Neural Networks

CISC 7026: Introduction to Deep Learning

University of Macau

1. We looked at linear and polynomial f
    1. Looked at both classification and regression
    2. They have problems
        1. Input features scale poorly
        2. Bad performance around edges
    3. Neural networks fix many of these problems
    4. What is a neural network?
        1. Draw linear model as neural network
    5. Based on theory of the brain
        1. Invented ages ago
        2. Only recently have we learned to harness them

6. Neuron theory
    1. Connectivity
    2. Activation function
7. Parallels between real/artificial neuron
8. Matrix/graph duality
9. Single layer perceptron
10. Issues with one layer
    1. Not universal function approximator
11. Backprops
    1. Provides a way to train nn
        1. Assigns “fault” for each neuron

2. Recall closed form for linear model
    1. We use the gradient of the linear model
3. We use a similar approach

1. Limitations of linear models
2. History and overview of neural networks
3. Neurons
4. Perceptron
5. Multilayer Perceptron
6. Backpropagation
7. Gradient descent

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

Linear models are useful for simple problems

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Issues with very complex problems

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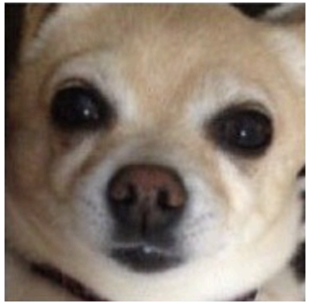
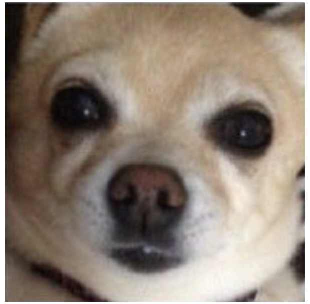


$$256 \times 256 \text{ pixels} = 65536 \text{ pixels}$$



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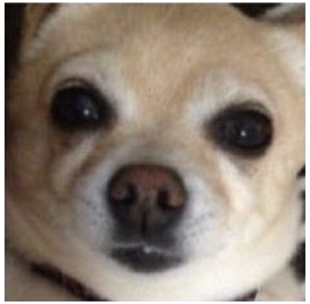
What does the design matrix look like for an n-degree polynomial?



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

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

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

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Polynomial regression scales poorly to high dimensional data

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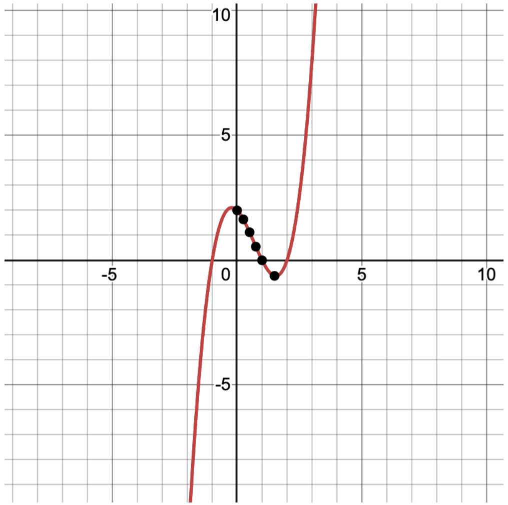

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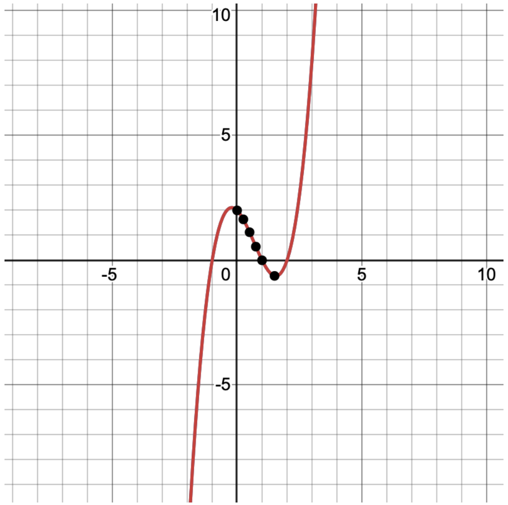

If breed of dog missing from training set, we still want to classify it as dog!

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Relax

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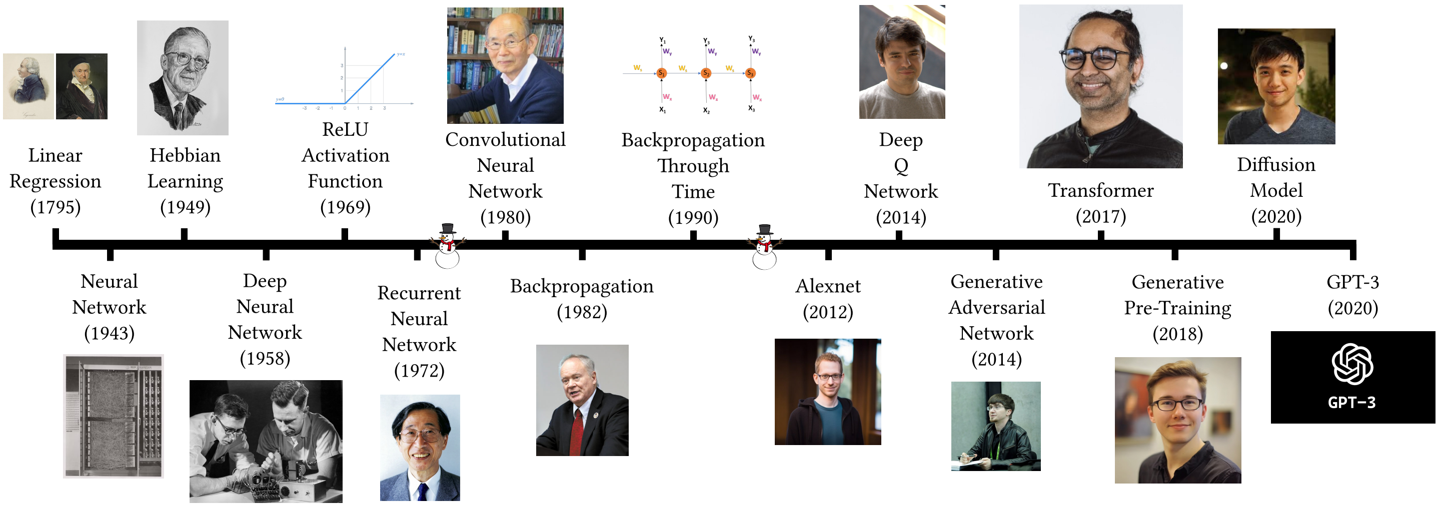

Brain: Biological neurons $\rightarrow$ Biological neural network

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Computer: Artificial neurons $\rightarrow$ Artificial neural network

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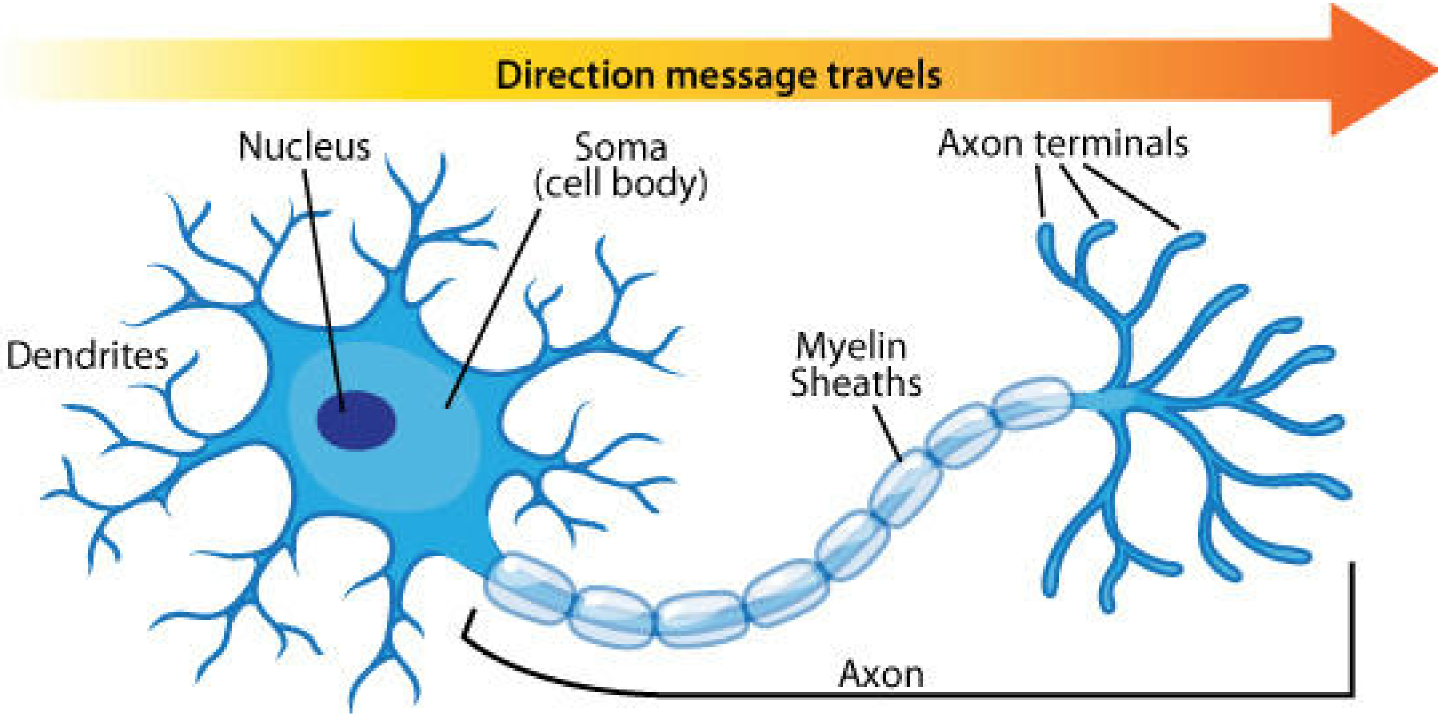

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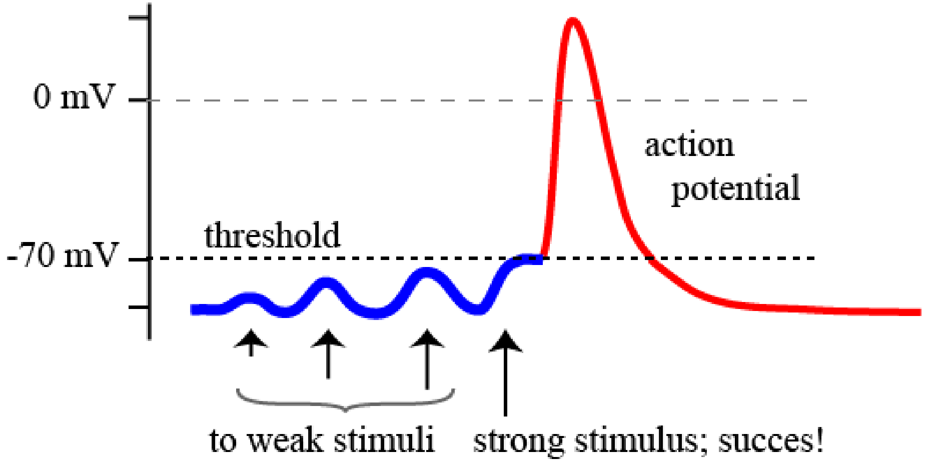

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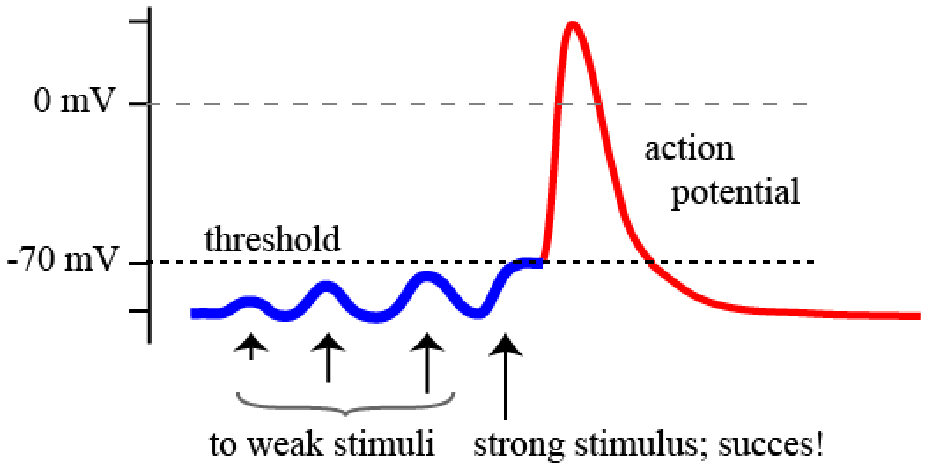
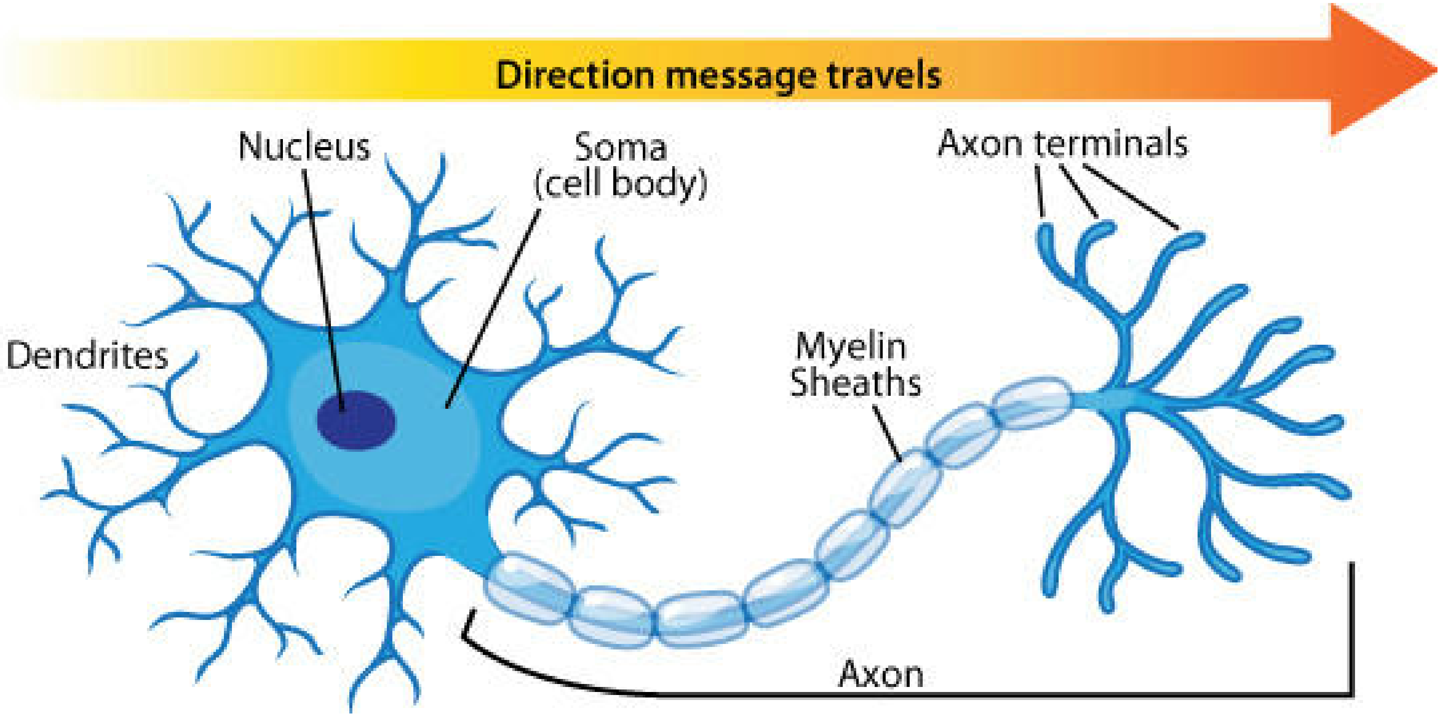
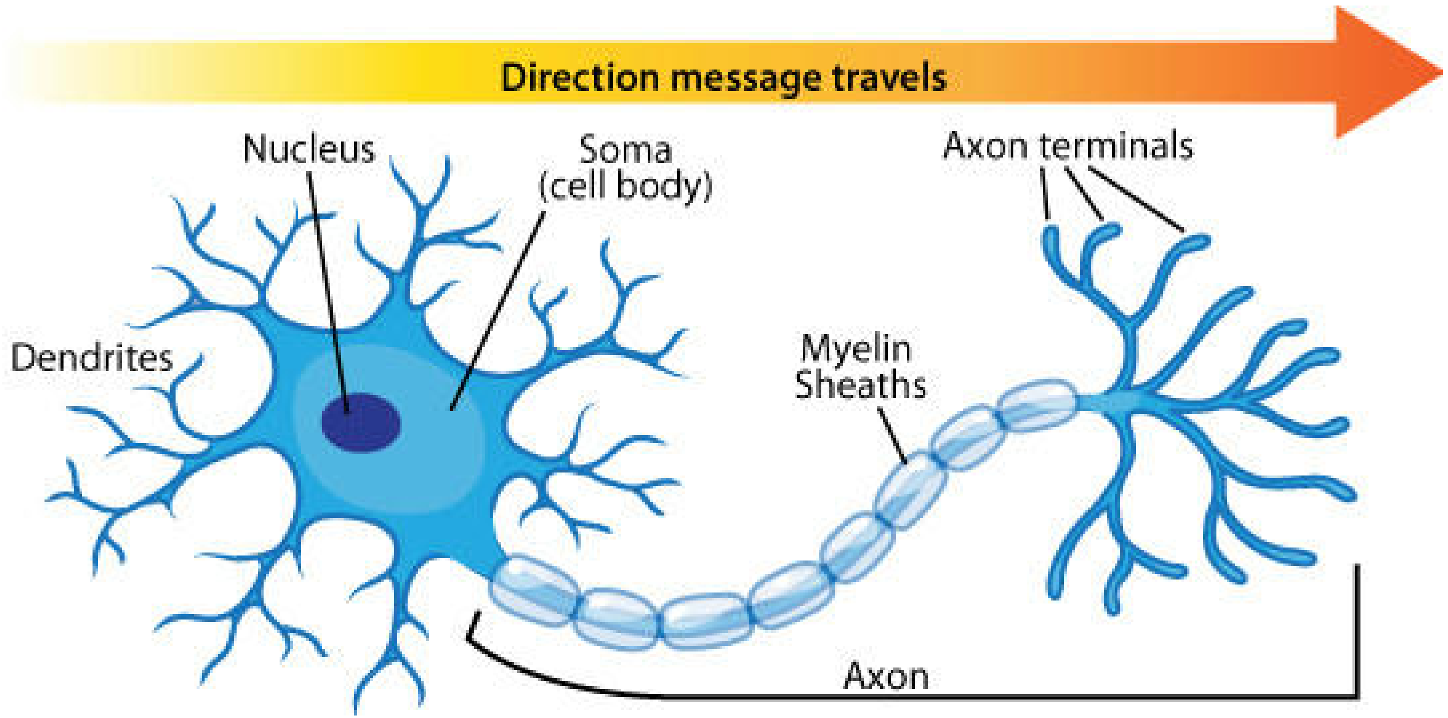


Pain triggers initial nerve impulse, sets of impulse chain into the brain


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



Question: How would you model a neuron mathematically?

Let us define a neuron as a function

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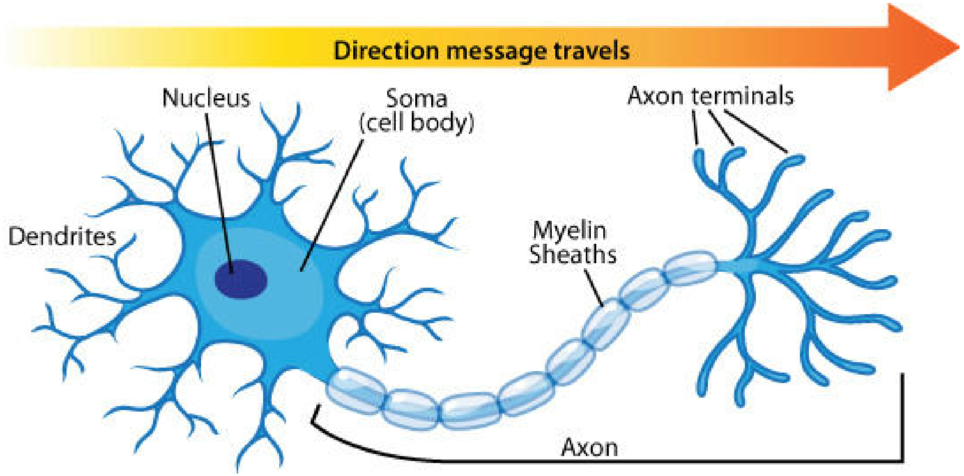

Neuron has a structure of dendrites

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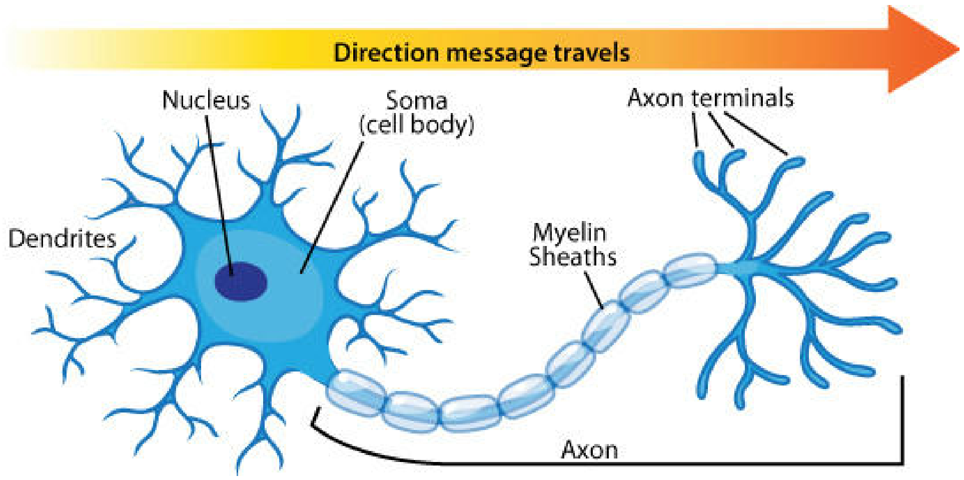

Neuron has a structure of dendrites

$$f\left(\begin{bmatrix}\theta_1 \\ \theta_2 \\ \vdots \\ \theta_n\end{bmatrix}\right) = f\left(\begin{bmatrix}1 \\ 0 \\ \vdots \\ 1\end{bmatrix}\right)$$

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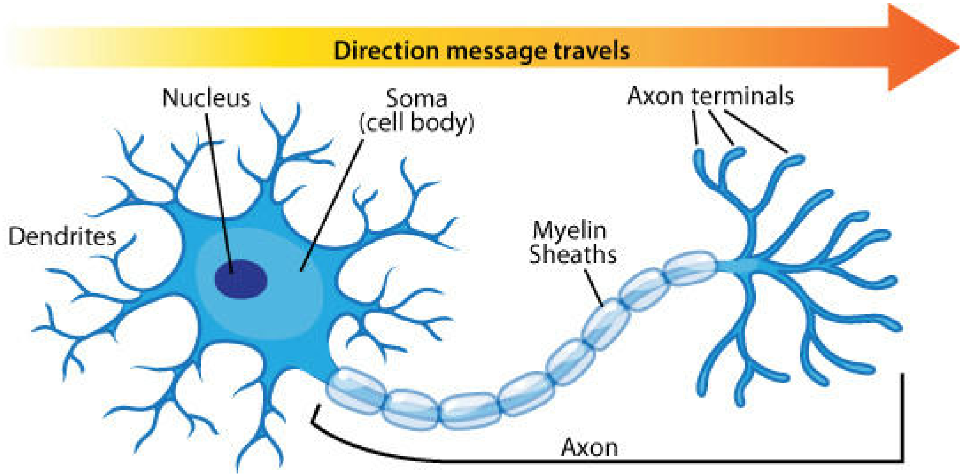

Each incoming dendrite has some voltage potential

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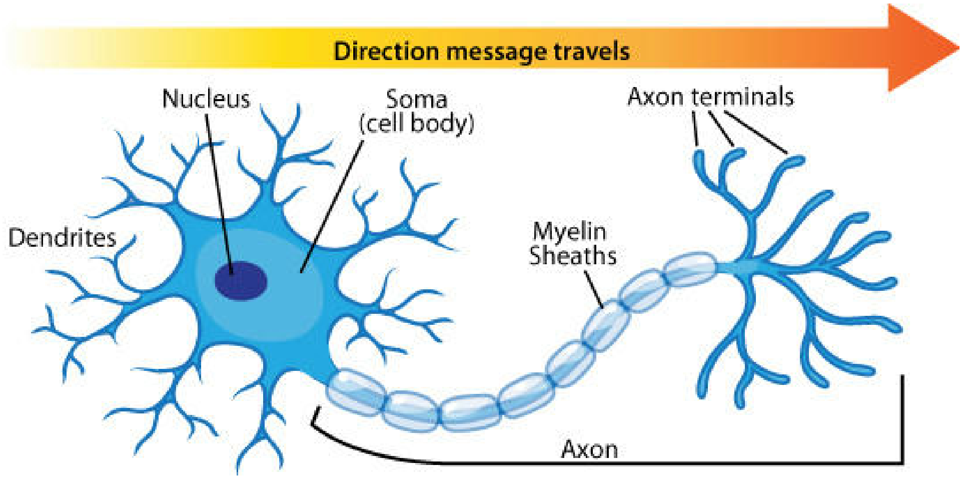

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$$\begin{bmatrix} x_1 \\ \vdots \\ x_n \end{bmatrix} = \begin{bmatrix} 0.5 \\ \vdots \\ -0.3 \end{bmatrix}$$

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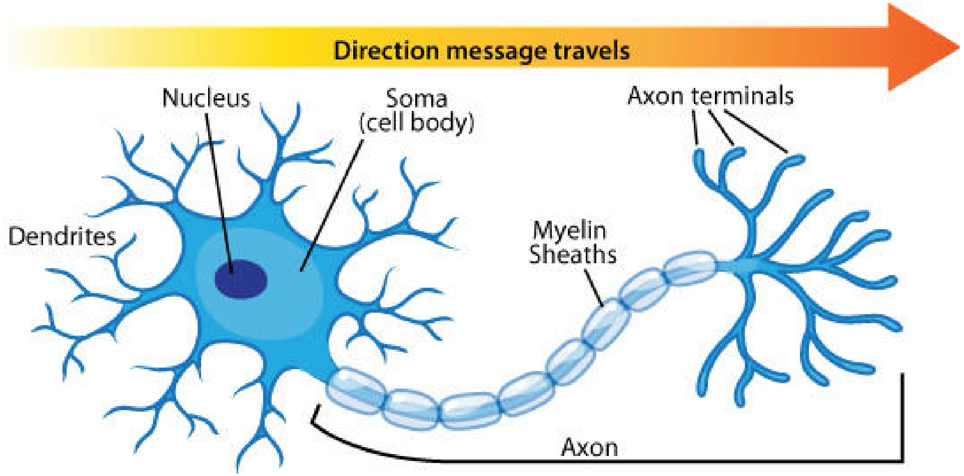

Voltage potentials sum together to give us the voltage in the cell body

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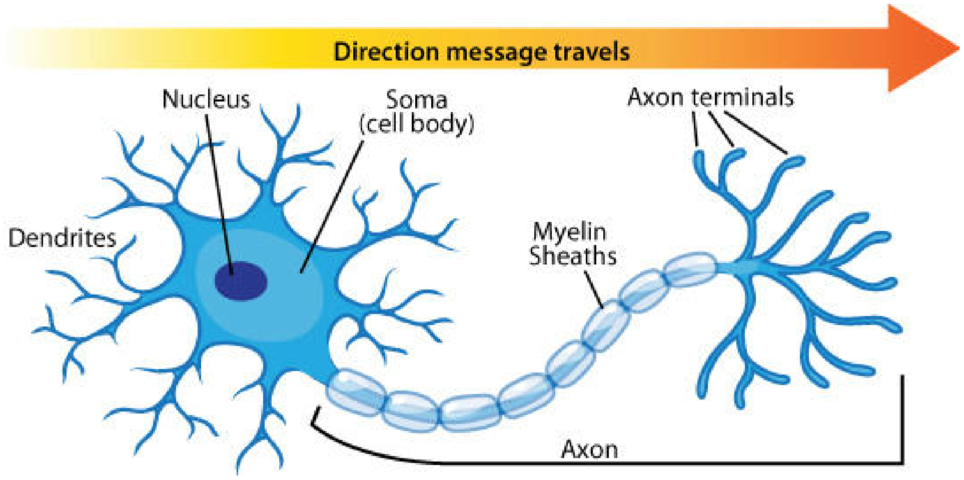

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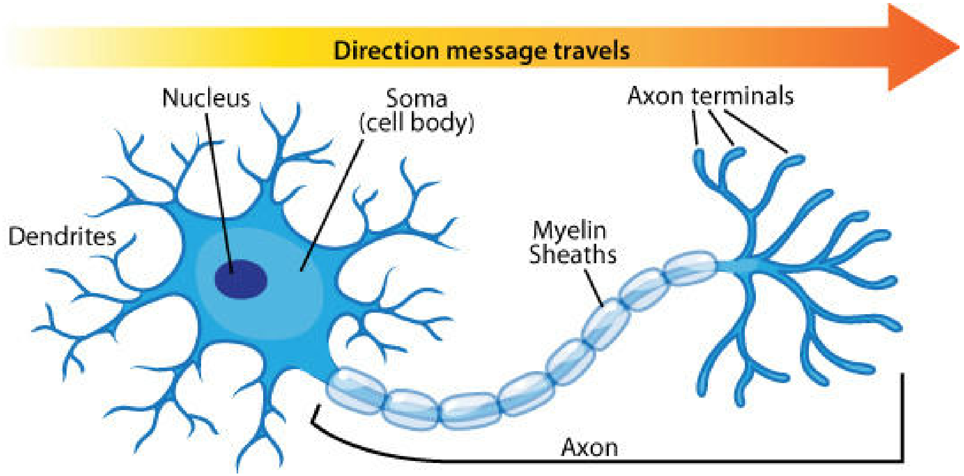

The axon fires only if the voltage is over a threshold

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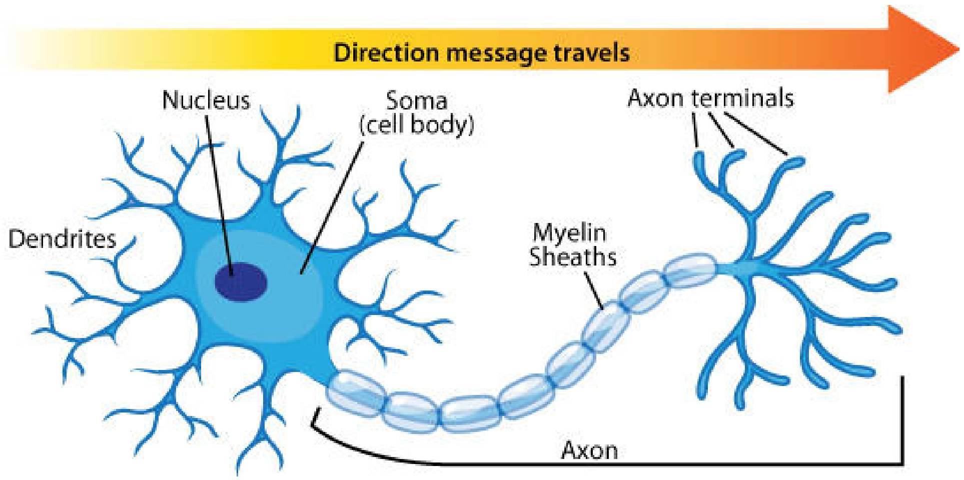

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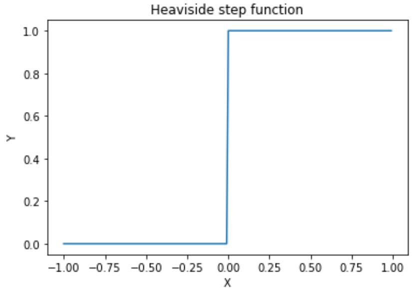

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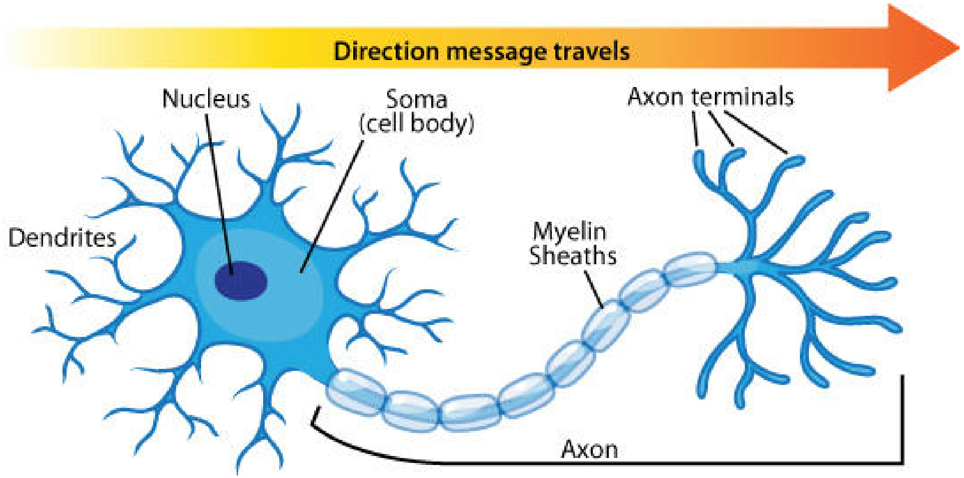

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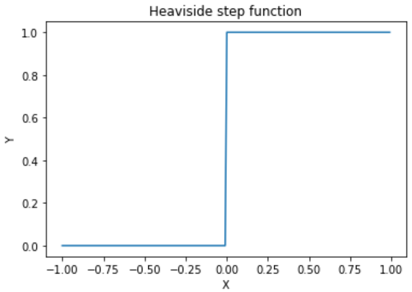

$$f\left(\begin{bmatrix} x_1 \\ \vdots \\ x_n \end{bmatrix}, \begin{bmatrix} \theta_1 \\ \vdots \\ \theta_n \end{bmatrix} \right) = \sigma\left(\sum_{i=1}^{n} x_i \theta_i \right)$$

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Answer: The linear model!

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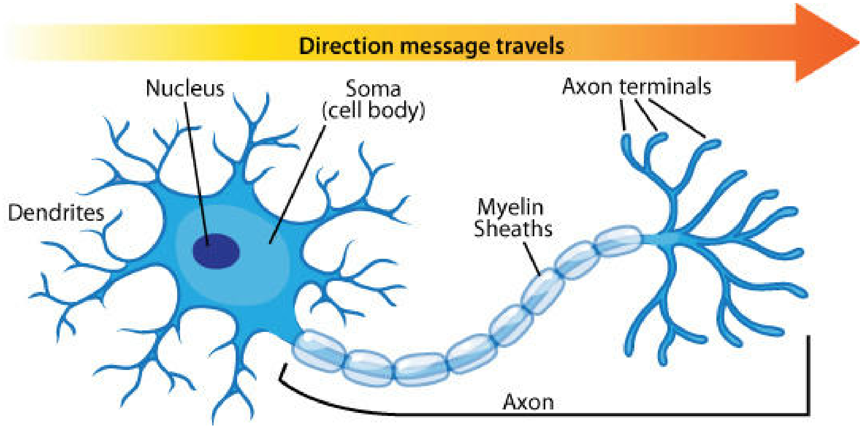

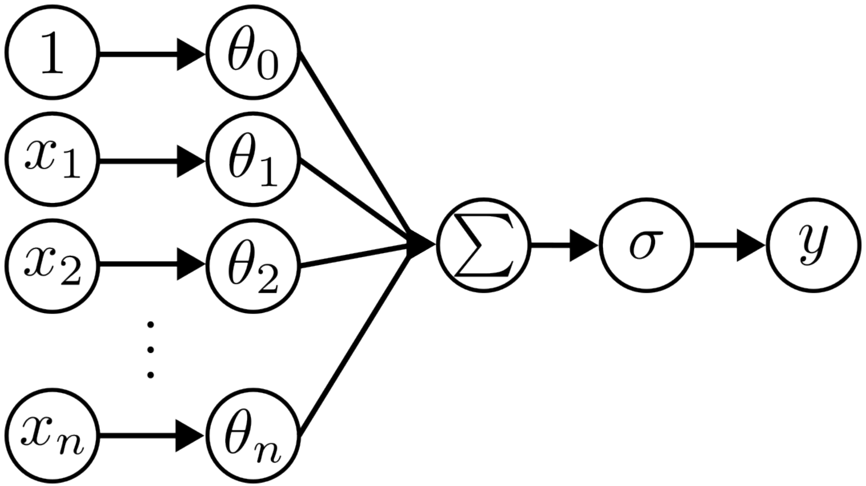

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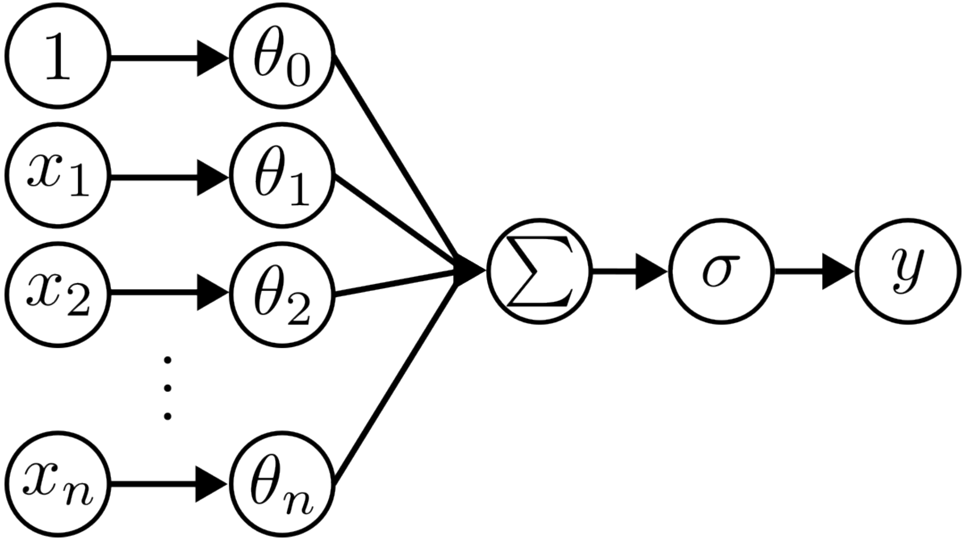
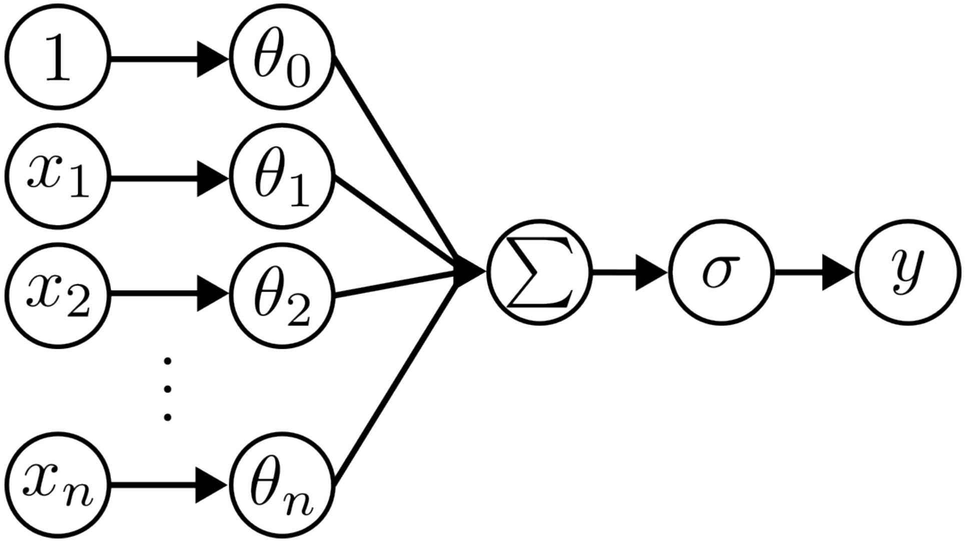
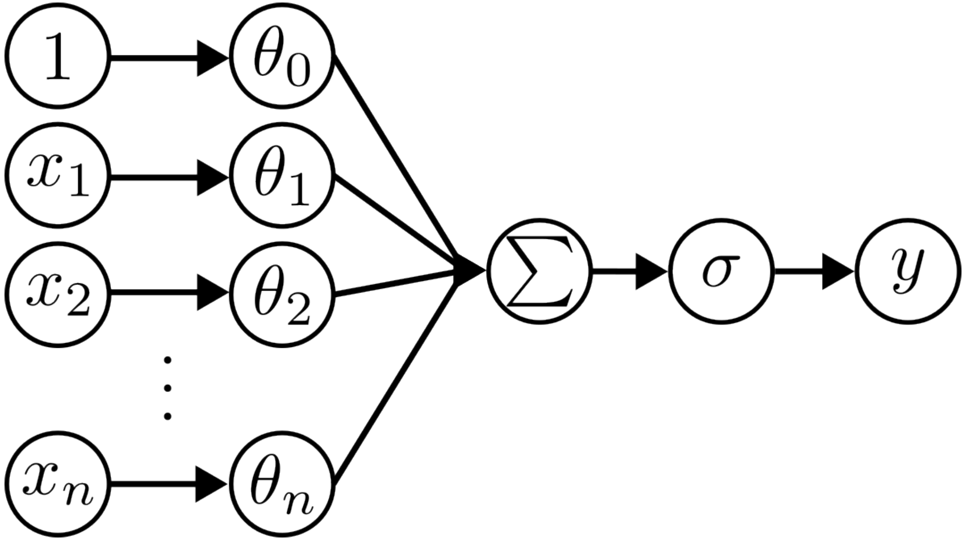
Relax


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



Recall that in machine learning we deal with functions



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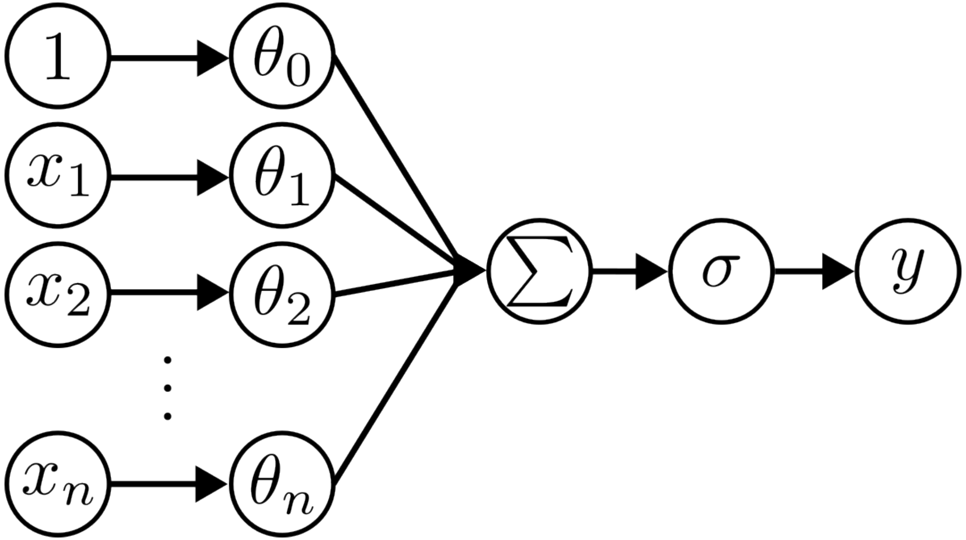
What kinds of functions can our neuron represent?



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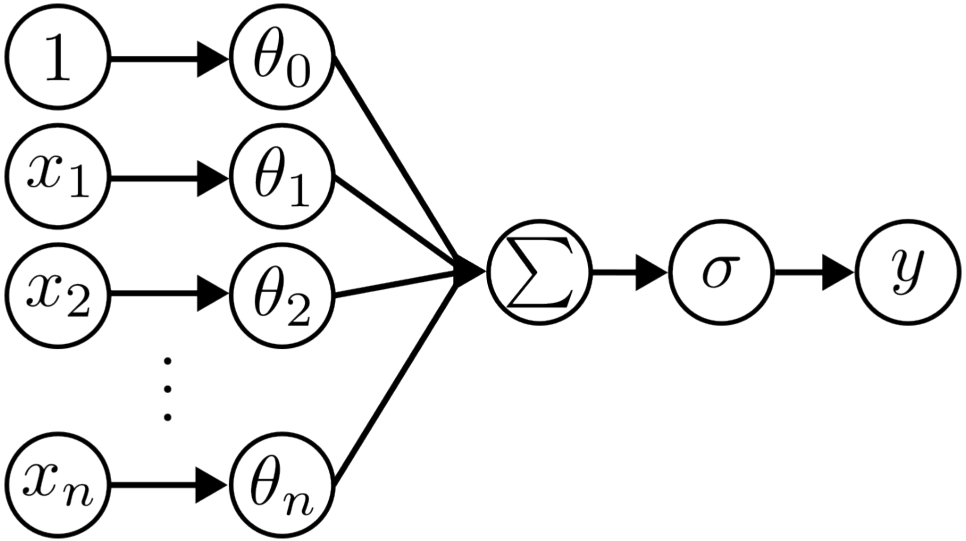
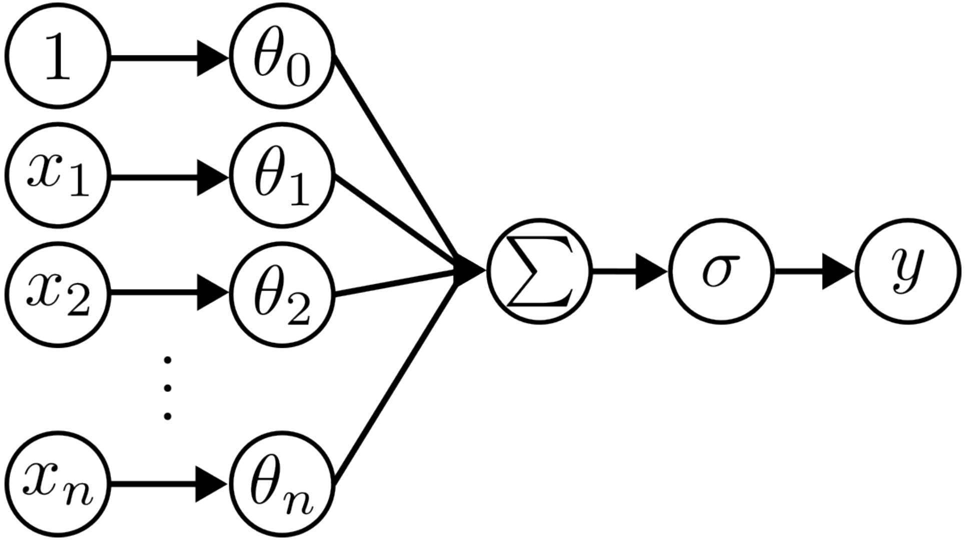
Let us start with a logical AND function

Recall the activation function (Heaviside step)





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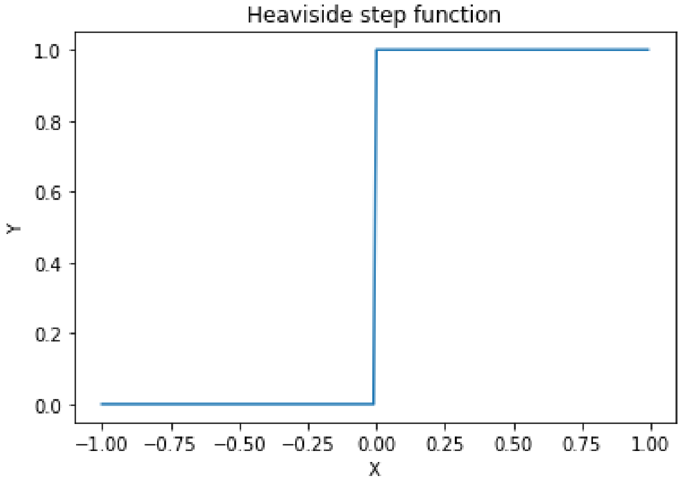

$$H(x) = \begin{cases} 1 \text{ if } x > 0 \\ 0 \text{ if } x \leq 0 \end{cases}$$

Implement AND using an artificial neuron

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

Implement AND using an artificial neuron

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

Implement AND using an artificial neuron

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

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

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 → Biological neural network

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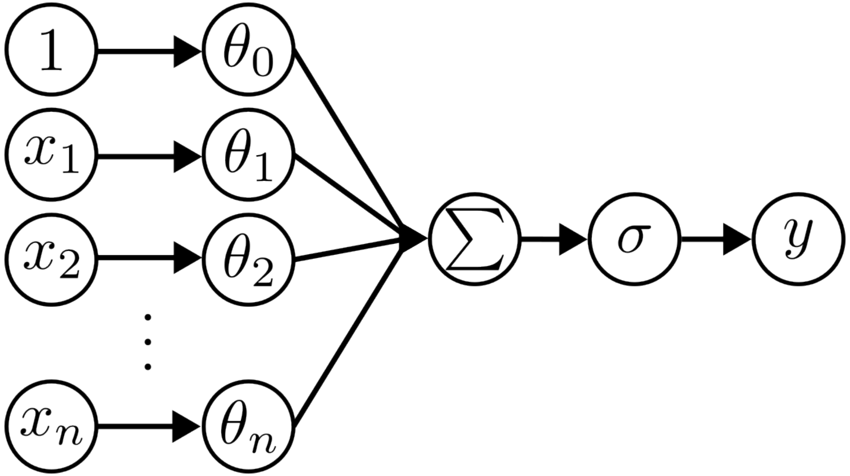
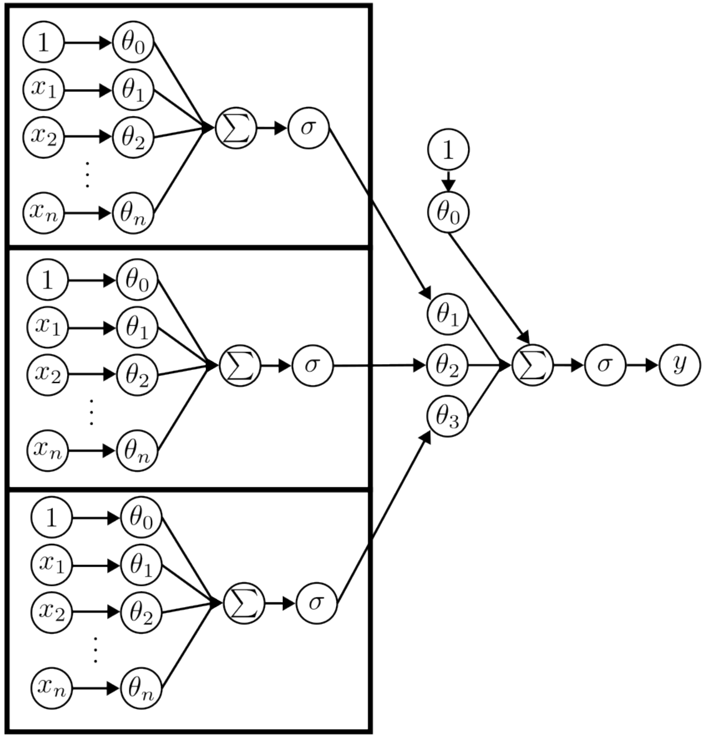
Computer: Artificial neurons $\rightarrow$ Artificial neural network

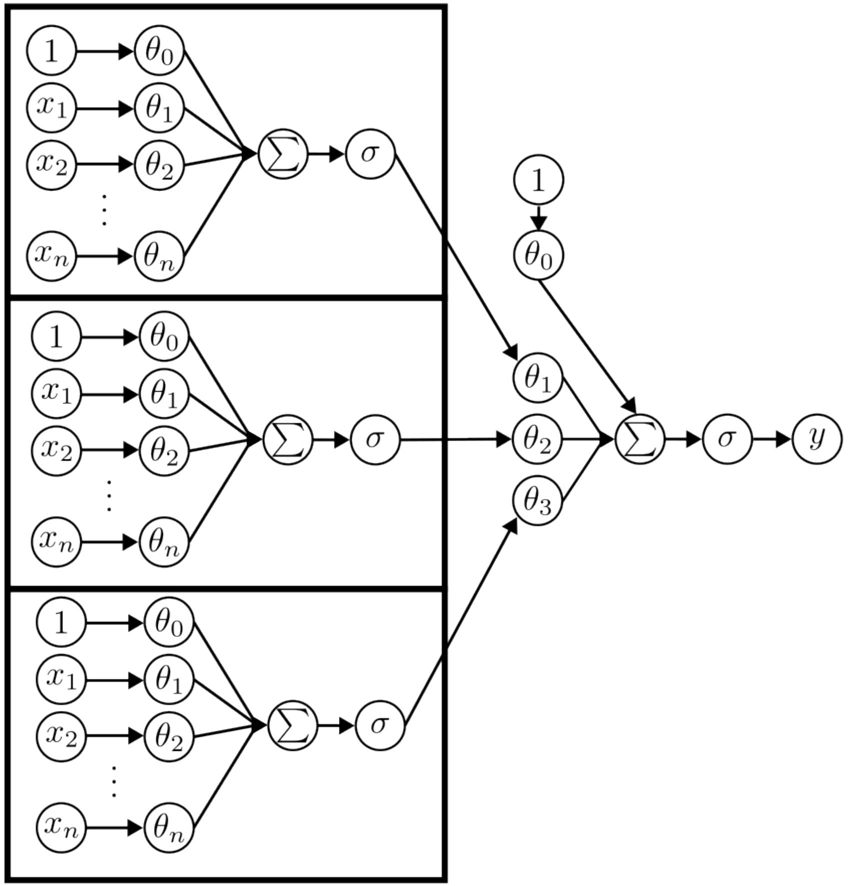
Connect artificial neurons into a network



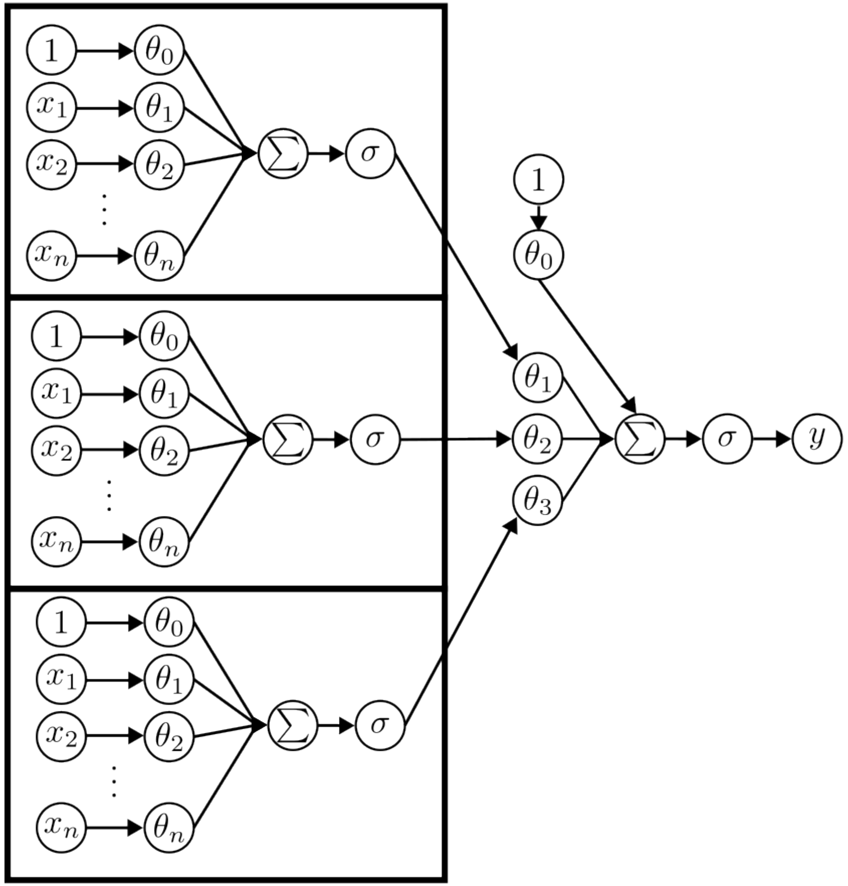
Neuron



Neural Network



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



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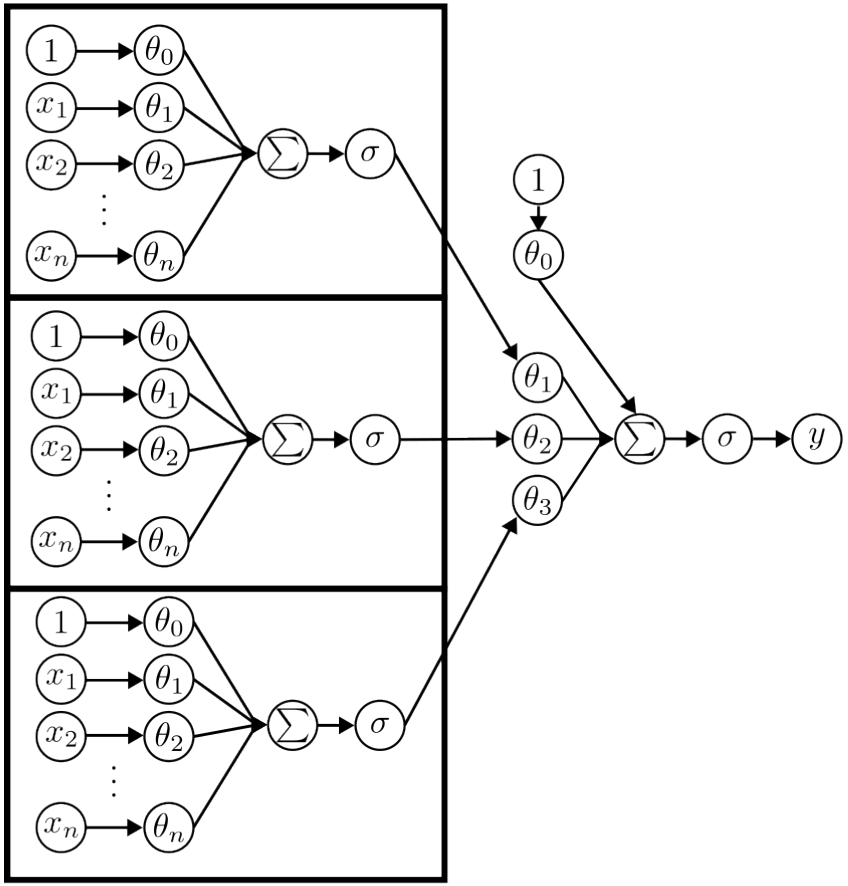

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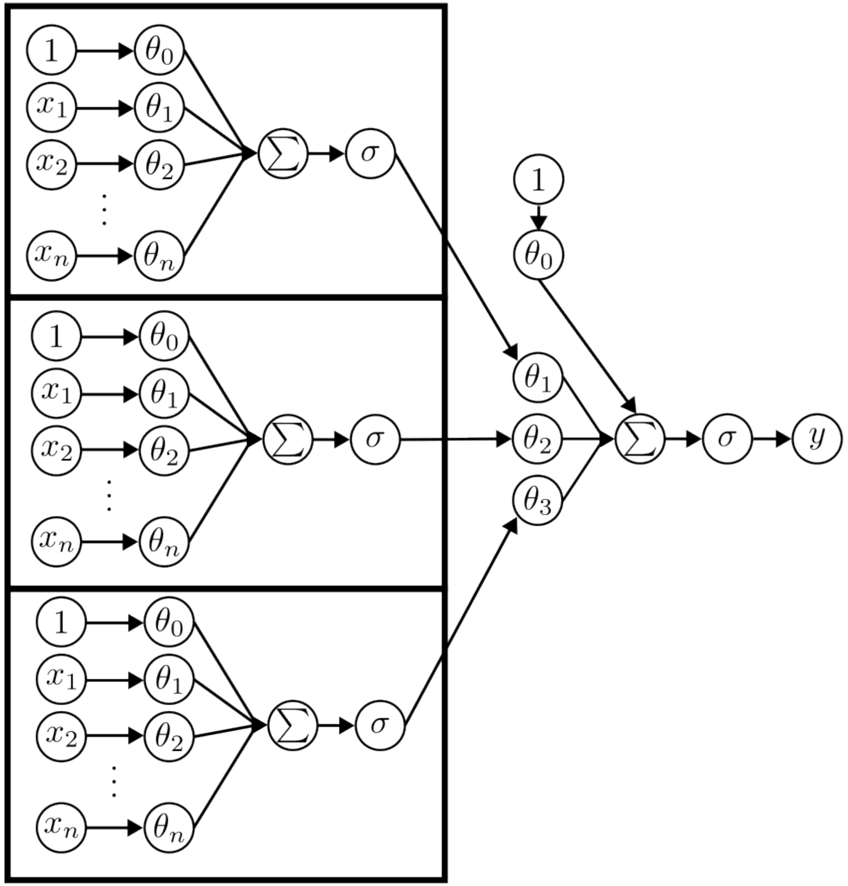
Today's powerful neural networks are both **wide** and **deep**



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

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

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

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For a single neuron:

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

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

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

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Use function composition

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

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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Implement XOR using a deep and wide neural network

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$$
\begin{aligned}
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+\theta_{3,2} \quad & \cdot \quad H\big(\theta_{2,0} + x_1 \theta_{2,1} + x_2 \theta_{2,2}\big)\big)
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$$\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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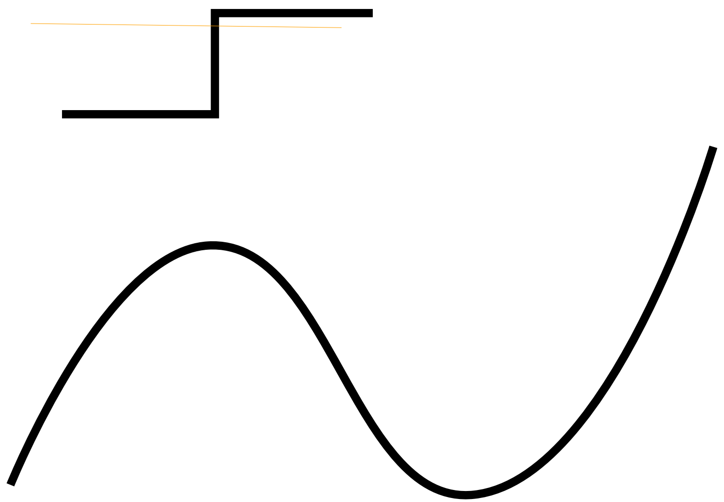

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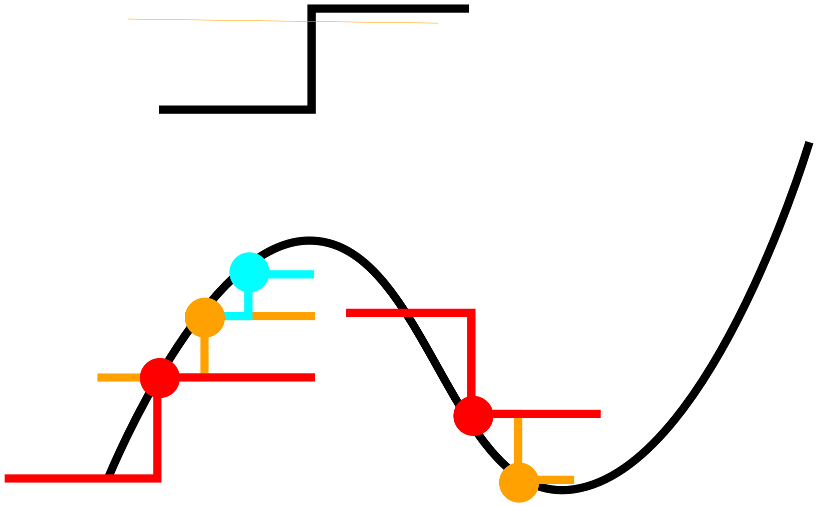

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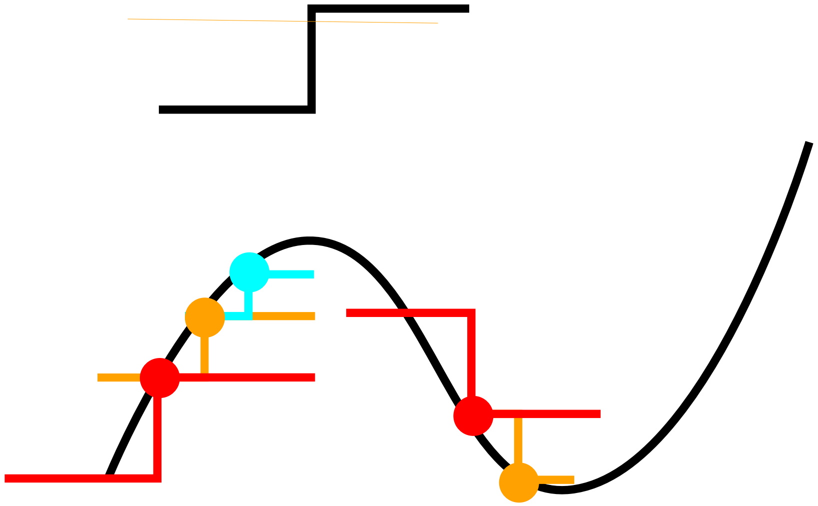

$$\text{Roughly, } \exists \boldsymbol{\theta} \Rightarrow \lim_{n \mapsto \infty} \left[\theta_{2,0} + \theta_{2,1} \sum_{j=1}^{n} \sigma(\theta_{1,0} + \theta_{1,j} x) \right] = g(x); \quad \forall g$$

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

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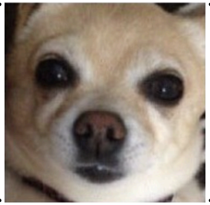
$g\Bigg($  $\Bigg) = \text{Dog}$

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

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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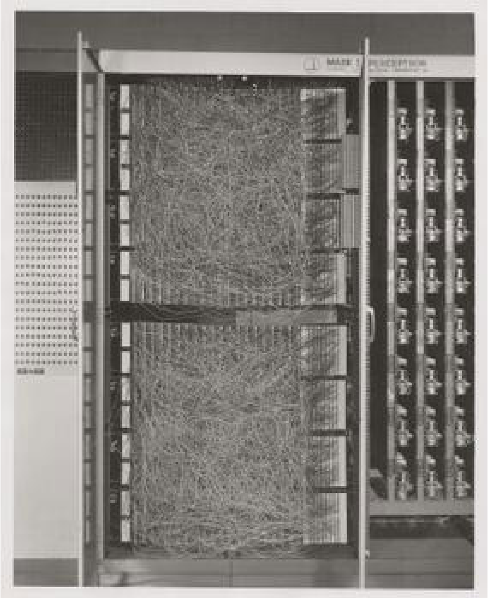
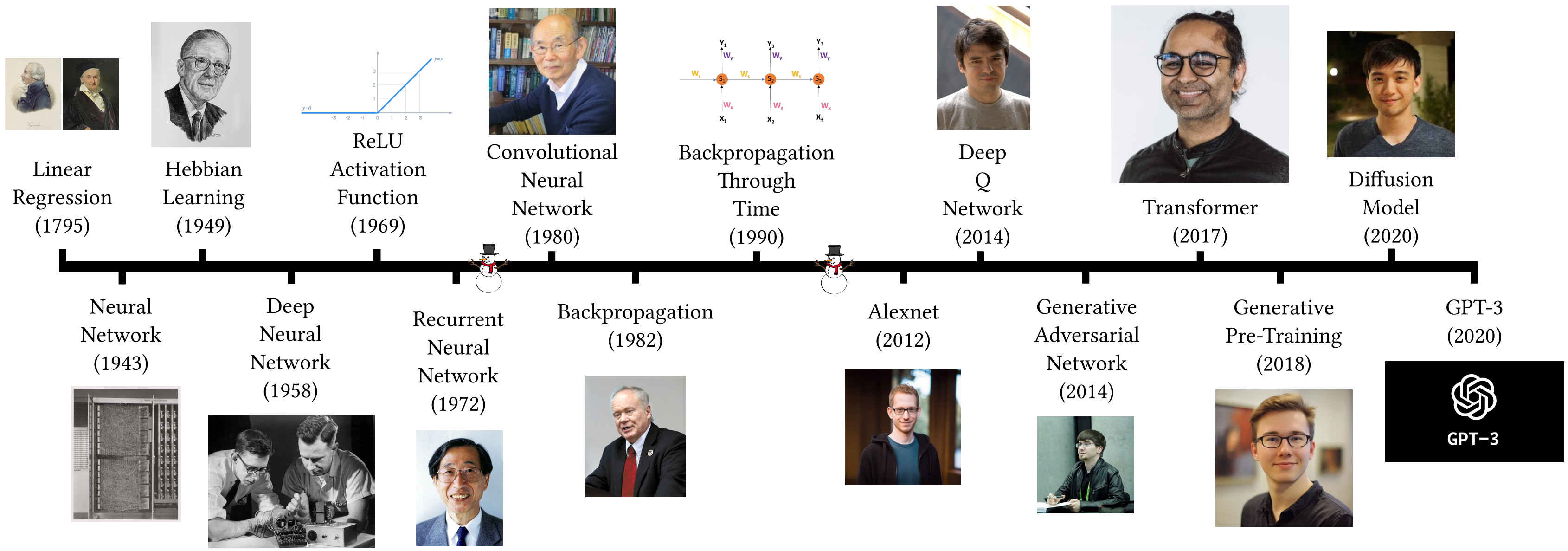
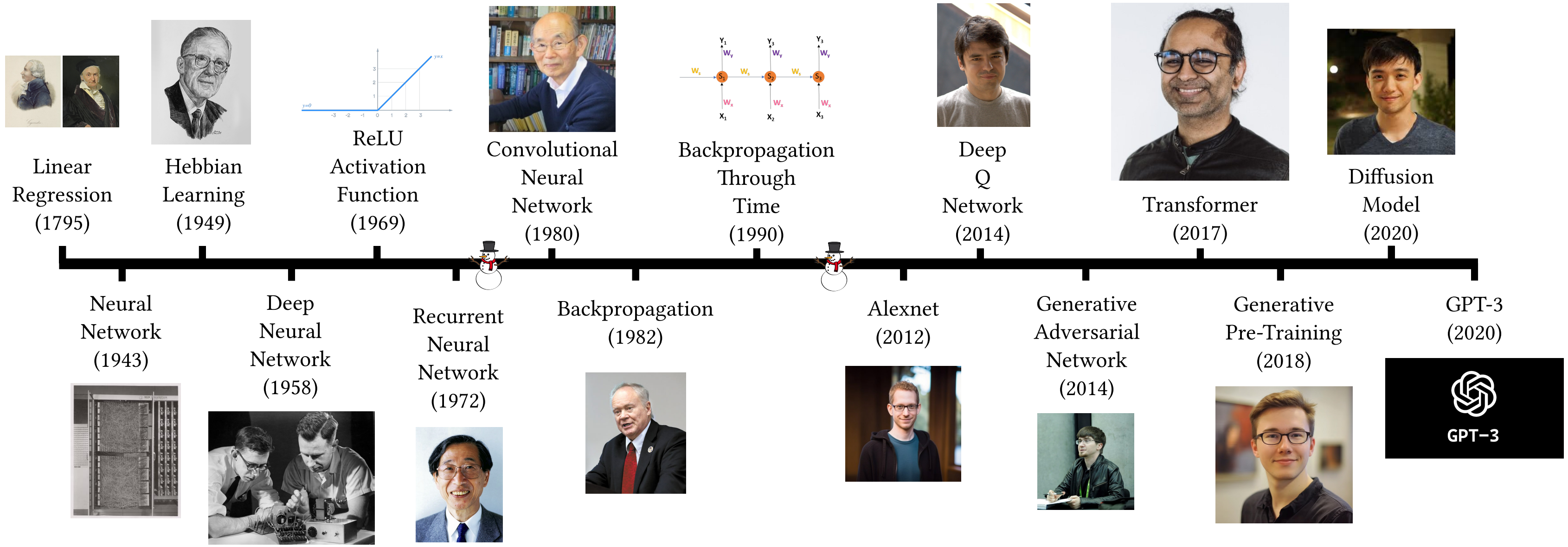


20×20 grid of pixels to process images


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

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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 neural networks in `torch` and `jax`

```python
import torch
from torch import nn

class MyNetwork(nn.Module):
  def __init__(self):
    super().__init__() # Required by pytorch
    self.input_layer = nn.Linear(5, 3) # 3 neurons, 5 inputs each
    self.output_layer = nn.Linear(3, 1) # 1 neuron with 3 inputs

  def forward(self, x):
    z = torch.heaviside(self.input_layer(x))
    y = self.output_layer(z)
    return y
```

```python
import jax, equinox
from jax import numpy as jnp
from equinox import nn

class MyNetwork(equinox.Module):
  input_layer: nn.Linear # Required by equinox
  output_layer: nn.Linear

  def __init__(self):
    self.input_layer = nn.Linear(5, 3, key=jax.random.PRNGKey(0))
    self.output_layer = nn.Linear(3, 1, key=jax.random.PRNGKey(1))

  def __call__(self, x):
    z = jnp.heaviside(self.input_layer(x))
    y = self.output_layer(z)
    return y
```