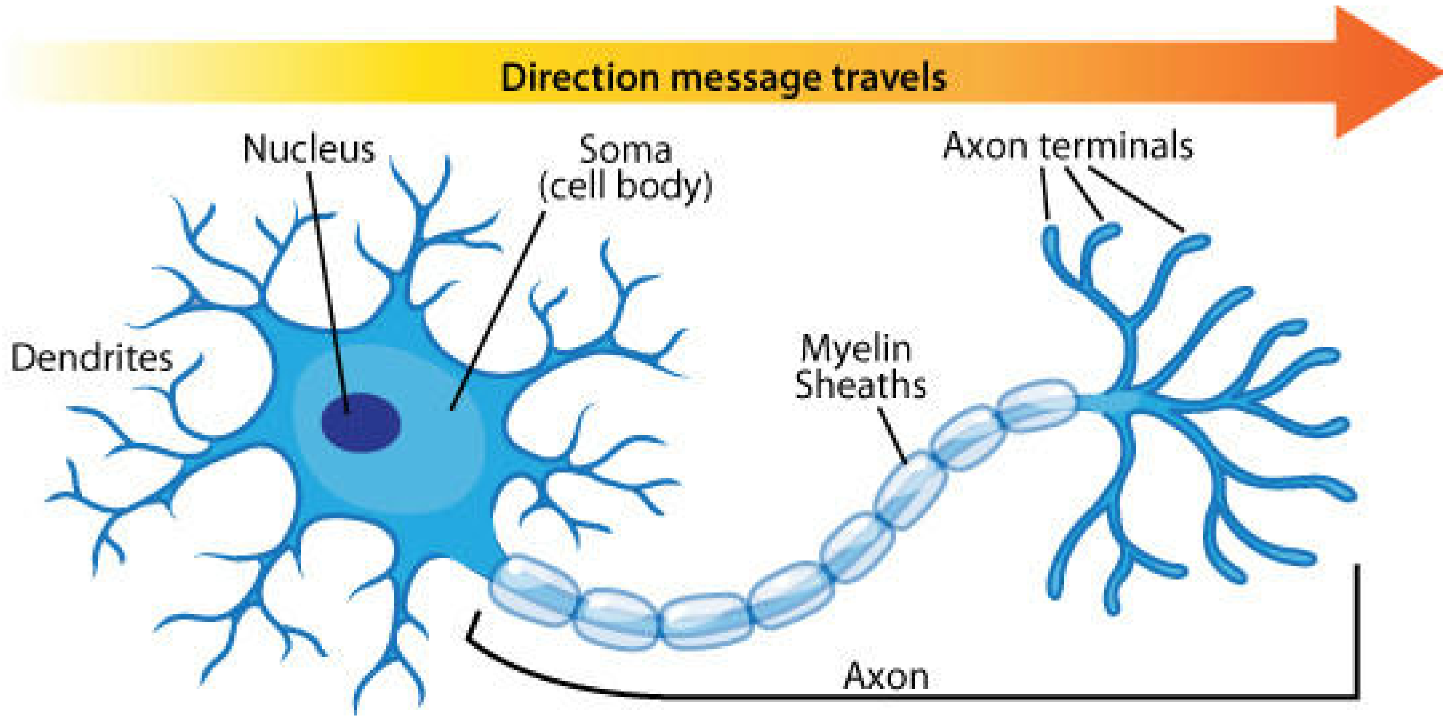
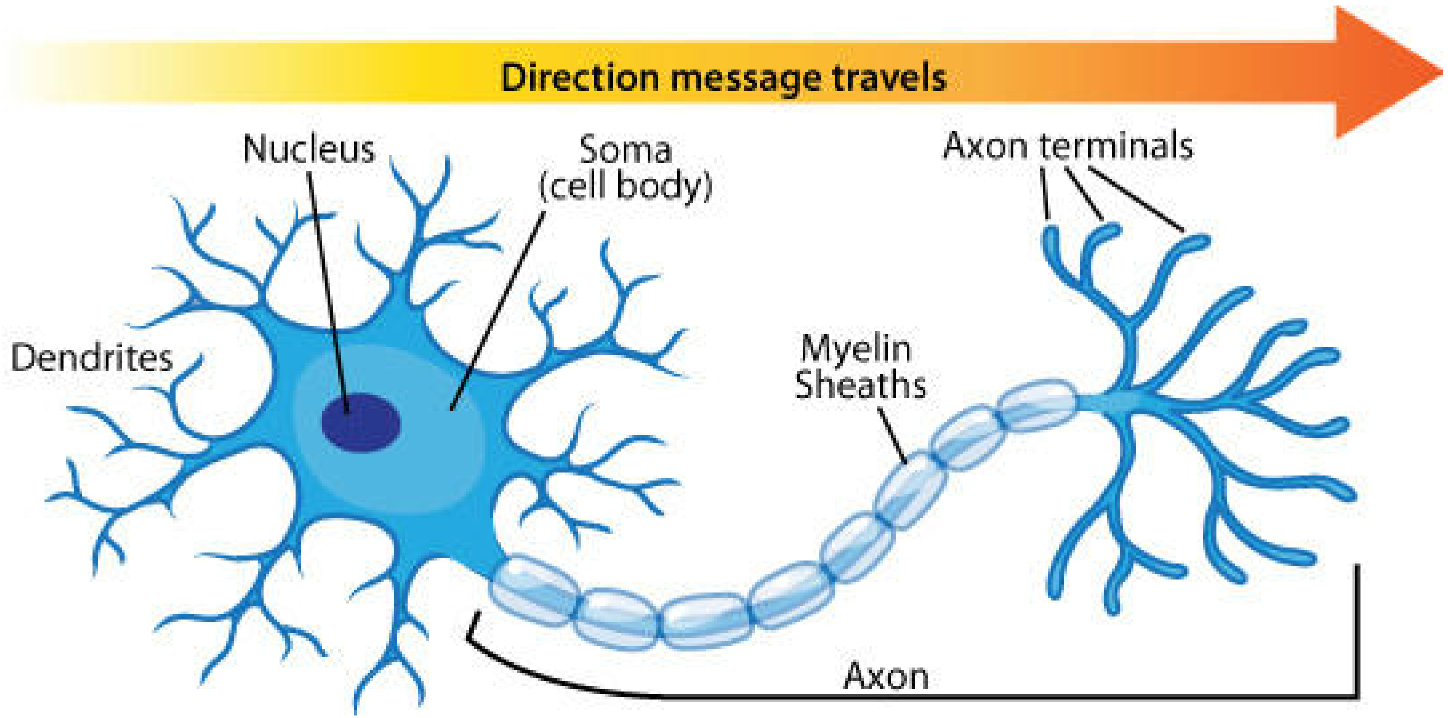
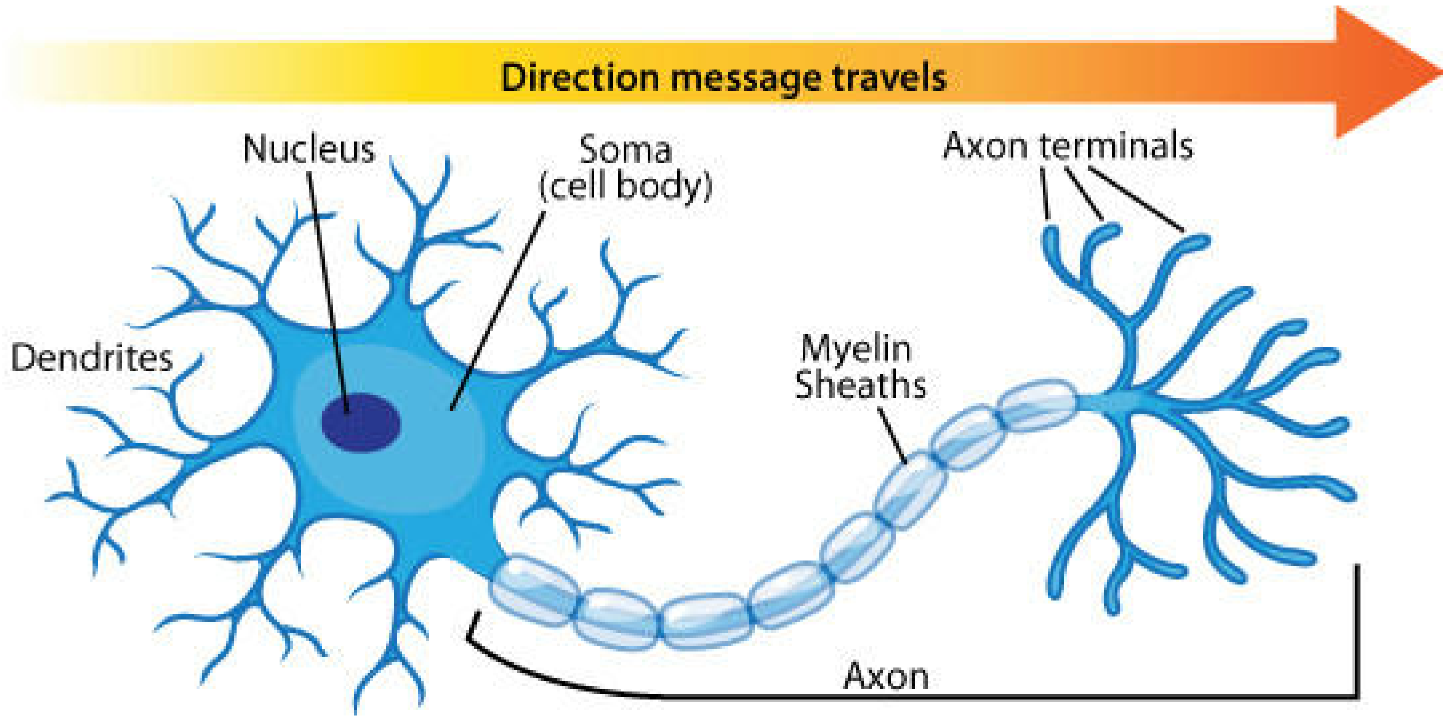


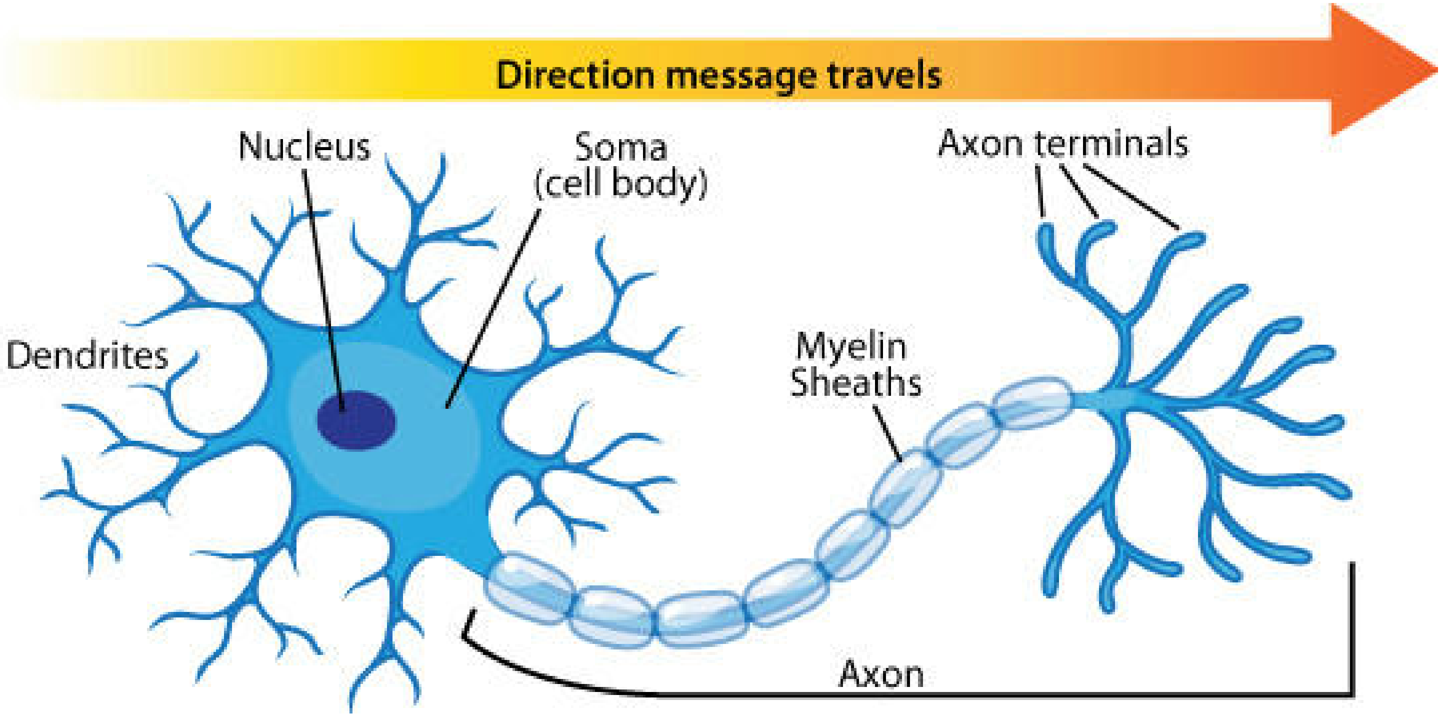
A simplified neuron consists of many parts



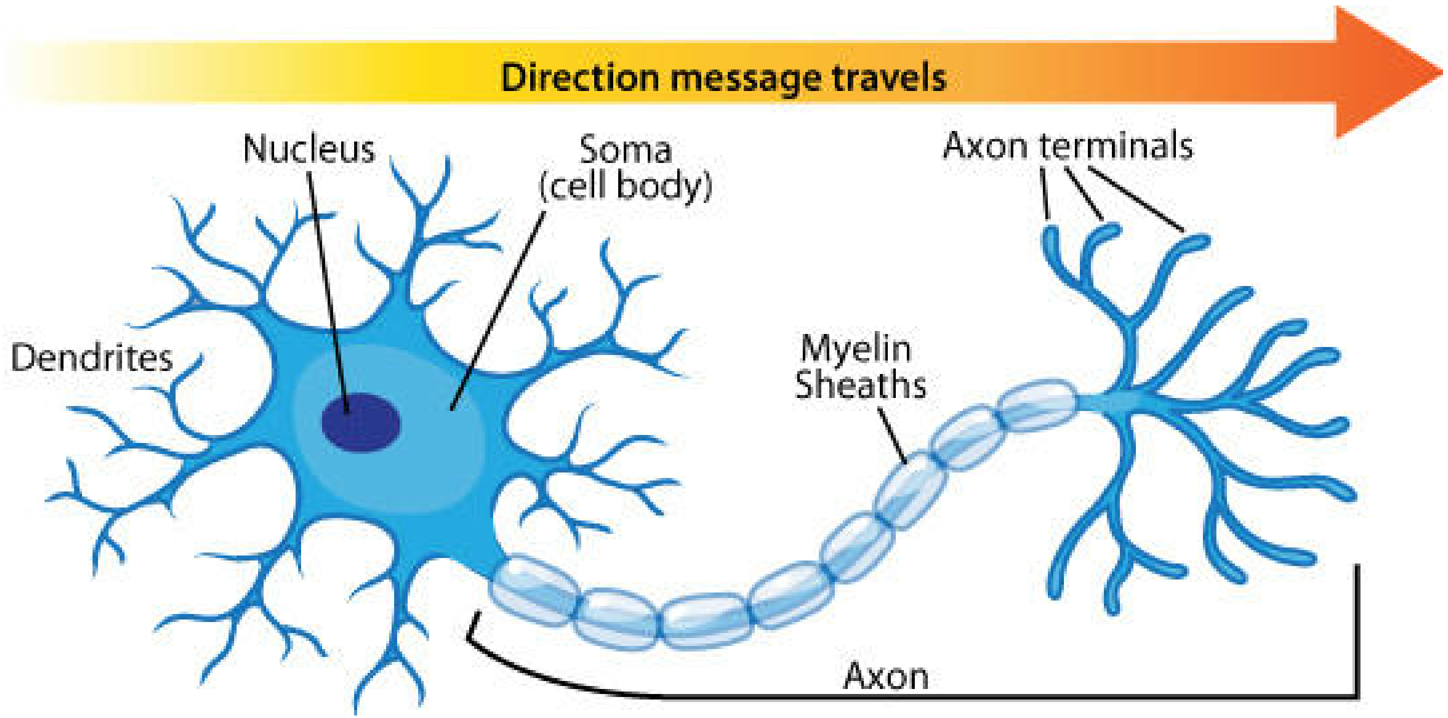
Neurons send and process messages from other neurons



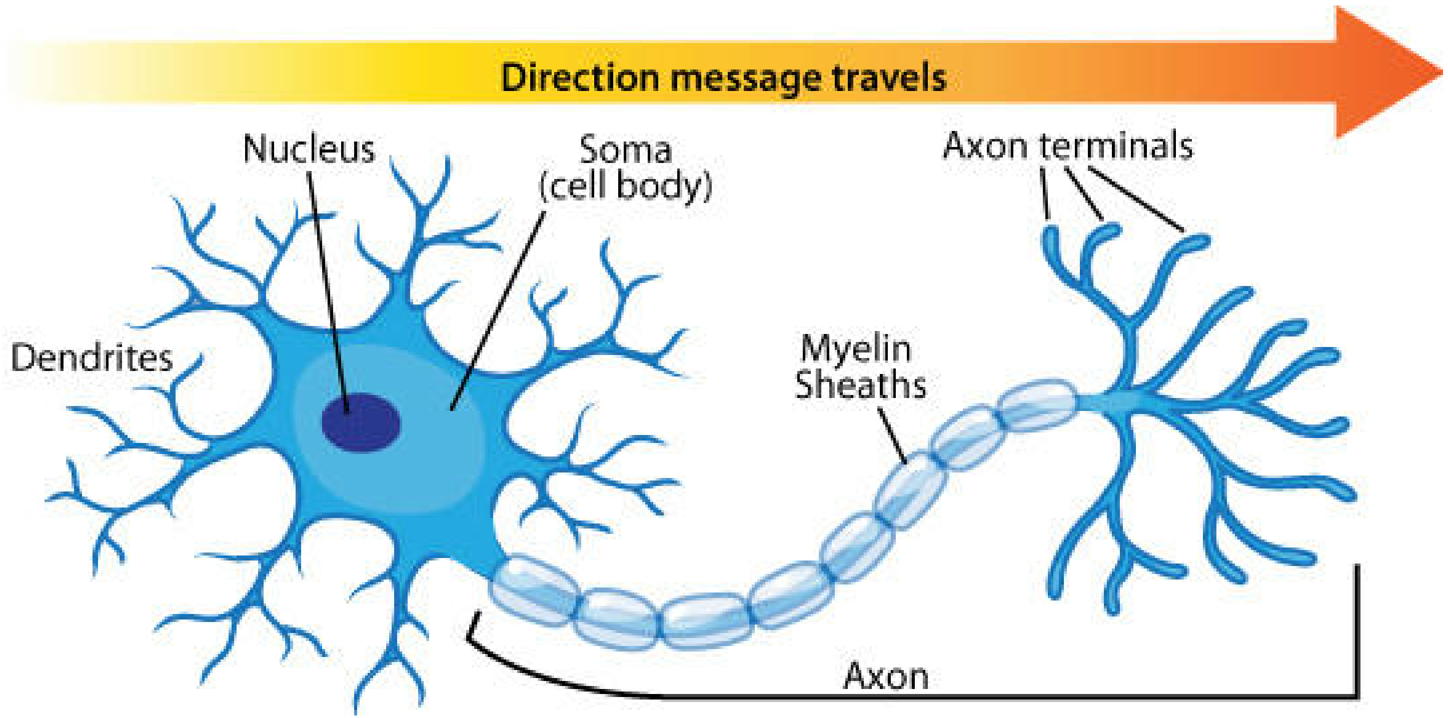
Incoming electrical signals travel along dendrites



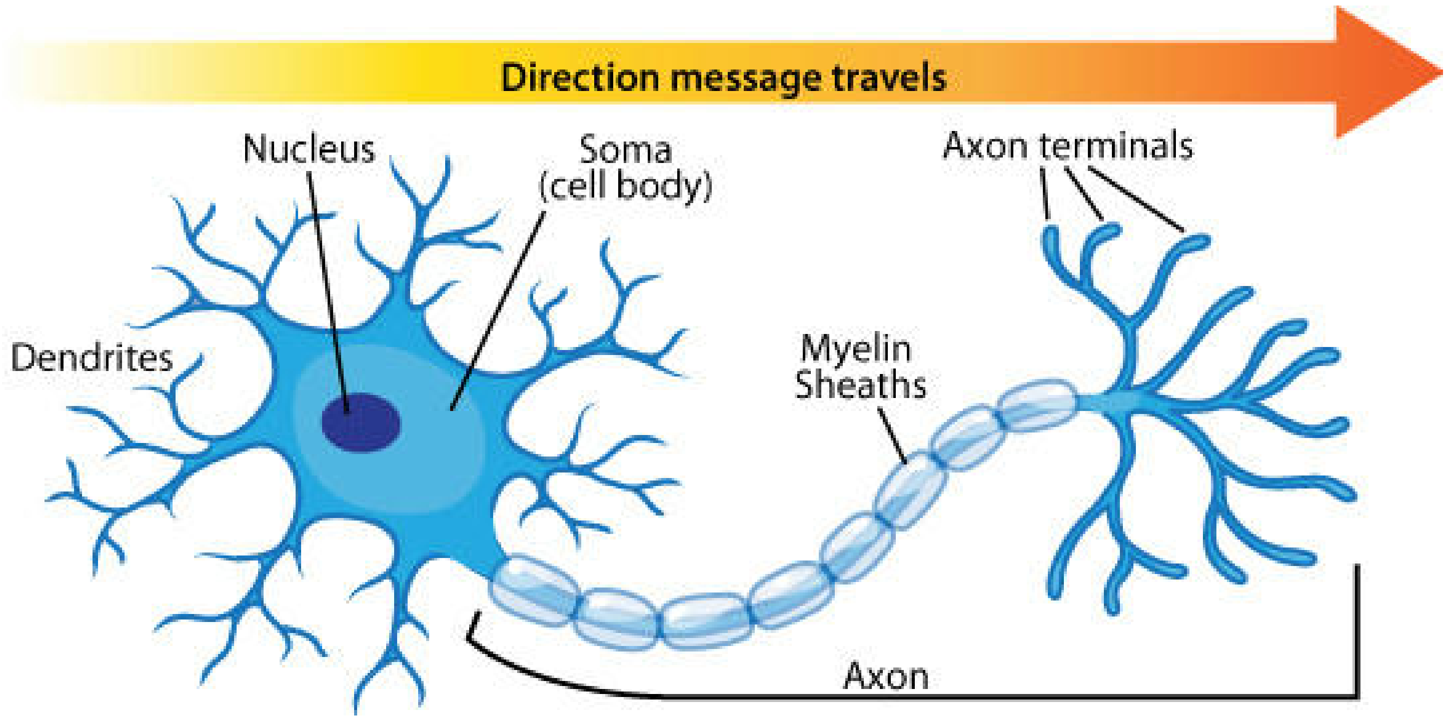
Dendrites are not all equal! Different dendrites have different diameters and structures



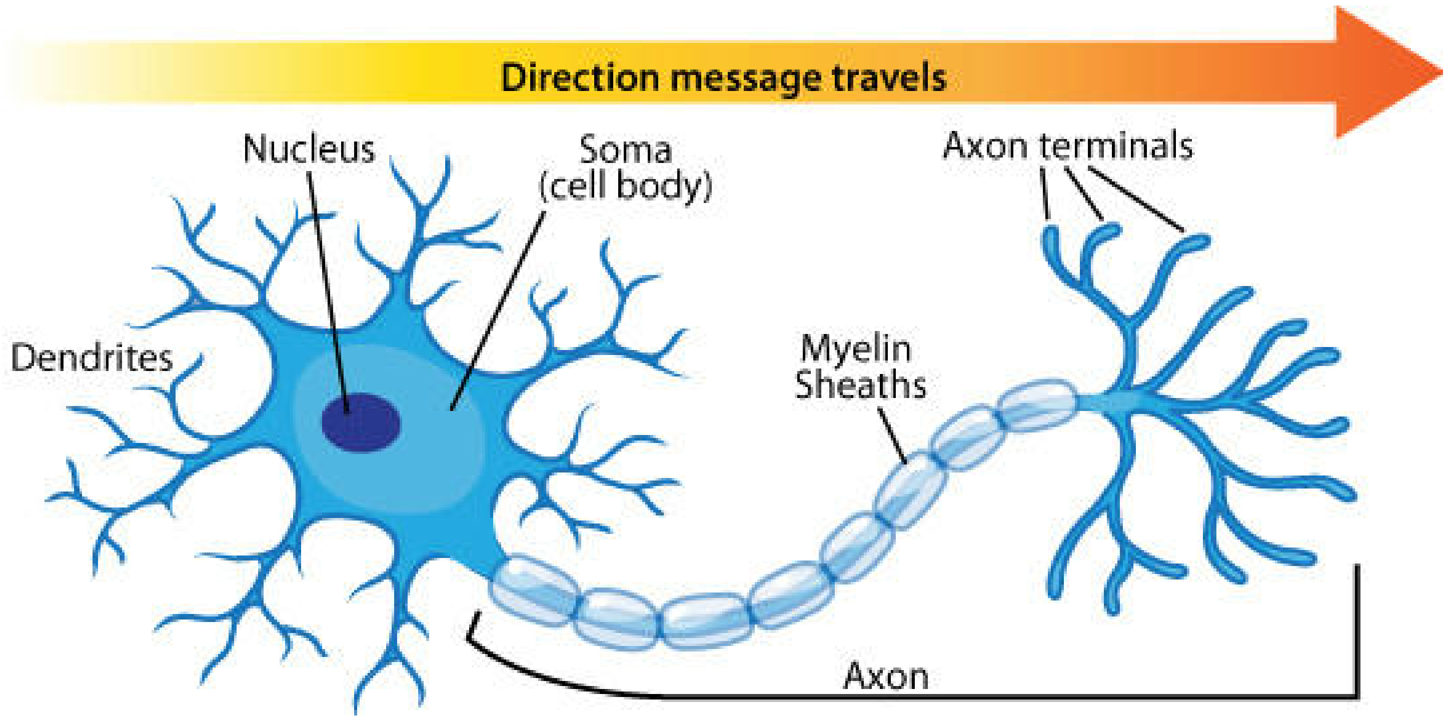
The axon outputs an electrical signal to other neurons



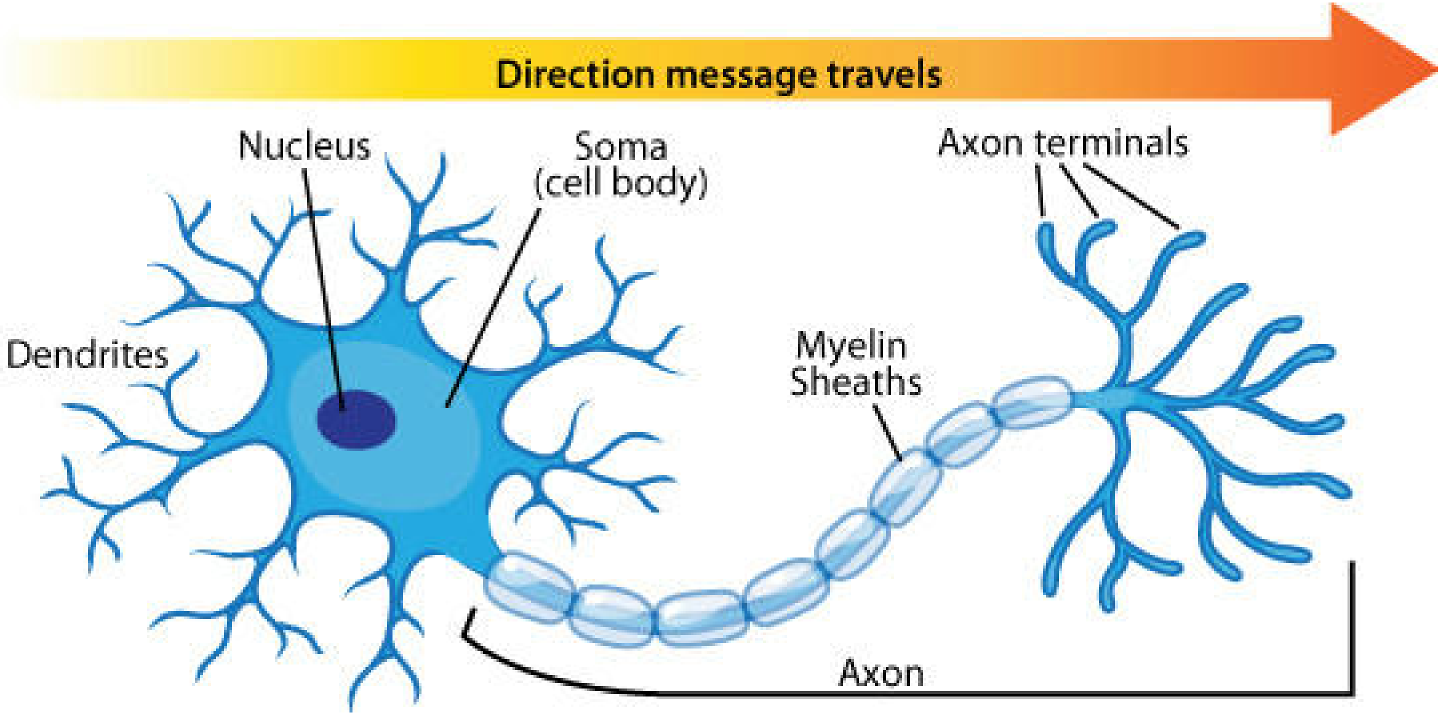
The axon terminals will connect to dendrites of other neurons



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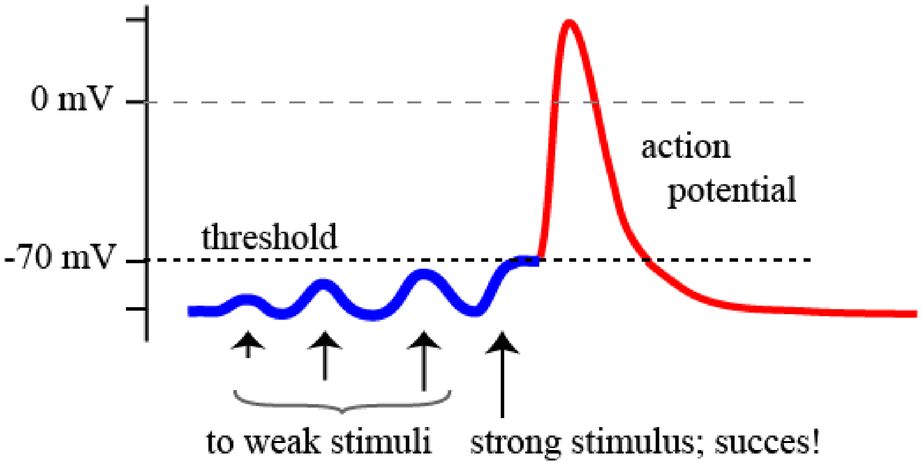
Incoming impulses (via dendrites) change the electric potential of the neuron



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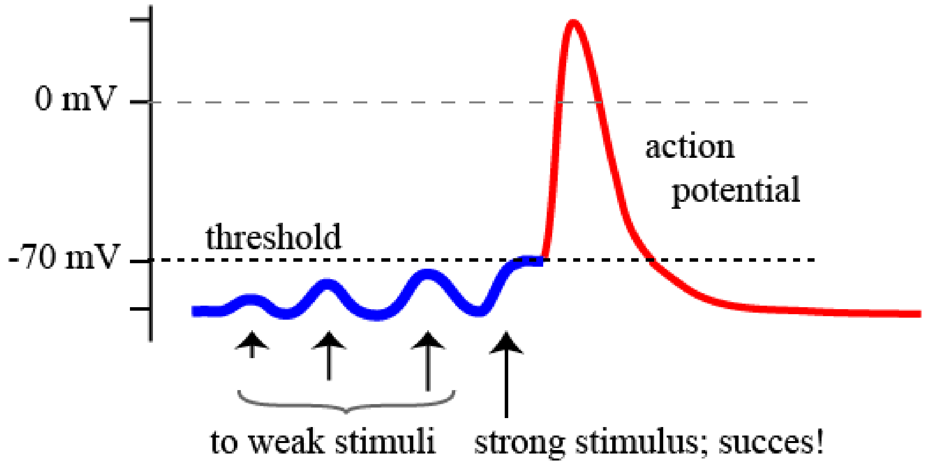

Recall that in a parallel circuit, we can sum voltages together

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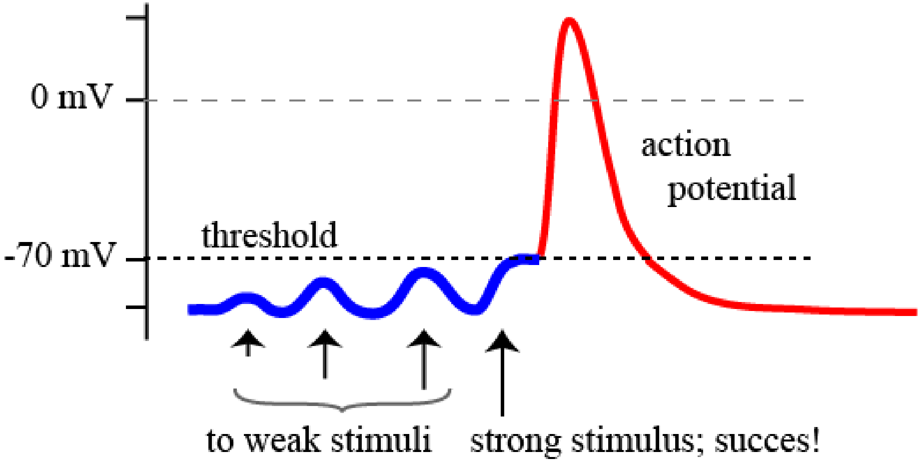
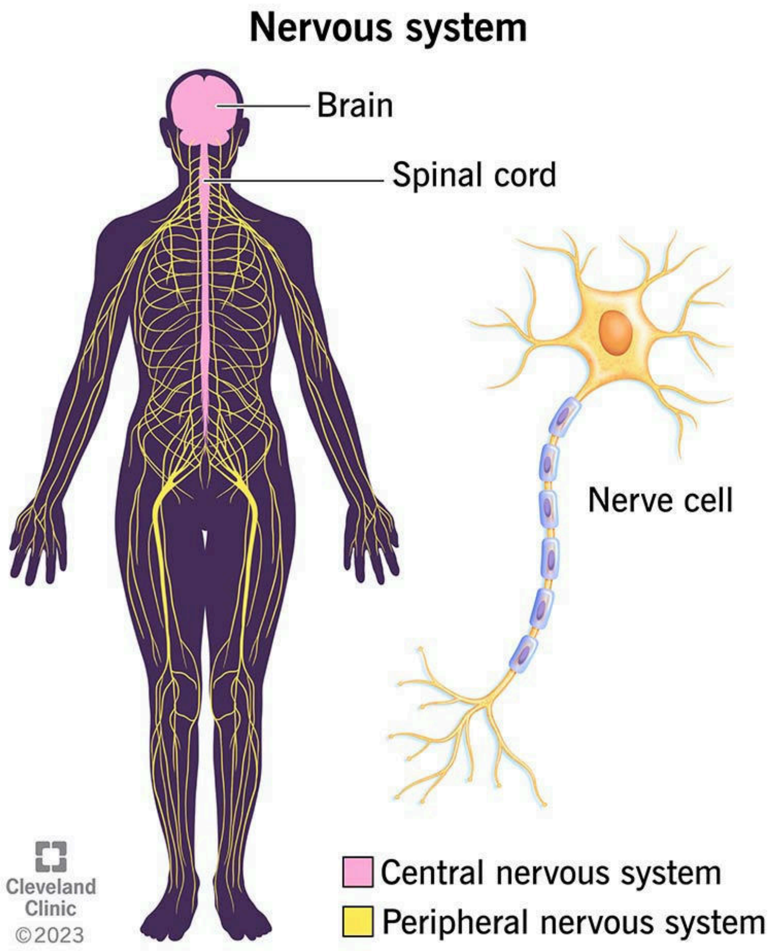


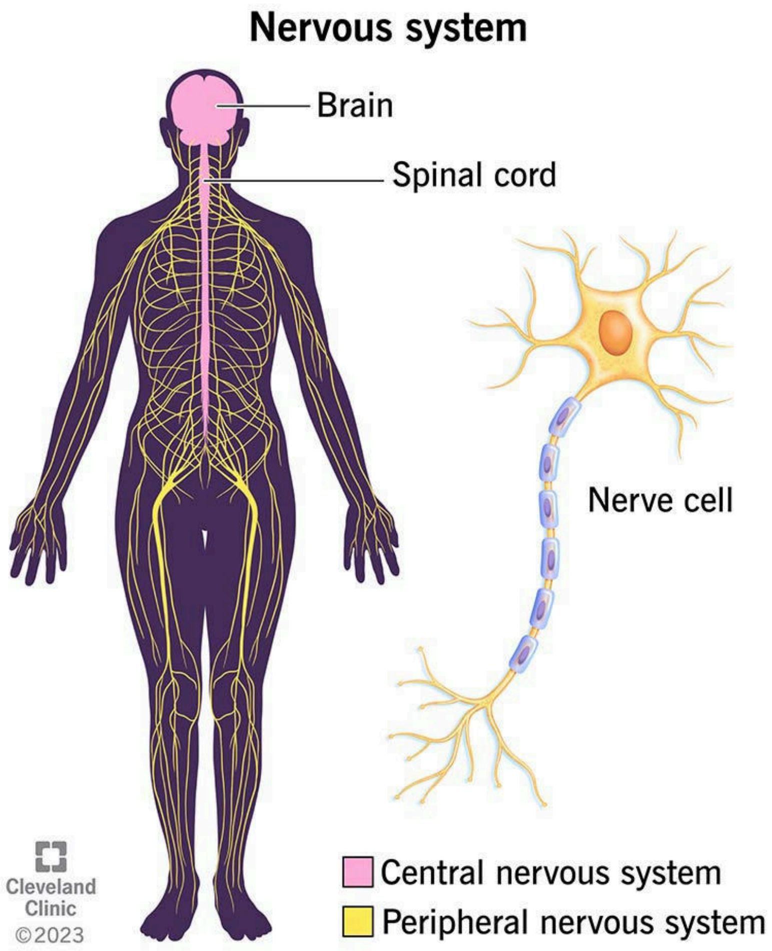
Recall that in a parallel circuit, we can sum voltages together

Many active dendrites will add together and trigger an impulse

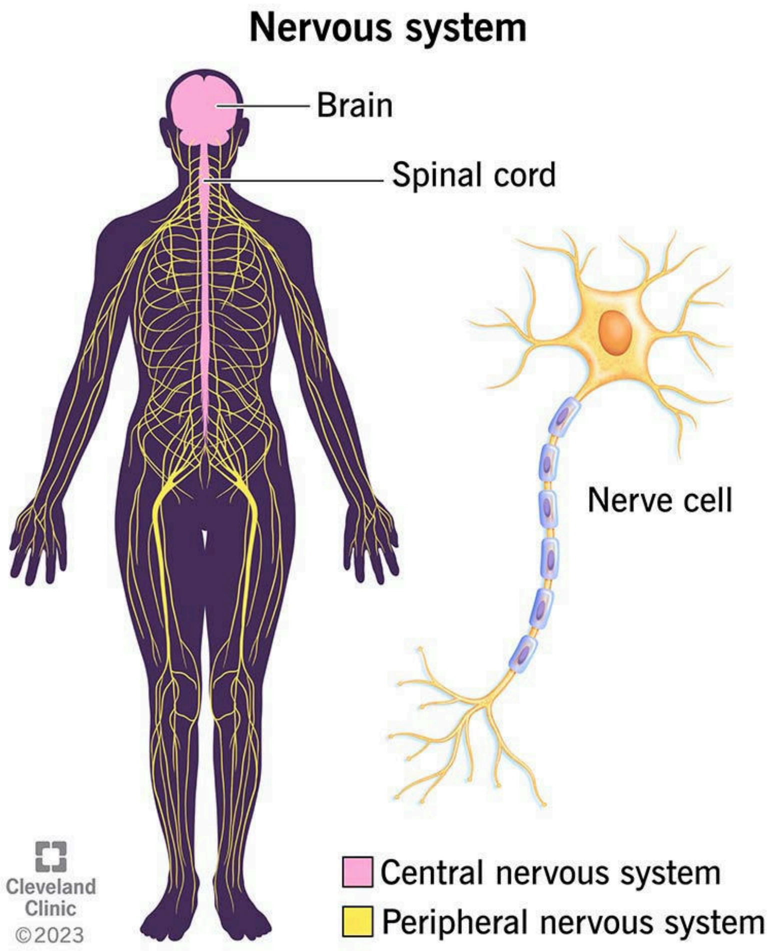
Pain triggers initial nerve impulse, starts a chain reaction into the brain



When the signal reaches the brain, we will think



After thinking, we will take action



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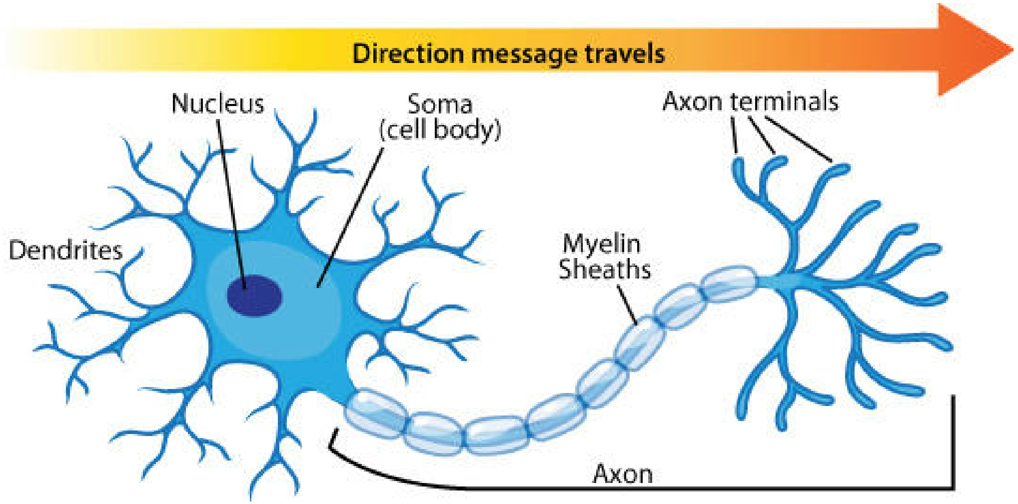
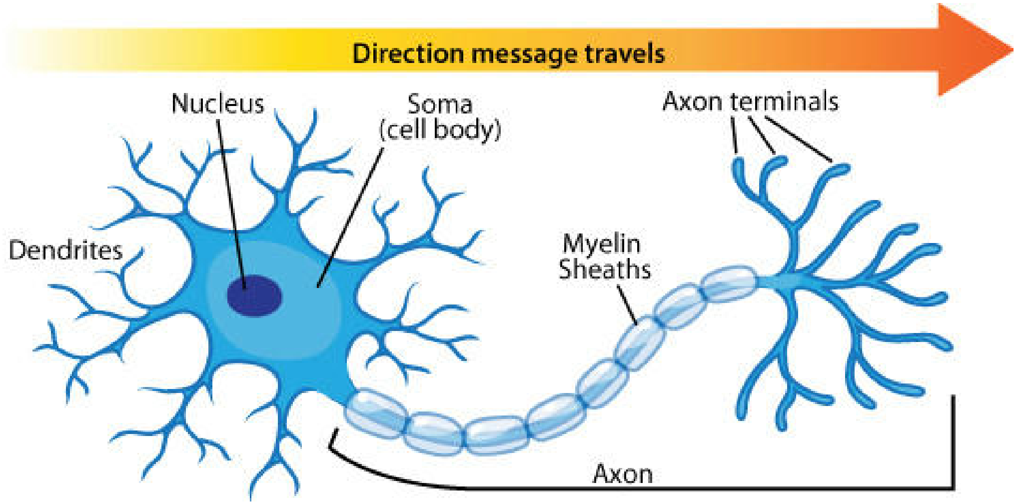
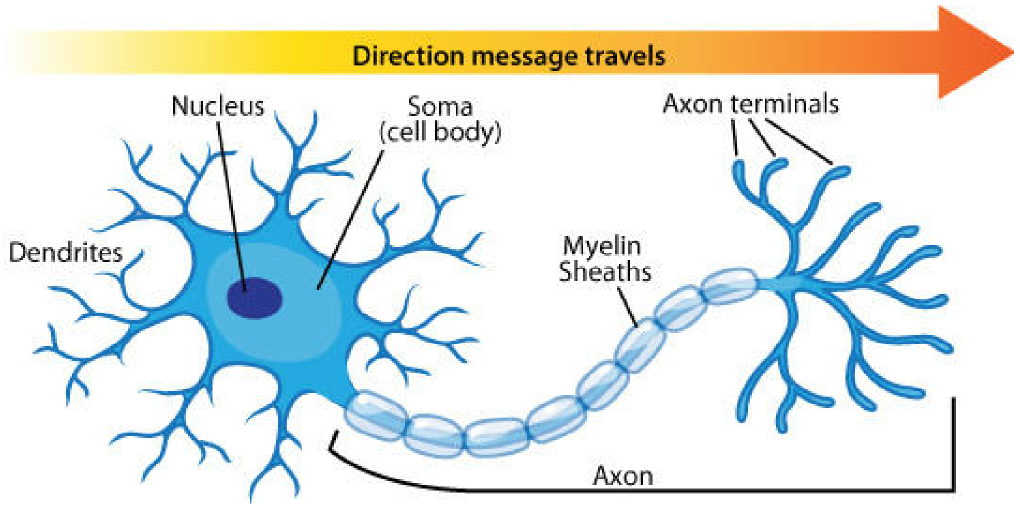


Direction message travels
Nucleus
Soma
(cell body)
Axon terminals
Dendrites
Myelin
Sheaths
Axon



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



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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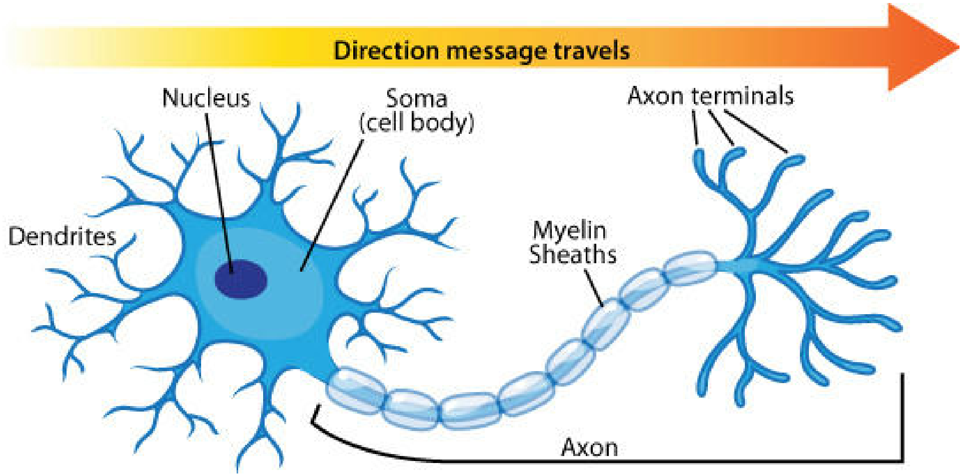

Neuron has a structure of dendrites

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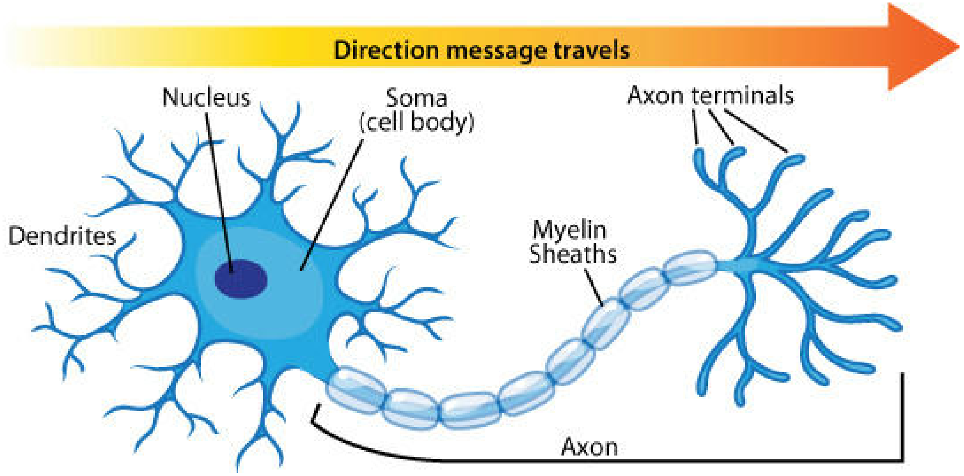
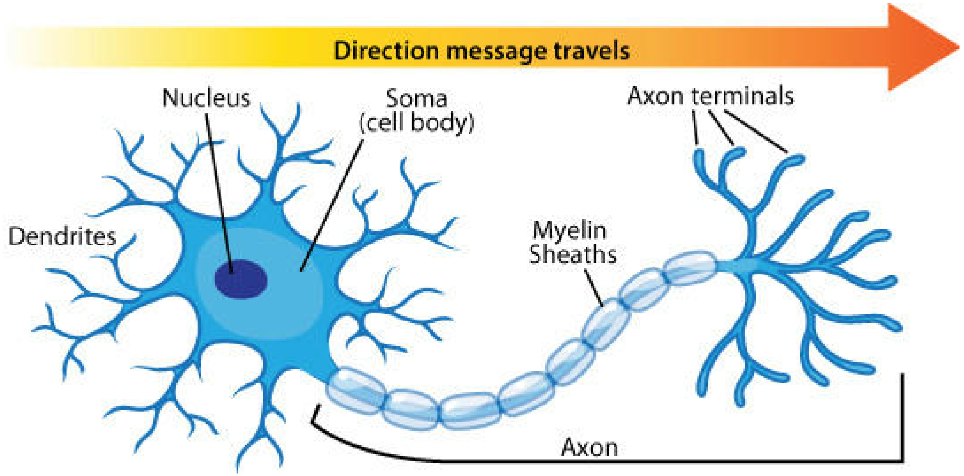


Neuron has a structure of dendrites

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

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

Let us implement an artifical neuron as a function



Each incoming dendrite has some voltage potential

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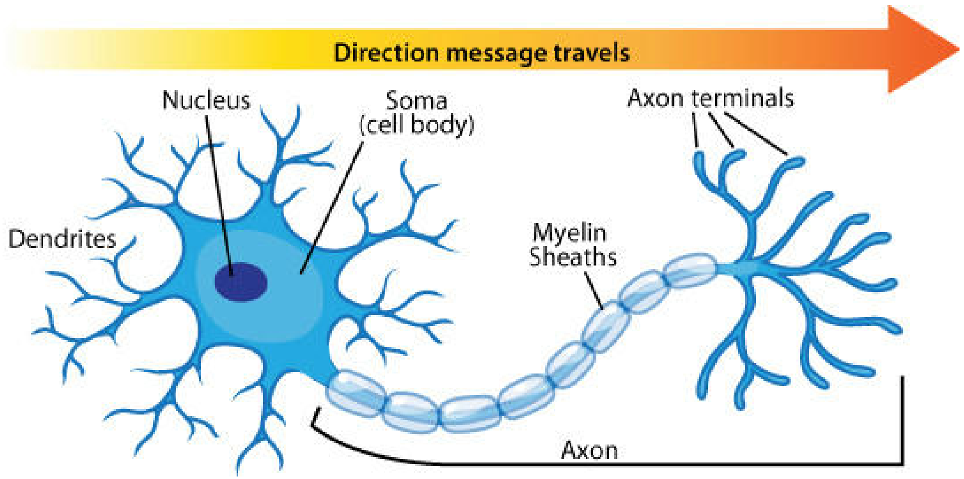

Each incoming dendrite has some voltage potential

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

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

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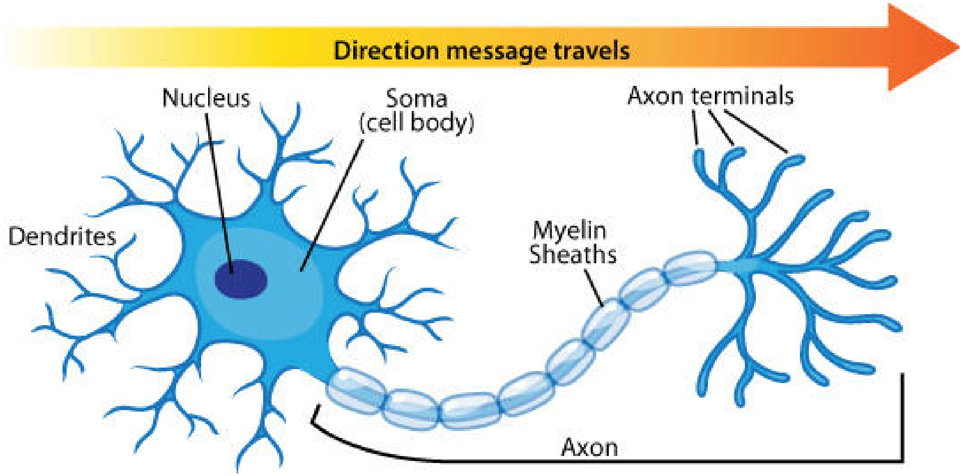

Voltage potentials sum together to give us the voltage in the cell body

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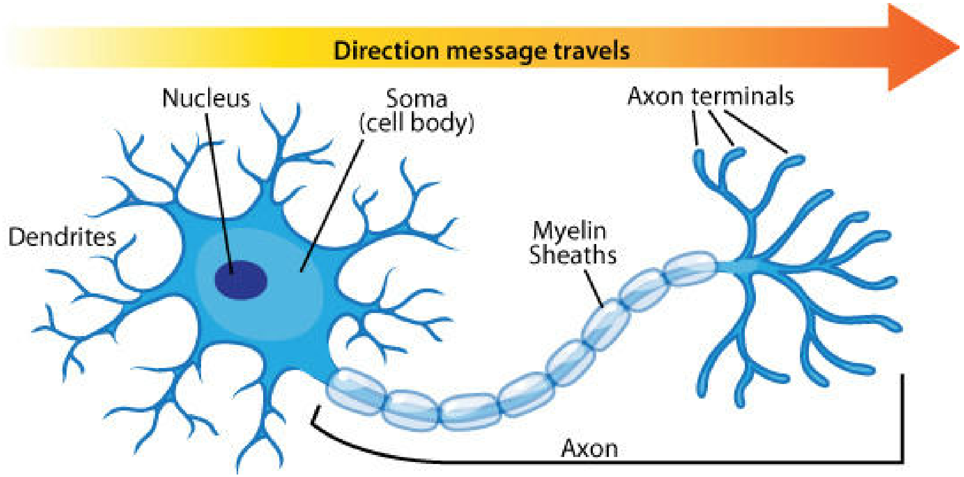

Voltage potentials sum together to give us the voltage in the cell body

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

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

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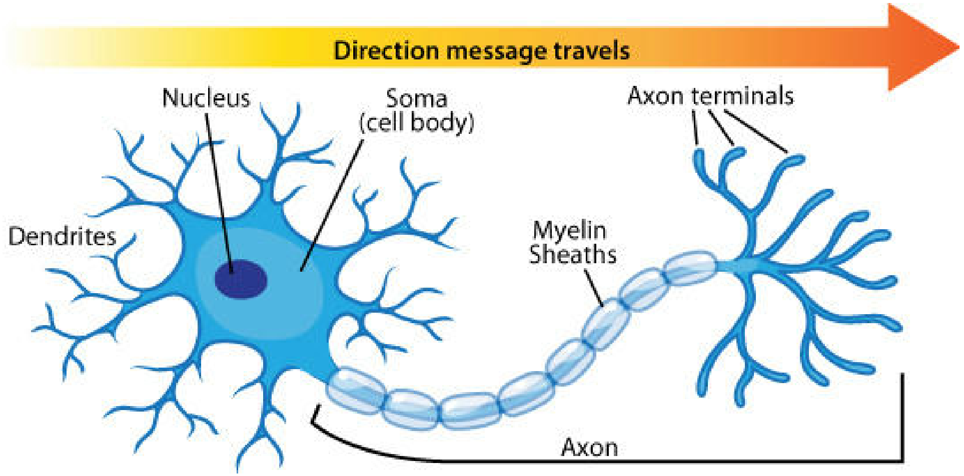

The axon fires only if the voltage is over a threshold

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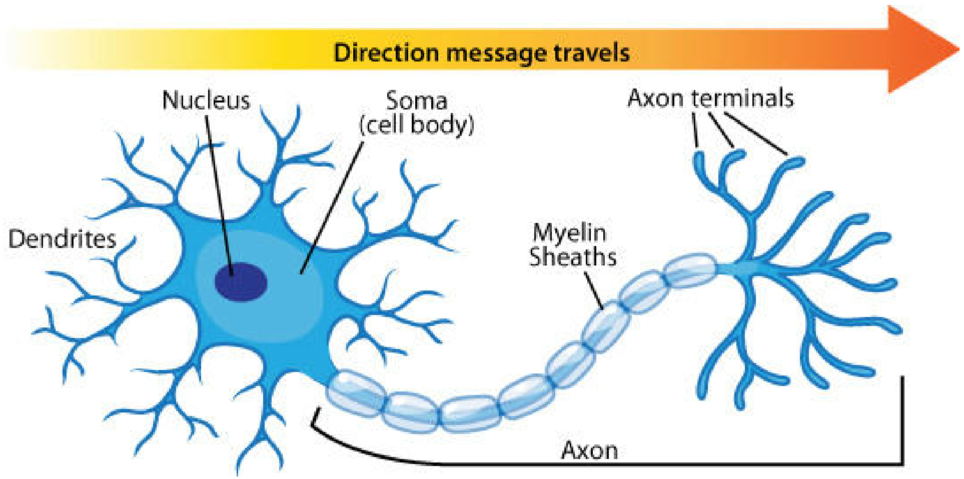

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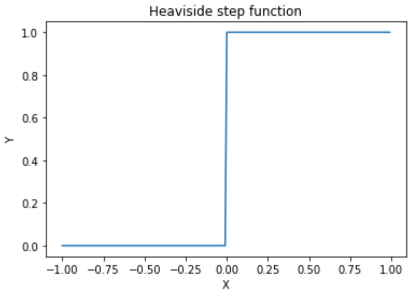
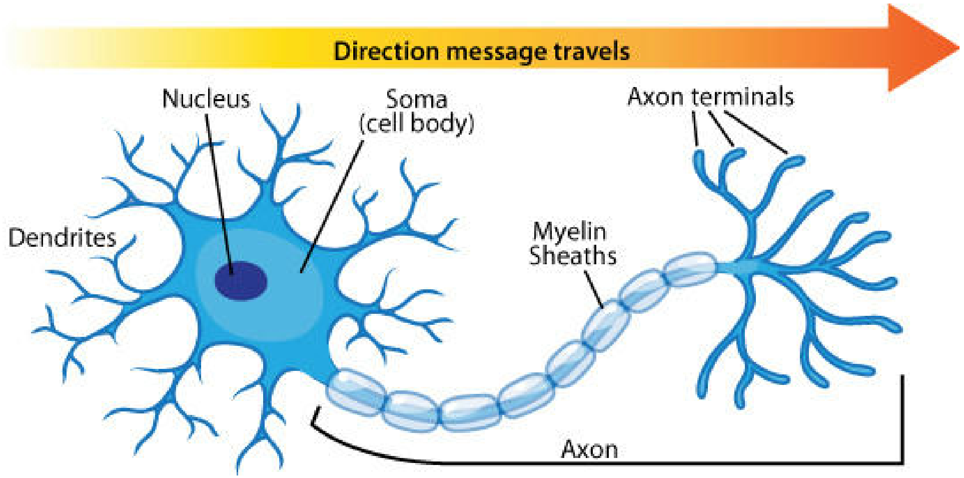
$$\sigma(x) =$$



Let us implement an artifical neuron as a function



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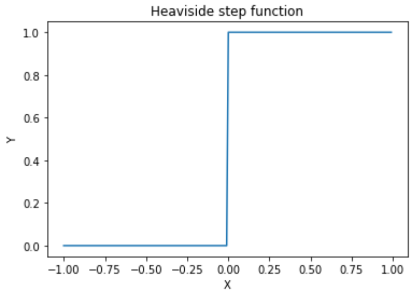
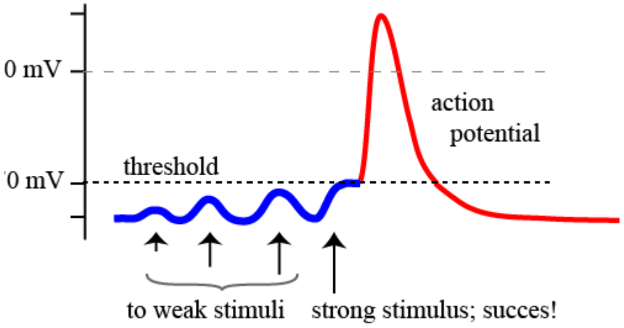
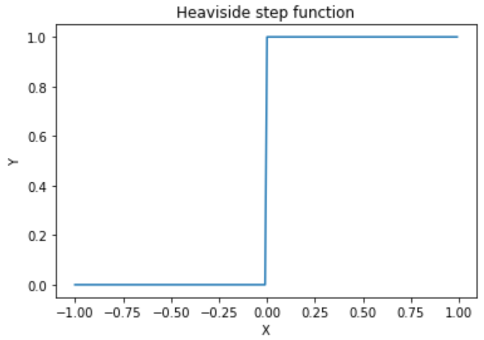


$$f\left(\begin{bmatrix} x_1 \\ \vdots \\ x_n \end{bmatrix}, \begin{bmatrix} \theta_1 \\ \vdots \\ \theta_n \end{bmatrix}\right) = \sigma\left(\sum_{j=1}^{d_x} x_j \theta_j\right)$$

Maybe we want to vary the activation threshold





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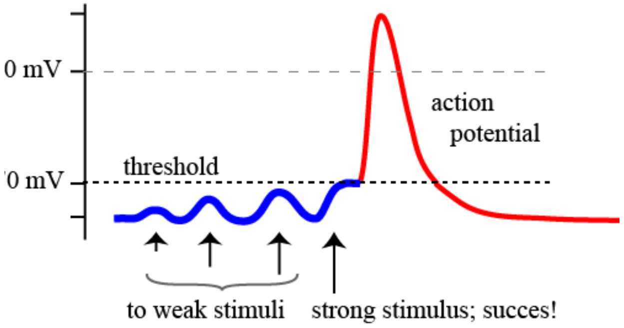

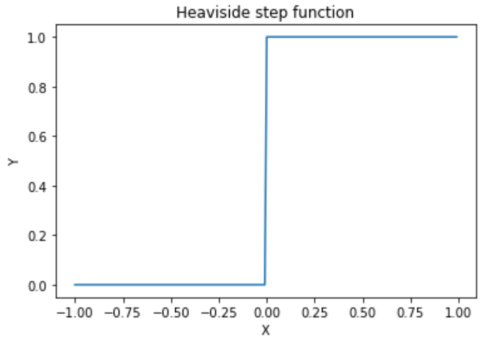

$$f\left(\begin{bmatrix} x_1 \\ \vdots \\ x_{d_x} \end{bmatrix}, \begin{bmatrix} \theta_0 \\ \theta_1 \\ \vdots \\ \theta_{d_x} \end{bmatrix}\right) = \sigma\left(\theta_0 + \sum_{j=1}^{d_x} \theta_j x_j\right)$$

$$f(\boldsymbol{x}, \boldsymbol{\theta}) = \theta_0 + \boldsymbol{\theta}_{1:d_x}^\top \boldsymbol{x}$$

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Let us write out the full equation for a neuron

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

$$f(\boldsymbol{x}, \boldsymbol{\theta}) = \theta_0 + \boldsymbol{\theta}_{1:d_x}^\top \boldsymbol{x}$$

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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!

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

We model a neuron using a linear model and activation function

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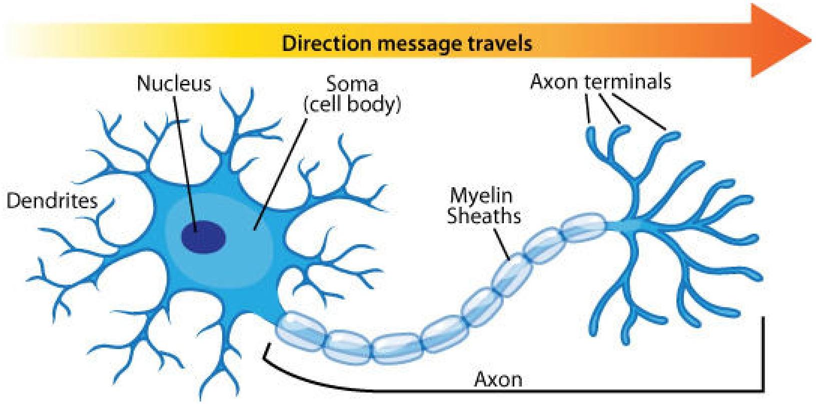

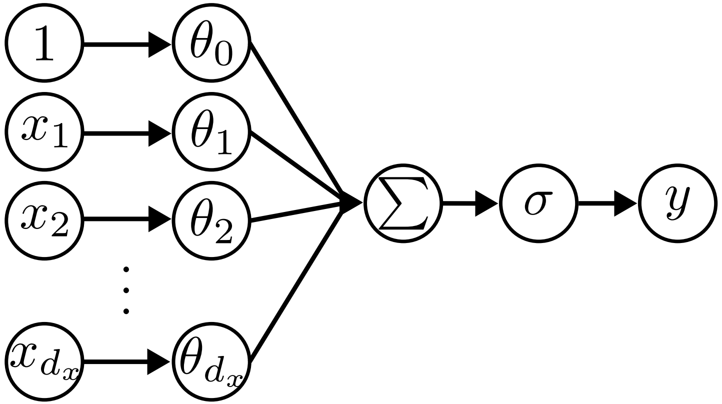

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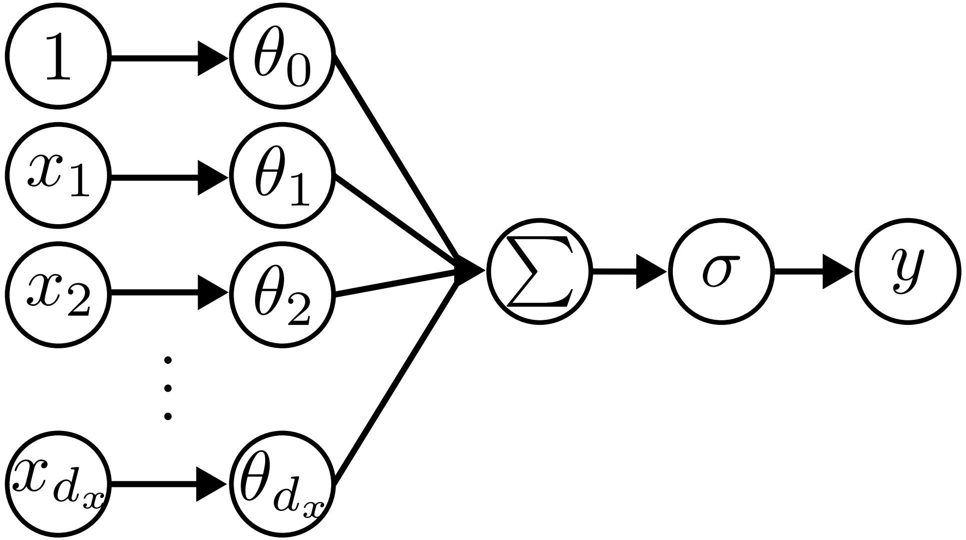
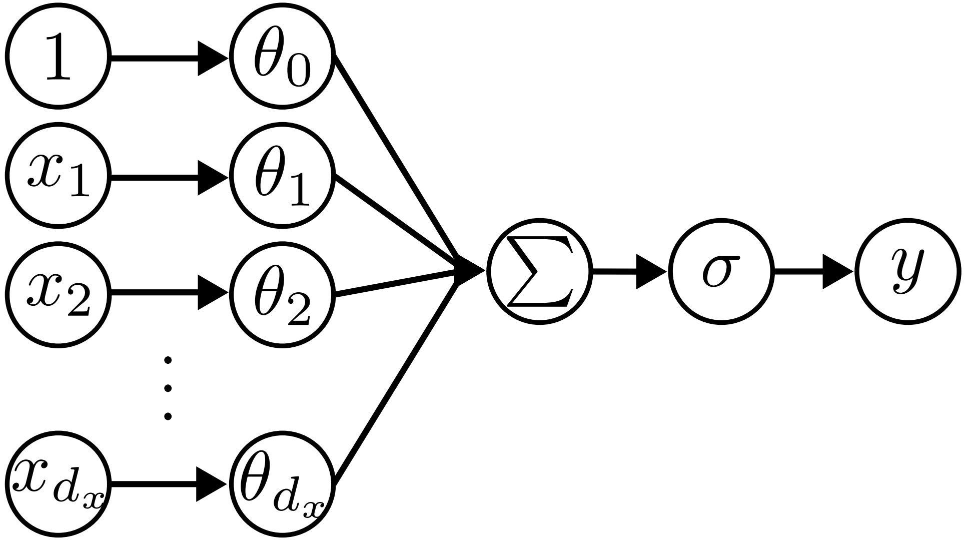
$$\boldsymbol{\theta} = \begin{bmatrix} b \\ \boldsymbol{w} \end{bmatrix}; \quad \begin{bmatrix} \theta_0 \\ \theta_1 \\ \vdots \\ \theta_{d_x} \end{bmatrix} = \begin{bmatrix} b \\ w_1 \\ \vdots \\ w_{d_x} \end{bmatrix}$$

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

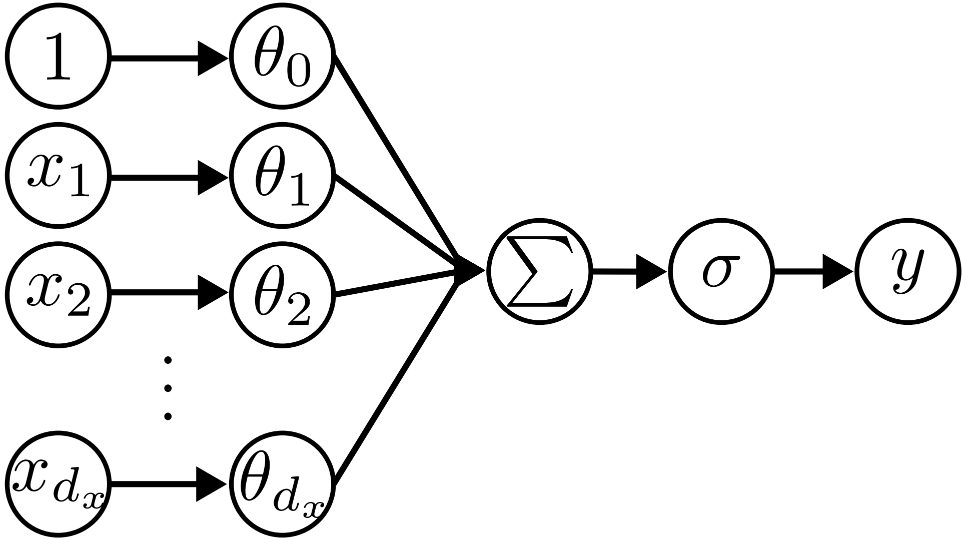
Relax



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

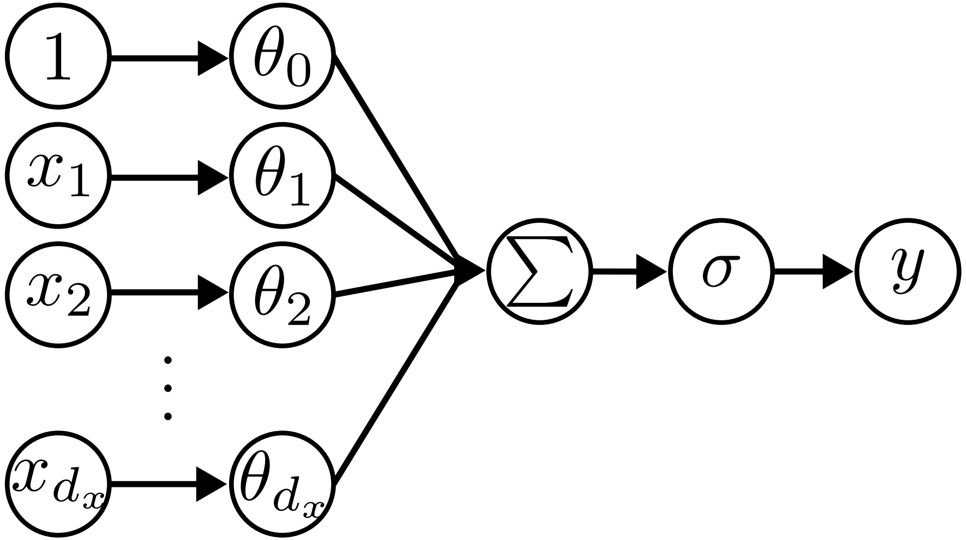


Recall that in machine learning we deal with functions



Recall that in machine learning we deal with functions

What kinds of functions can our neuron represent?

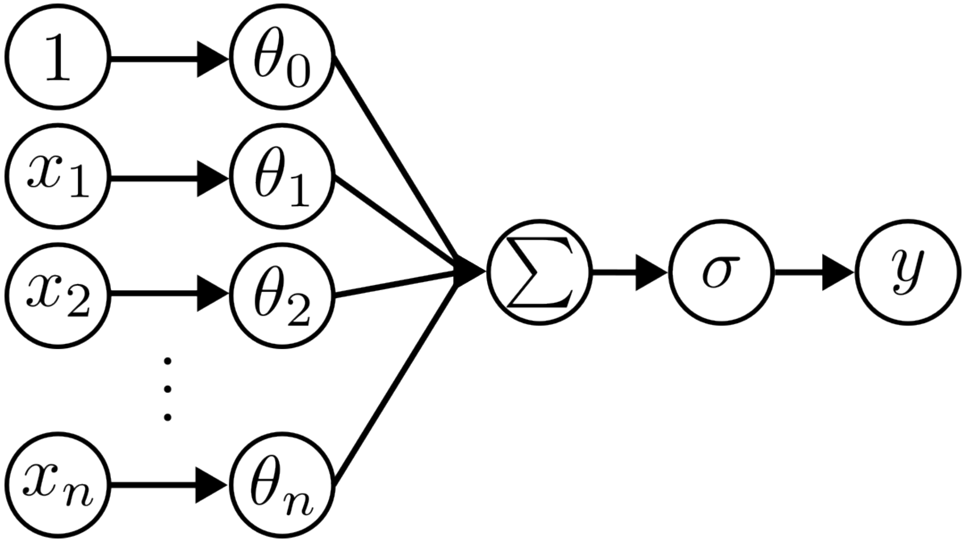


Recall that in machine learning we deal with functions

What kinds of functions can our neuron represent?

Let us start with a logical AND function

Recall the activation function (Heaviside step)



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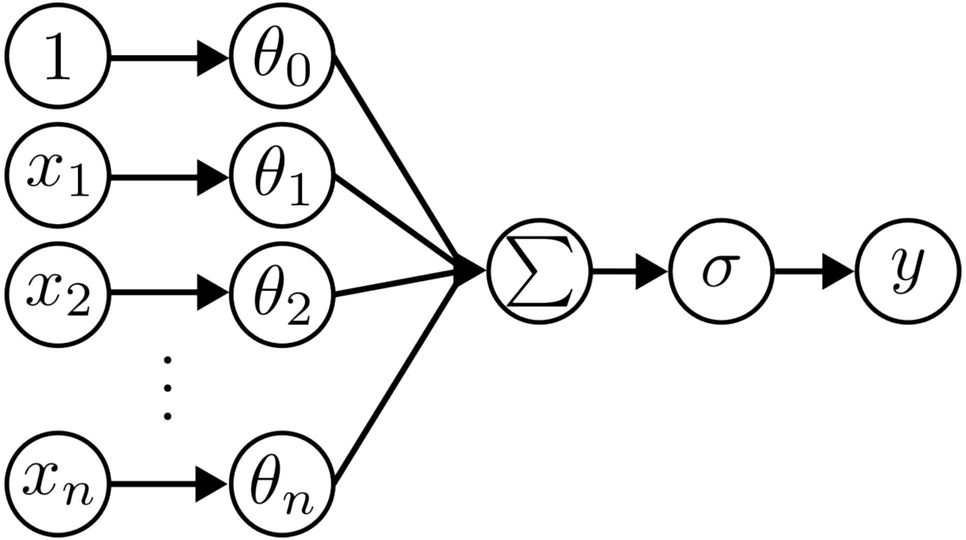

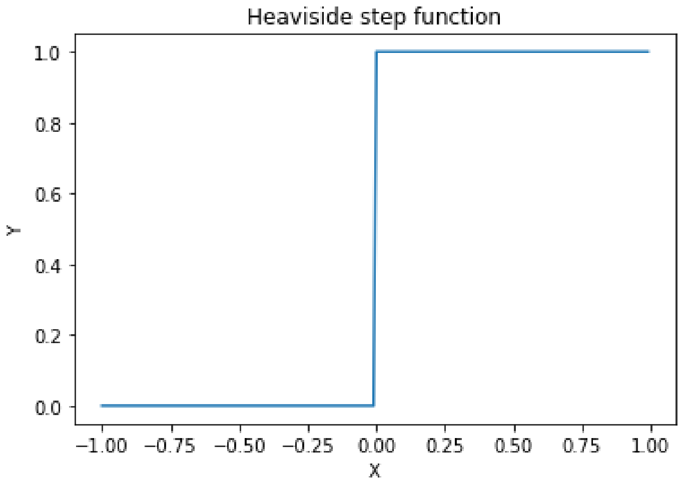

$$H(x) = \begin{cases} 1 \text{ if } x > 0 \\ 0 \text{ if } x \leq 0 \end{cases}$$

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

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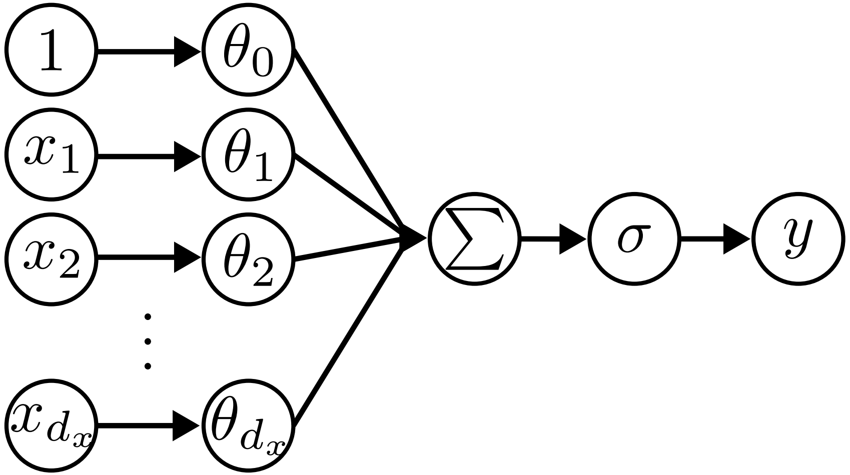
Let us think back to biology, maybe it has an answer

Brain: Biological neurons $\rightarrow$ Biological neural network

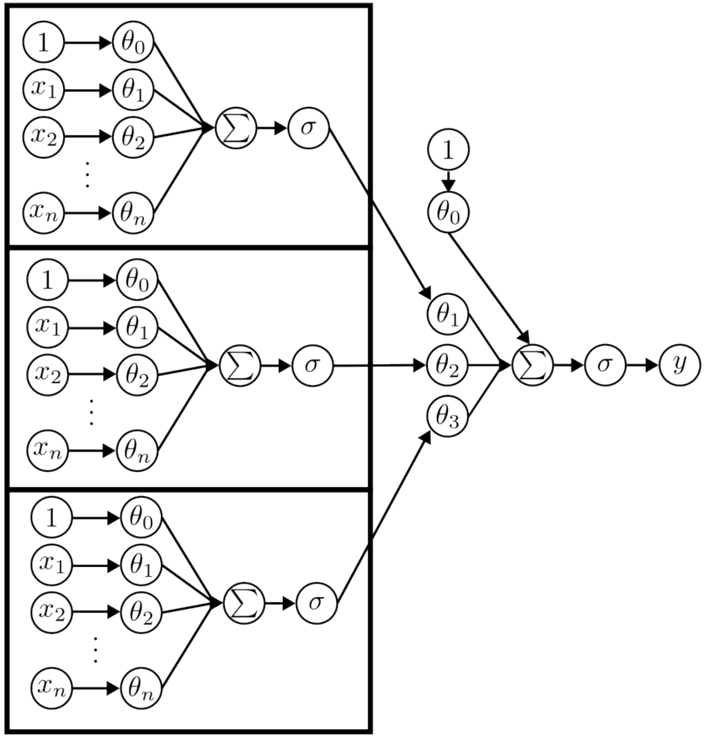
Brain: Biological neurons $\to$ Biological neural network

Computer: Artificial neurons $\to$ Artificial neural network

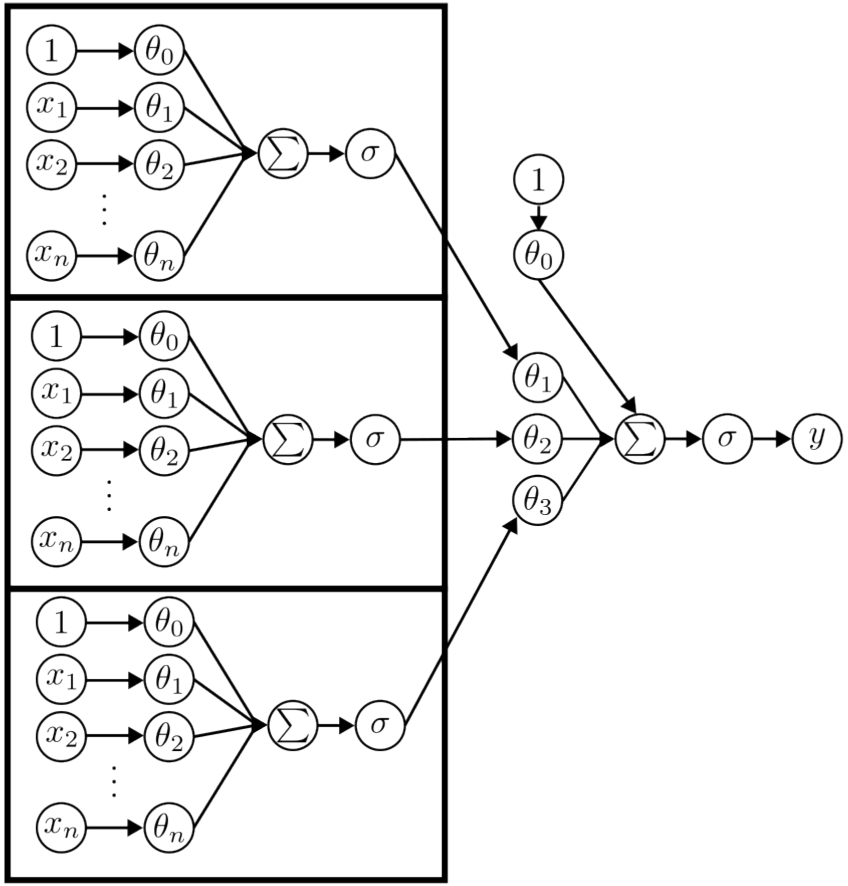
Connect artificial neurons into a network



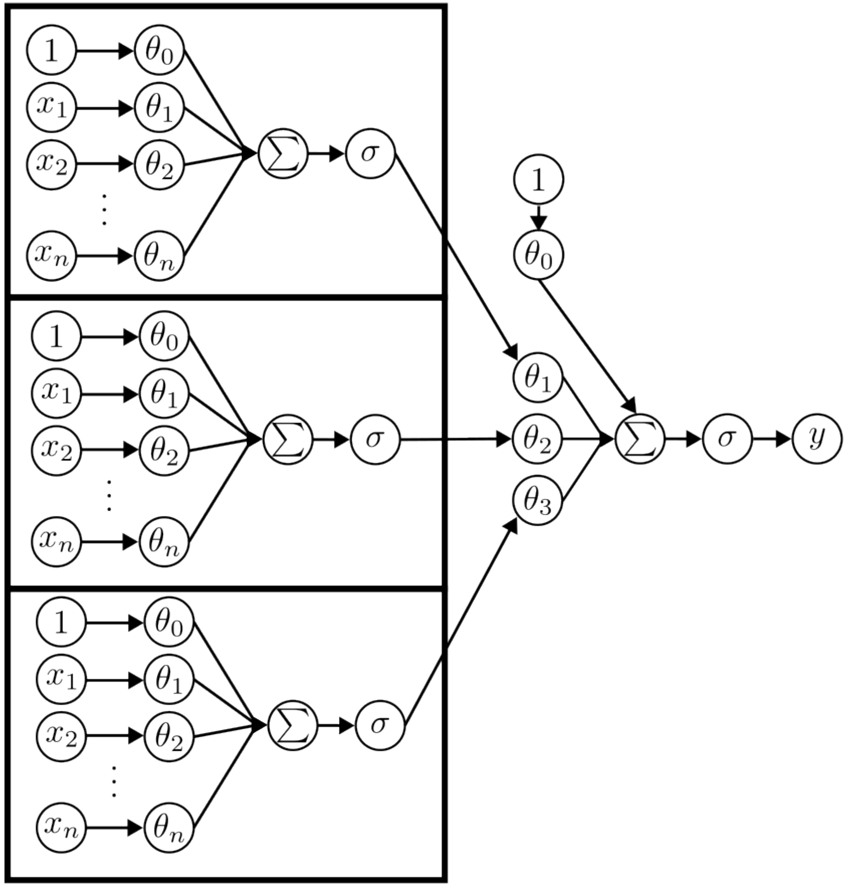
Neuron



Neural Network



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



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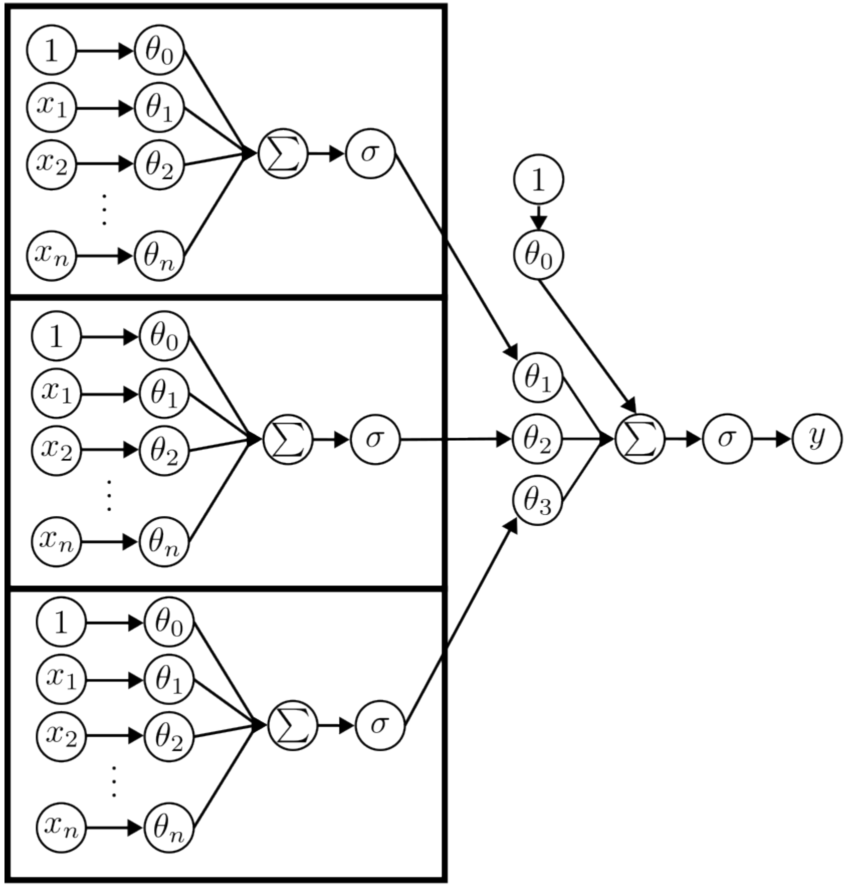
Adding neurons in **series** creates a **deep** neural network



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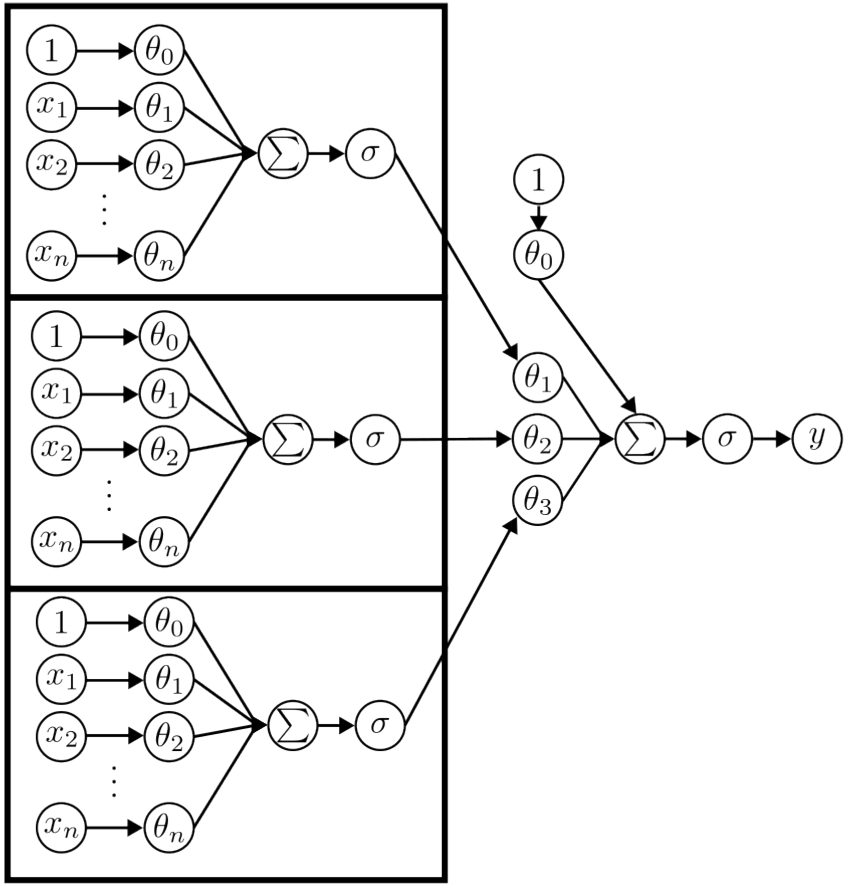
Today's powerful neural networks are both **wide** and **deep**



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

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. Perceptron
10. Multilayer Perceptron

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

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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 $\boldsymbol{\theta}, \boldsymbol{\psi}, \boldsymbol{\rho}$

$$f_1(\boldsymbol{x}, \boldsymbol{\theta}) = \boldsymbol{\theta}_{\cdot,0} + \boldsymbol{\theta}_{\cdot,1:n} \boldsymbol{x} \quad f_2(\boldsymbol{x}, \boldsymbol{\psi}) = \boldsymbol{\psi}_{\cdot,0} + \boldsymbol{\psi}_{\cdot,1:n} \boldsymbol{x} \quad \dots \quad f_\ell(\boldsymbol{x}, \boldsymbol{\rho}) = \boldsymbol{\rho}_{\cdot,0} + \boldsymbol{\rho}_{\cdot,1:n} \boldsymbol{x}$$

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

Written more plainly as

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

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$$\vdots$$

$$\boldsymbol{y} = f_\ell(\boldsymbol{x}, \boldsymbol{\rho}) = \boldsymbol{\rho}_{\cdot,0} + \boldsymbol{\rho}_{\cdot,1:n} \boldsymbol{z}_{(d_x)-1}$$

Written more plainly as

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

$$\boldsymbol{z}_2 = f_2(\boldsymbol{z}_{\mathbf{1}}, \psi) = \boldsymbol{\psi}_{\cdot,0} + \boldsymbol{\psi}_{\cdot,1:n}\boldsymbol{z}_1$$

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Implement XOR using a deep and wide neural network

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Implement XOR using a deep and wide neural network

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

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

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$$

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

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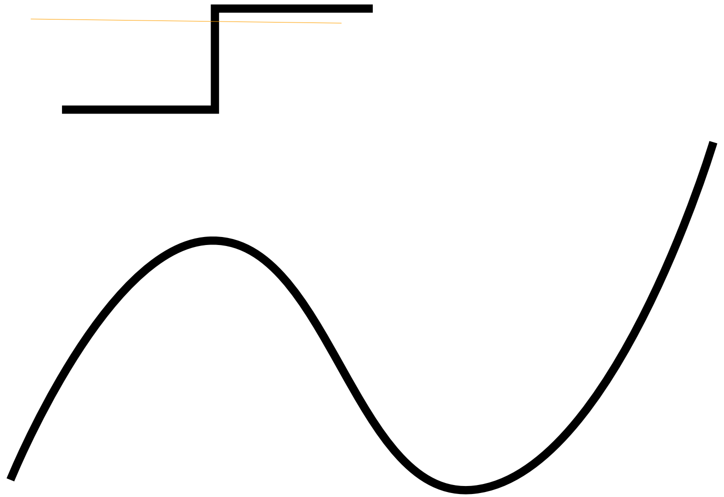

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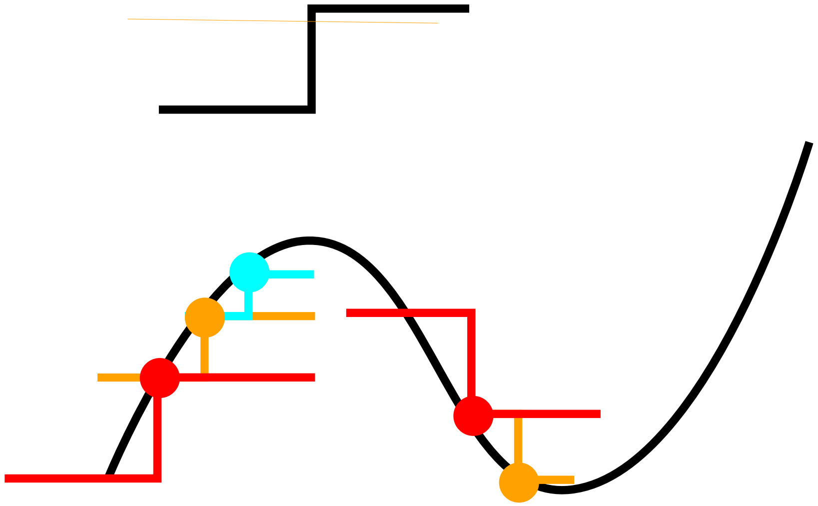

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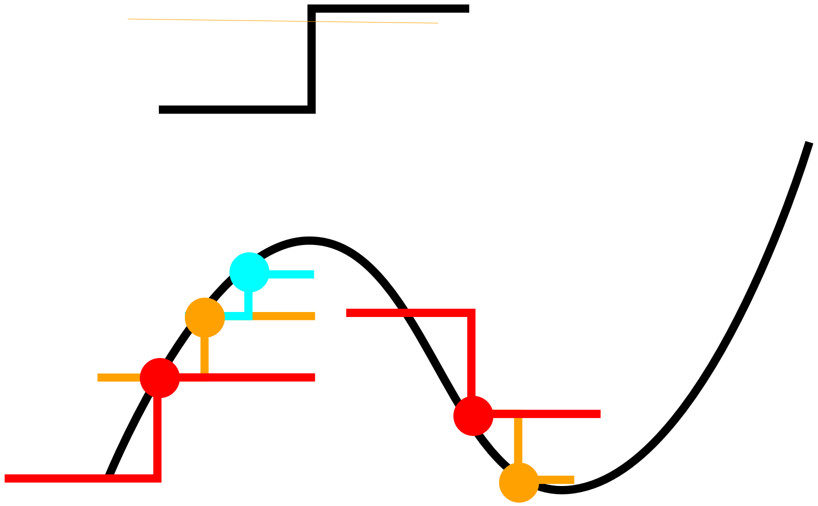

$$\text{Roughly, } \exists \boldsymbol{\theta} \Rightarrow \lim_{n \mapsto \infty} \left[\theta_{2,0} + \theta_{2,1} \sum_{j=1}^{n} \sigma\left(\theta_{1,0} + \theta_{1,j} x\right) \right] = g(x); \quad \forall g$$

More formally, a wide and deep neural network is a **universal function approximator**

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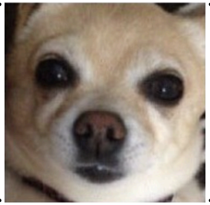
$g\Bigg($  $\Bigg) = \text{Dog}$

$g\Bigg($  $\Bigg) = \text{Muffin}$

Very powerful finding! The basis of deep learning.

All the models we examine in this course will use this neural network structure internally

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Relax

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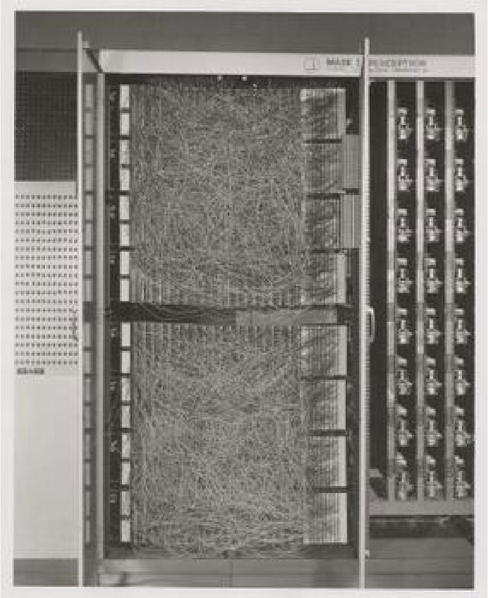
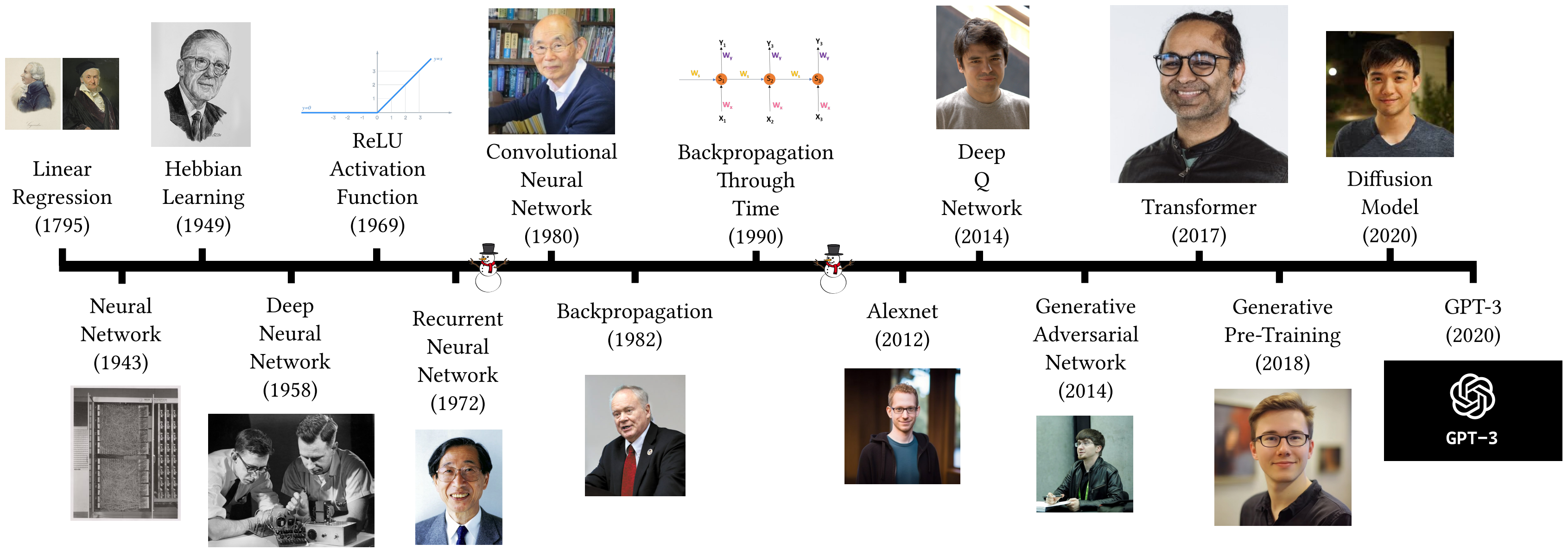
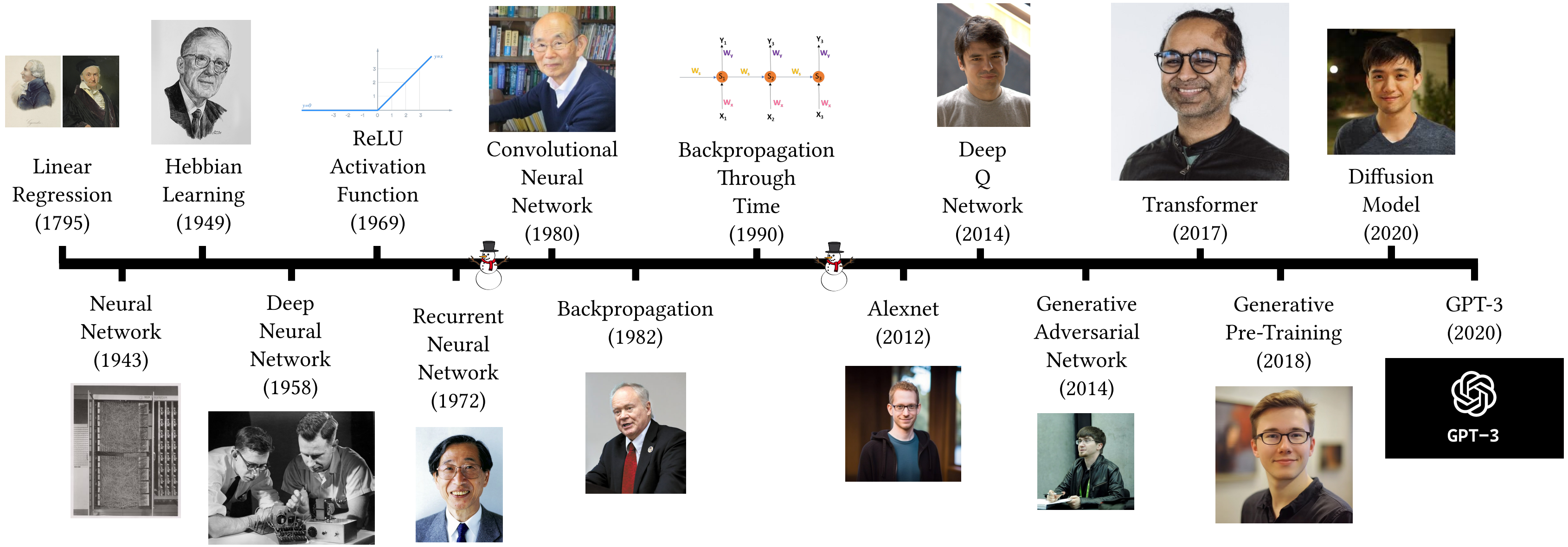


20×20 grid of pixels to process images


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

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

or

$$f(\boldsymbol{x}, (\boldsymbol{b}, \boldsymbol{W})) = \sigma(\boldsymbol{b} + \boldsymbol{W} \boldsymbol{x})$$

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