Introdução à Aprendizagem Automática (IAA)

SUSANA BRÁS

SUSANA.BRAS@UA.PT

IAA – L9

Artificial Neural Networks

- Nonlinear Classifier
- Neuron model
- Activation function
- Binary vs multiclass classification
- Cost function
- Backpropagation error

Data Matrix

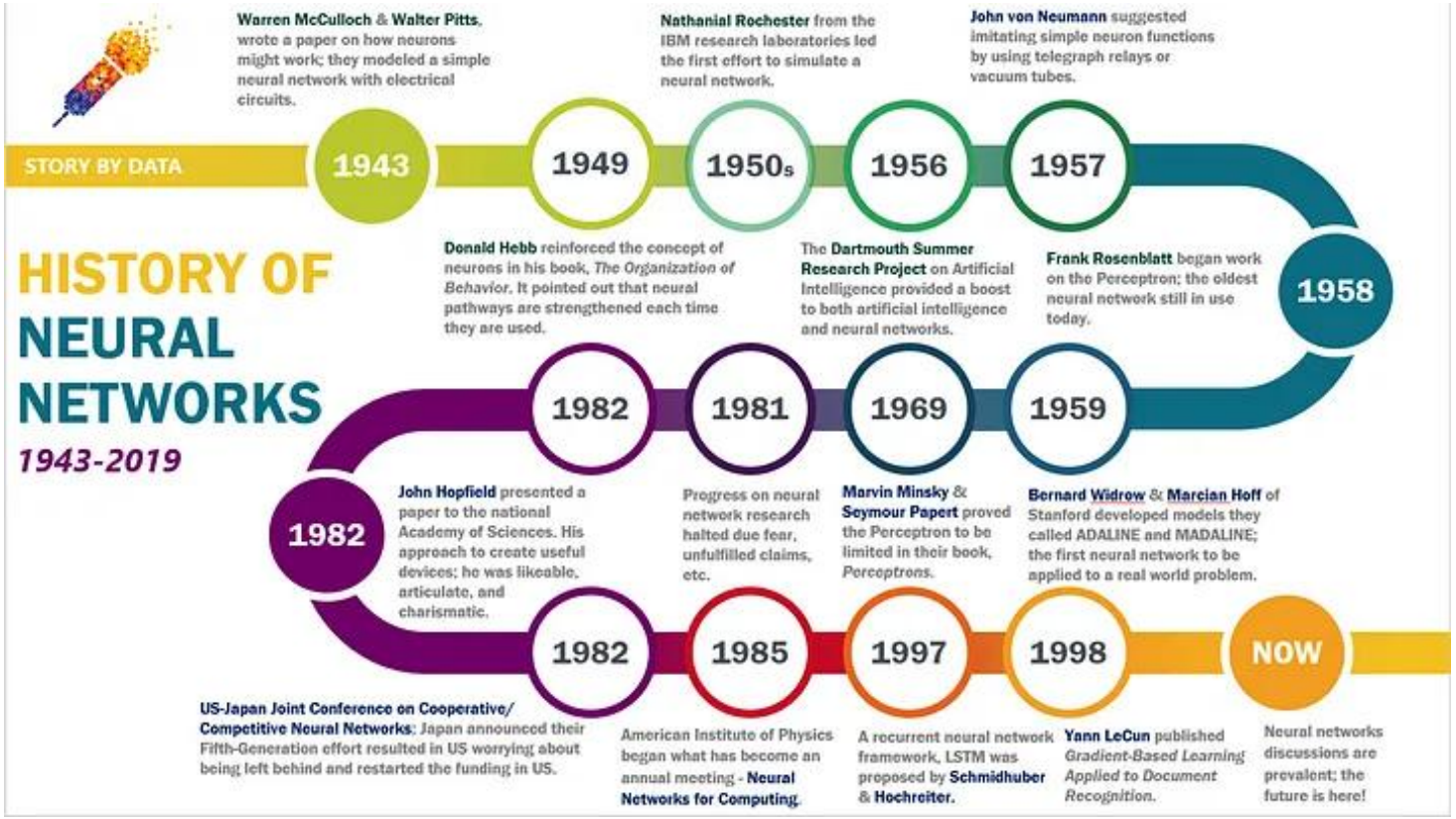
matrix X (mxn)	feature x_1	feature x_2	.....	feature x_n	Target Y
Example 1	$x_1^{(1)}$	$x_2^{(1)}$		$x_n^{(1)}$	$Y^{(1)}$
Example 2	$x_1^{(2)}$	$x_2^{(2)}$		$x_n^{(2)}$	$Y^{(2)}$
…					
Example i	$x_1^{(i)}$	$x_2^{(i)}$		$x_n^{(i)}$	$Y^{(i)}$
…					
…					
Example m	$x_1^{(m)}$	$x_2^{(m)}$		$x_n^{(m)}$	$Y^{(m)}$

x – input vector of features, attributes
y – output vector of labels, ground truth, target
m - number of training examples
n – number of features
$h_\theta(x)$ - model (hypothesis)
θ - vector of model parameters

Training set: data matrix X (m rows, n columns)

Artificial Neural Networks (ANN)

NN History



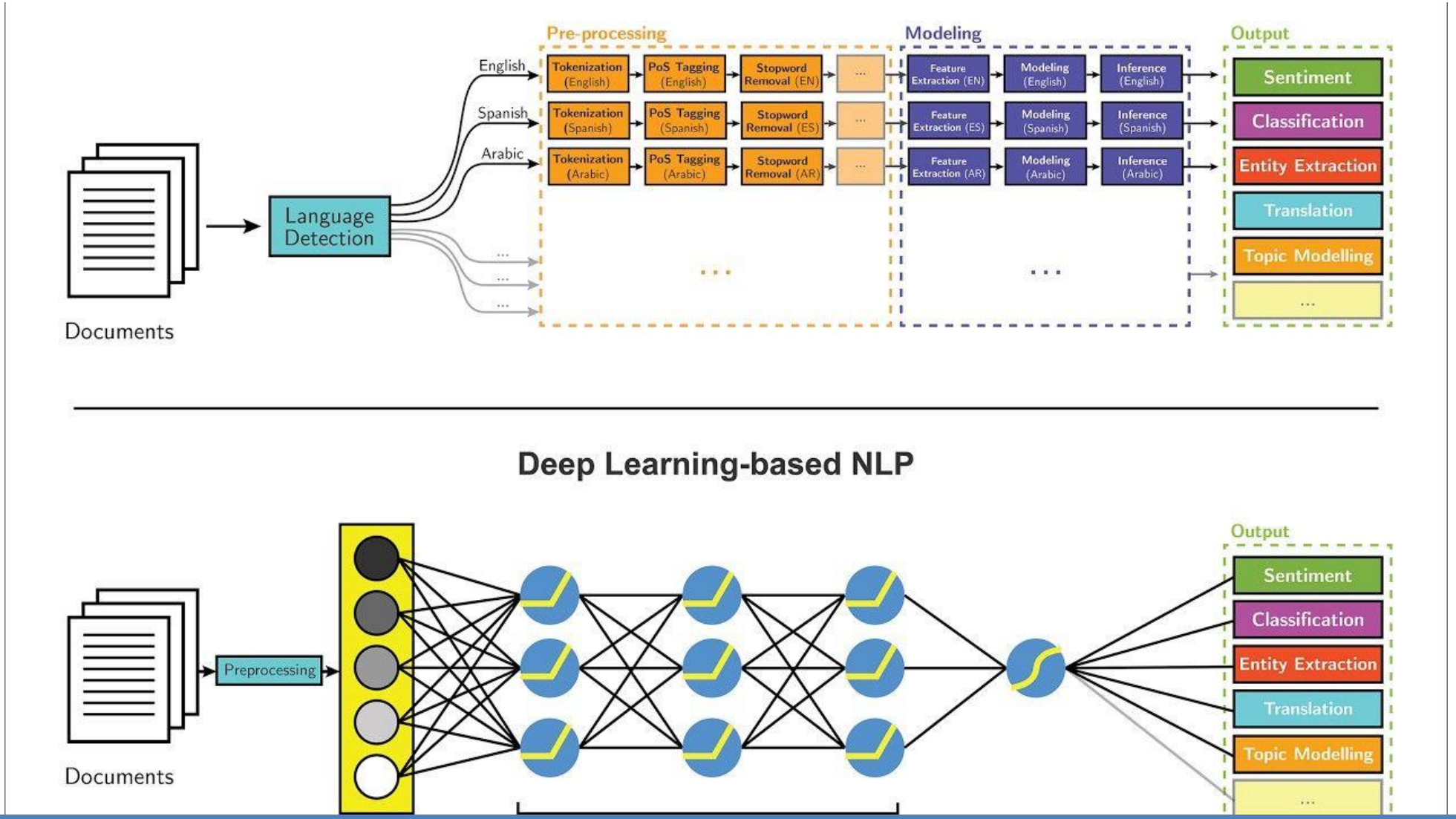
Only with the advent of hyper-fast processing, massive data storage capabilities, and access to computing resources where neural networks were able to advance to the point they have reached today.

Developments are still being made in this field; one of the most important types of neural networks in use today, the transformer, dates to 2017.

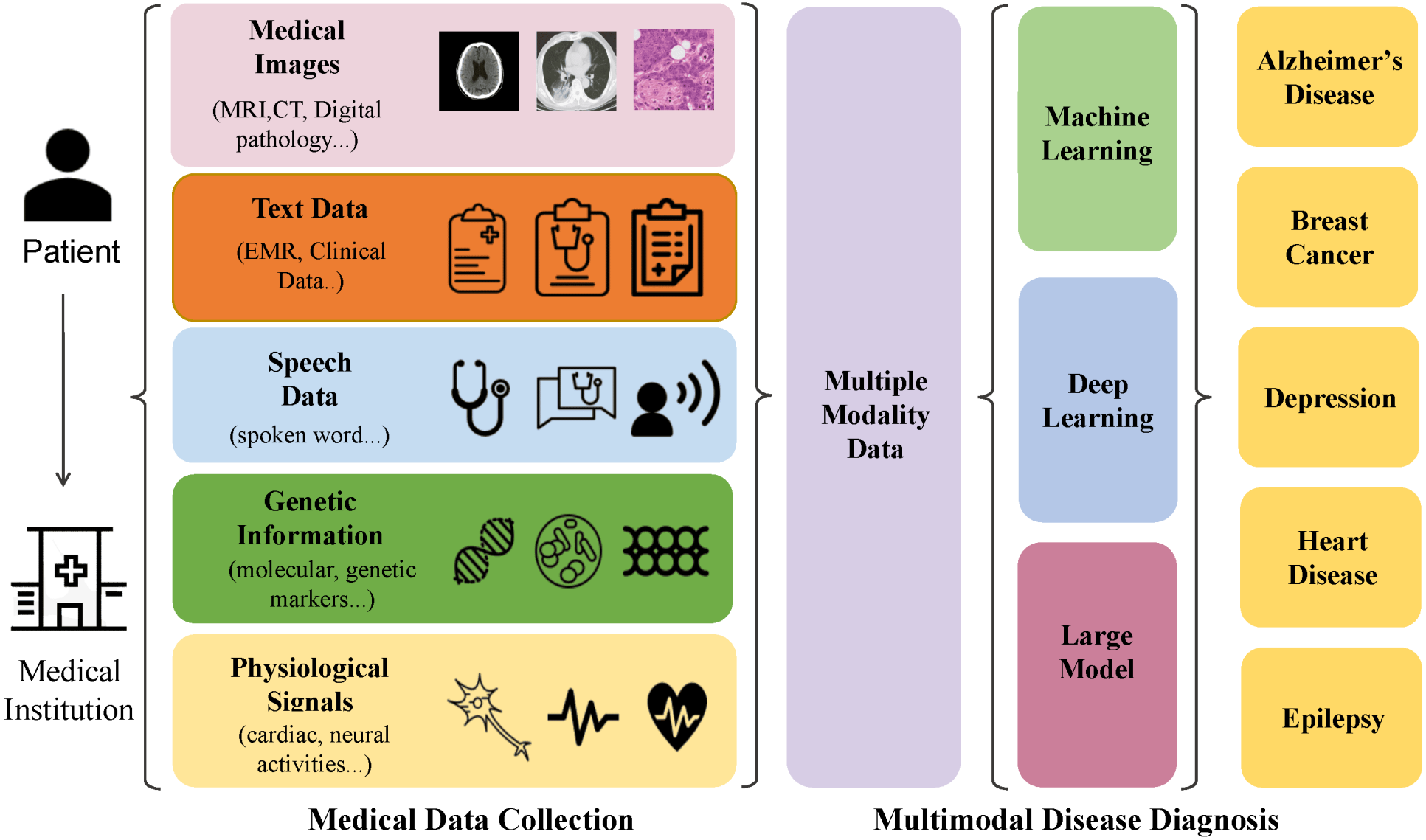
Nonlinear Separable Data

- Let us have 100 nonlinear separable features:
  - If using quadratic combinations of the features to get a nonlinear decision boundary, we end up with 5000 features
- Logistic regression and SVM are not efficient for such complex nonlinear models

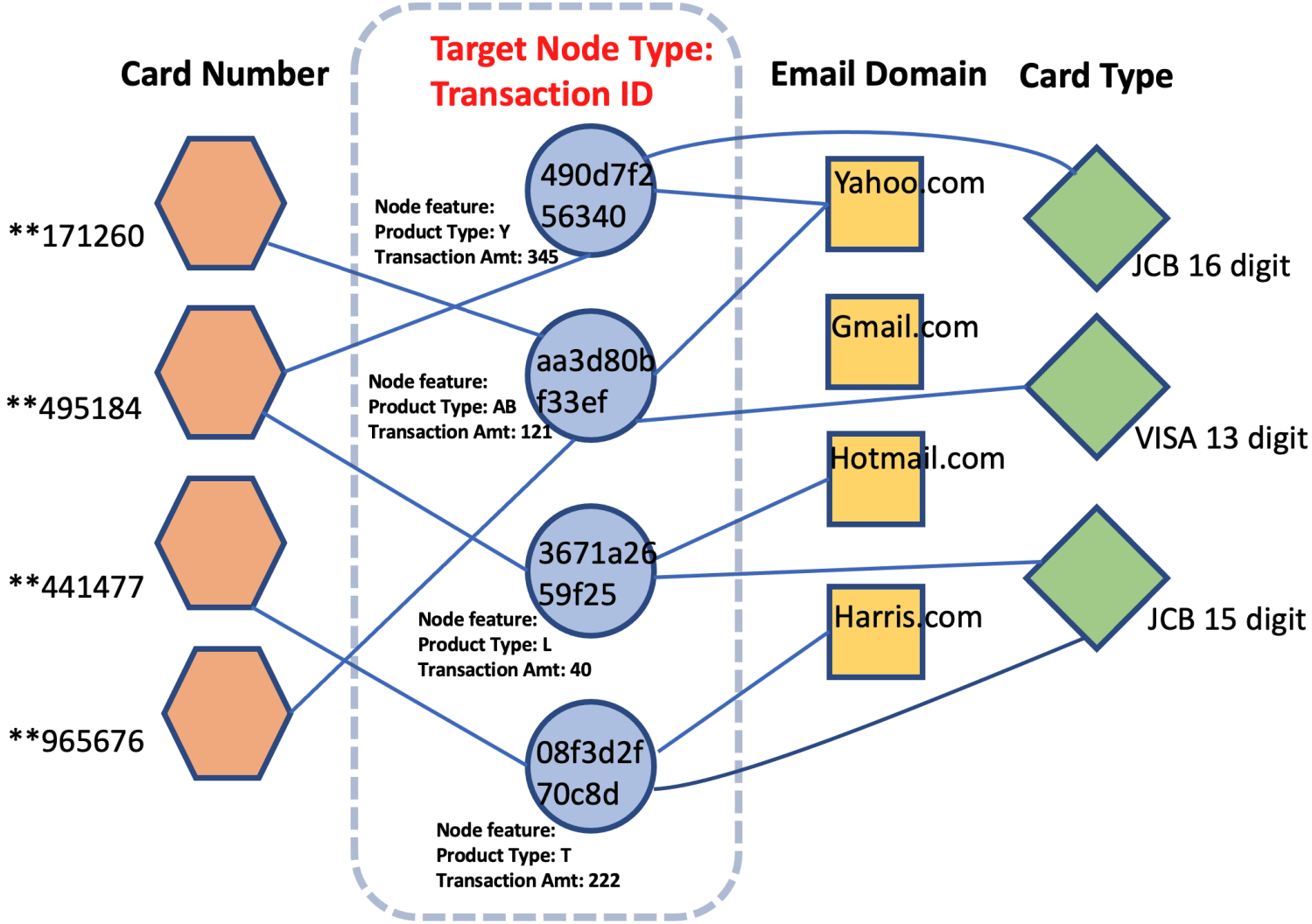
Applications



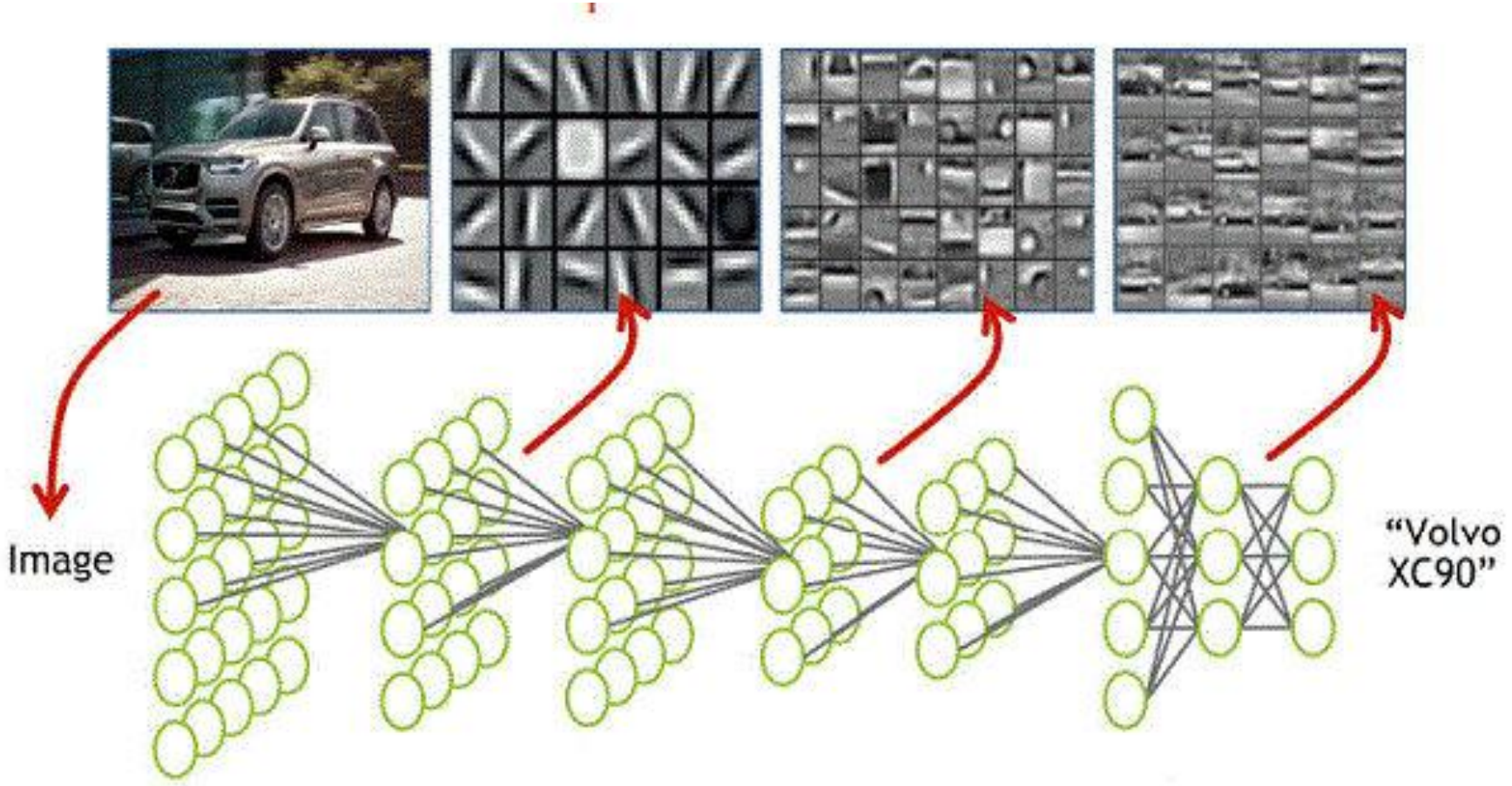
Applications



Applications

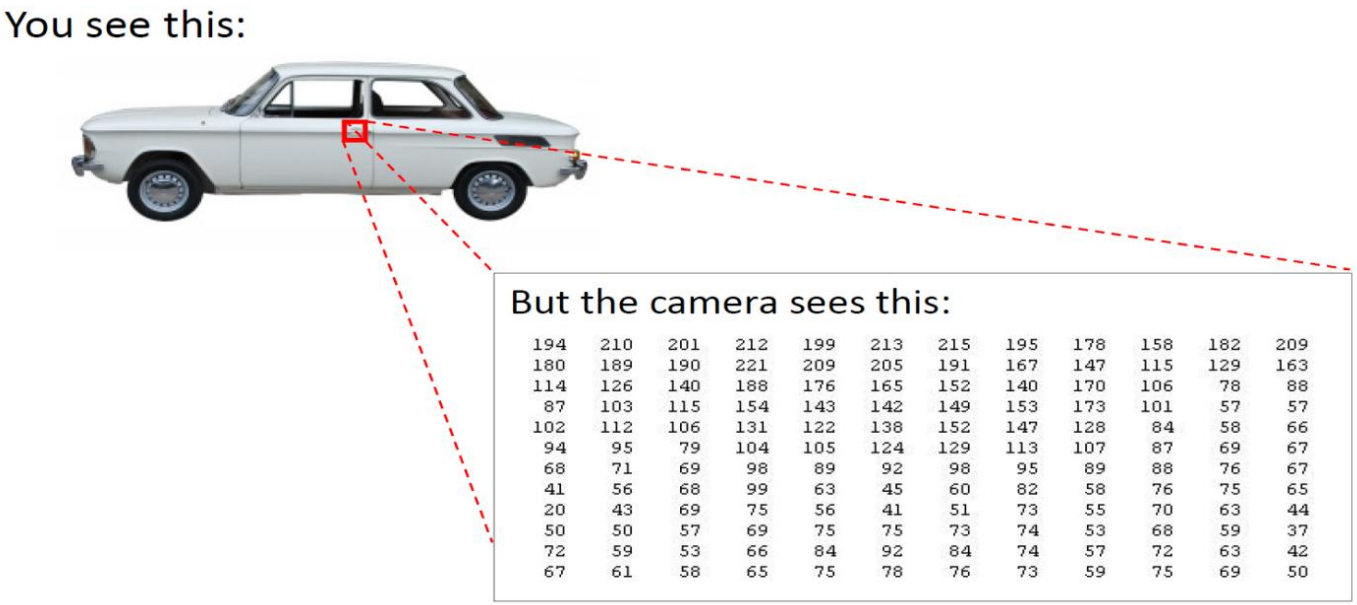


Applications



Applications

For a small peace of the car image we may have too many features (pixels)



Large Scale Data

50 x 50 pixel images→ 2500 pixels

$n = 2500$ (7500 if RGB)

$$x = \begin{bmatrix} \text{pixel 1 intensity} \\ \text{pixel 2 intensity} \\ \vdots \\ \text{pixel 2500 intensity} \end{bmatrix}$$

50 x 50 pixel images:

2500 pixels (features) for a gray scale image

7500 pixels (features) for a RGB image

If using quadratic features => 3 million features

Complex nonlinear models.

Neural Networks were designed and planned to fit complex nonlinear models.

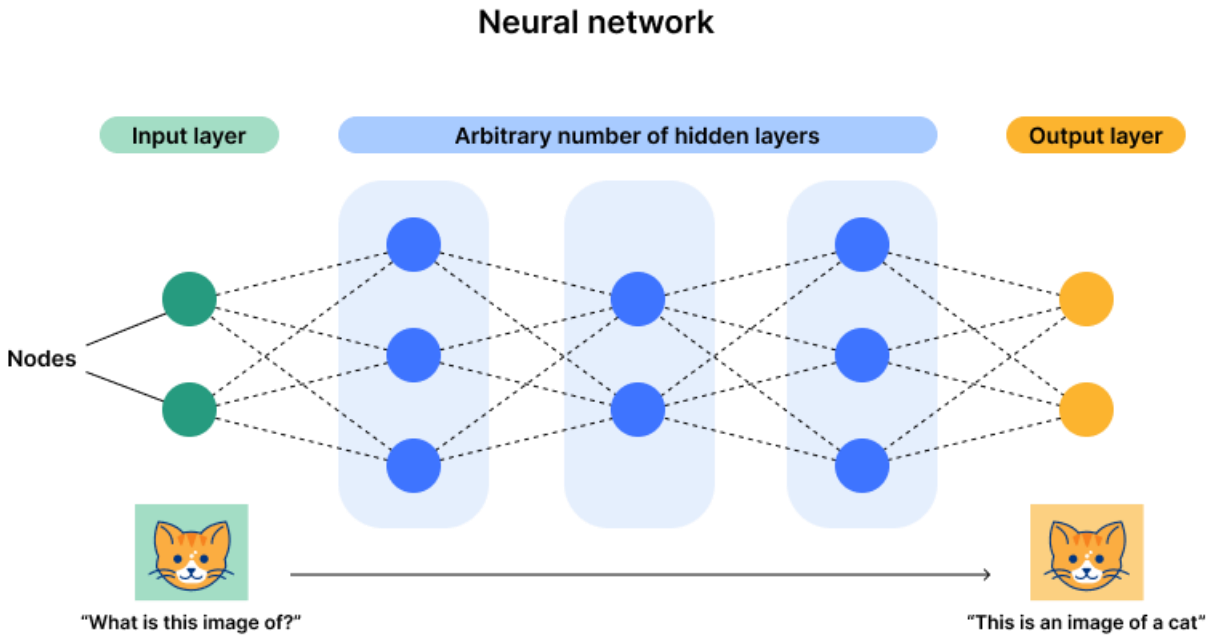
NN

A neural network, or artificial neural network, is a computing architecture based on a model of how a human brain works — hence the name "neural.“

NN are made up of a collection of processing units called "nodes.“

These nodes pass data to each other, just like how in a brain, neurons pass electrical impulses to each other.

NN are used in machine learning, which refers to a category of computer programs that learn without definite instructions, they learn from data.



https://www.cloudflare.com/learning/ai/what-is-neural-network/

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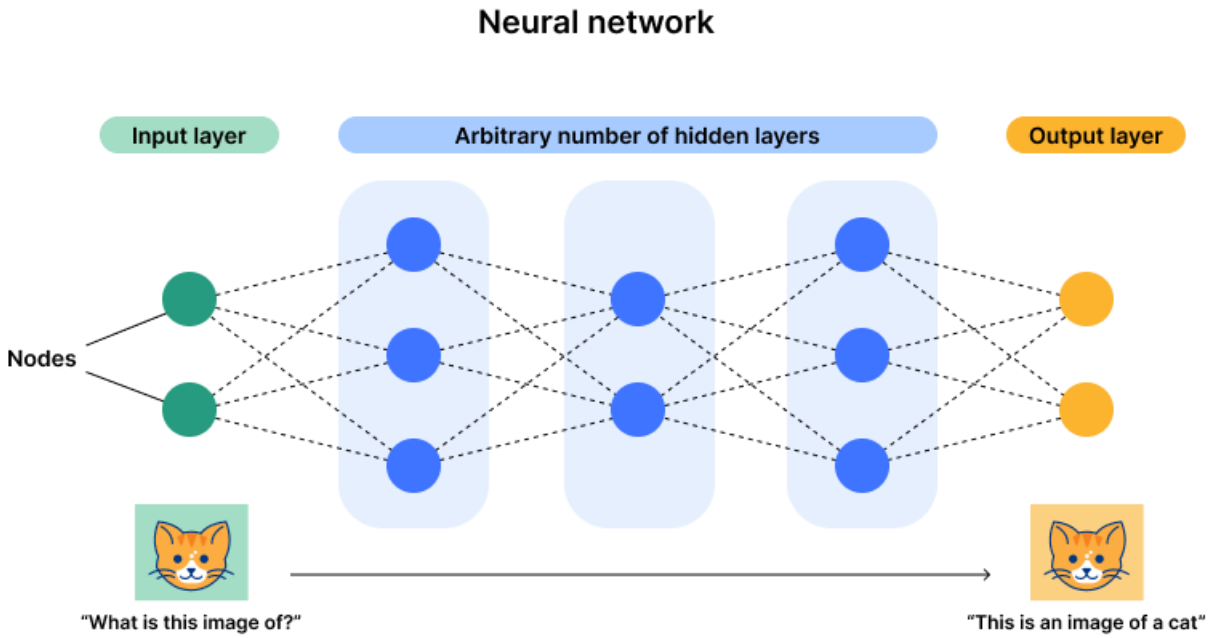

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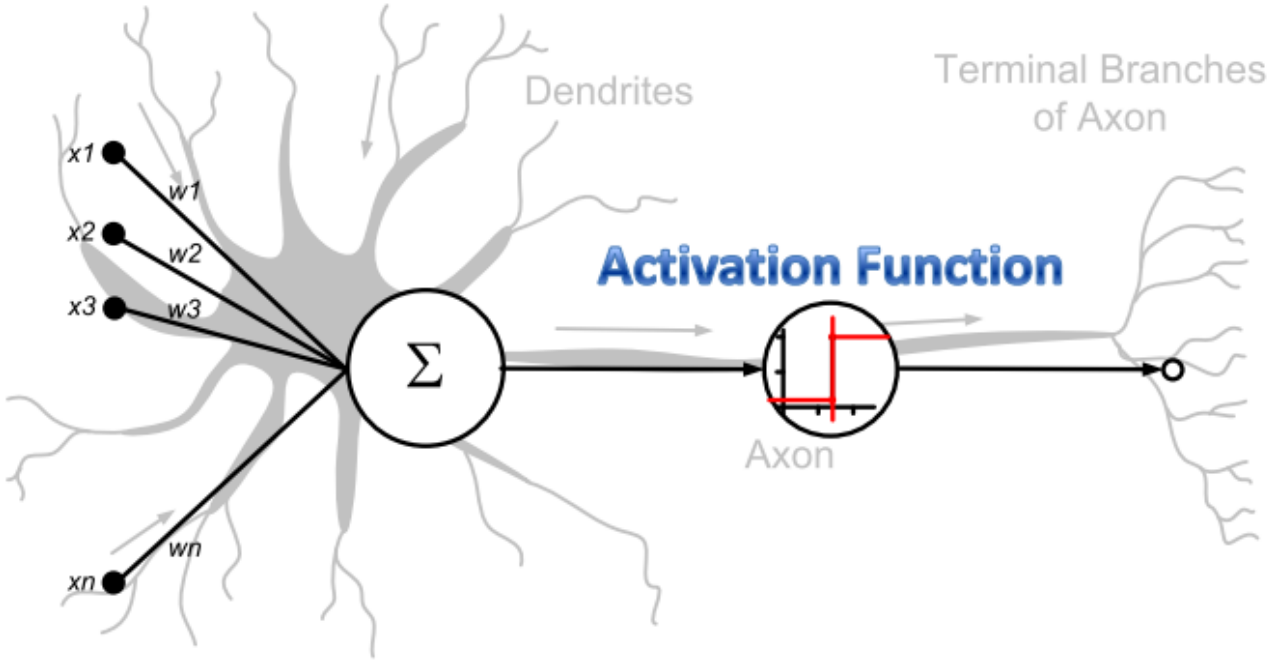
Neuron Model

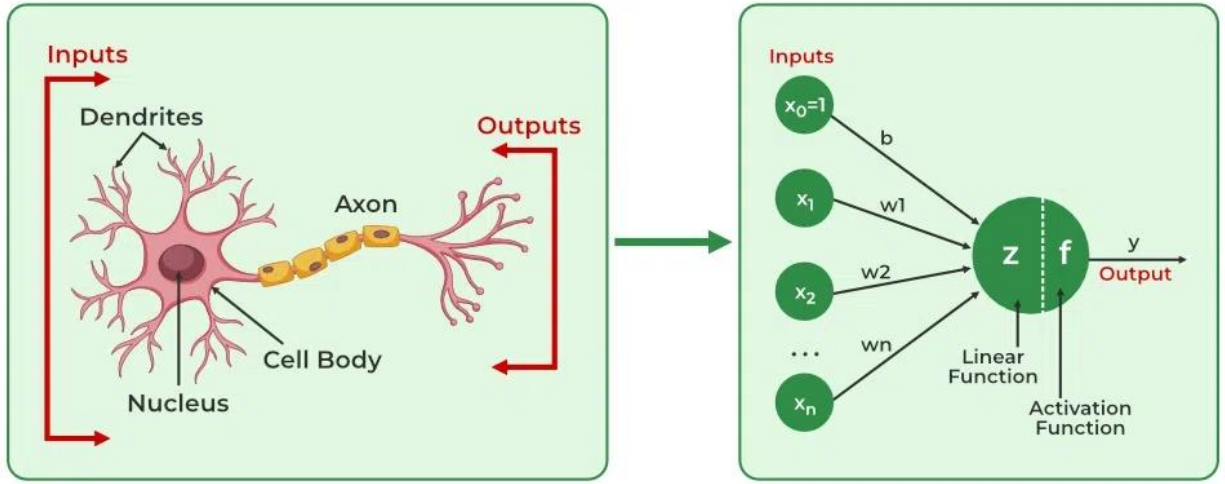
Origins: NN models inspired by biological neuron structures and computations.



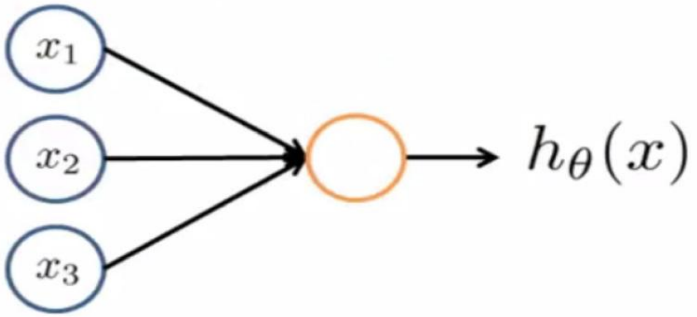
NN are particularly useful for complex tasks where traditional machine learning algorithms fail.

The main **advantage** of NN is their ability to learn **intricate patterns** and relationships in data, even when the data is **highly dimensional or unstructured**.

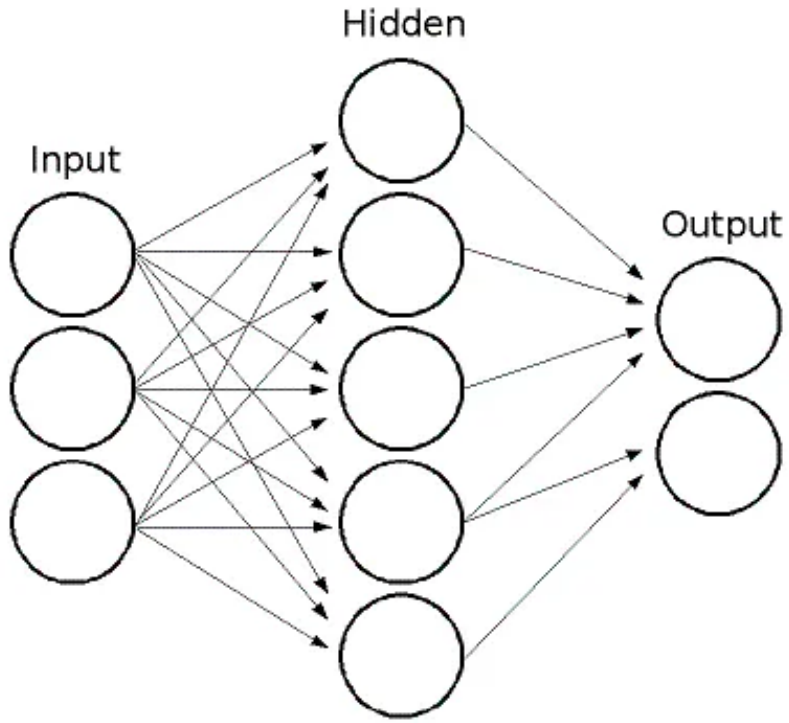
Neuron Model



Model of an artificial neuron (unit, node)



NN - Principle



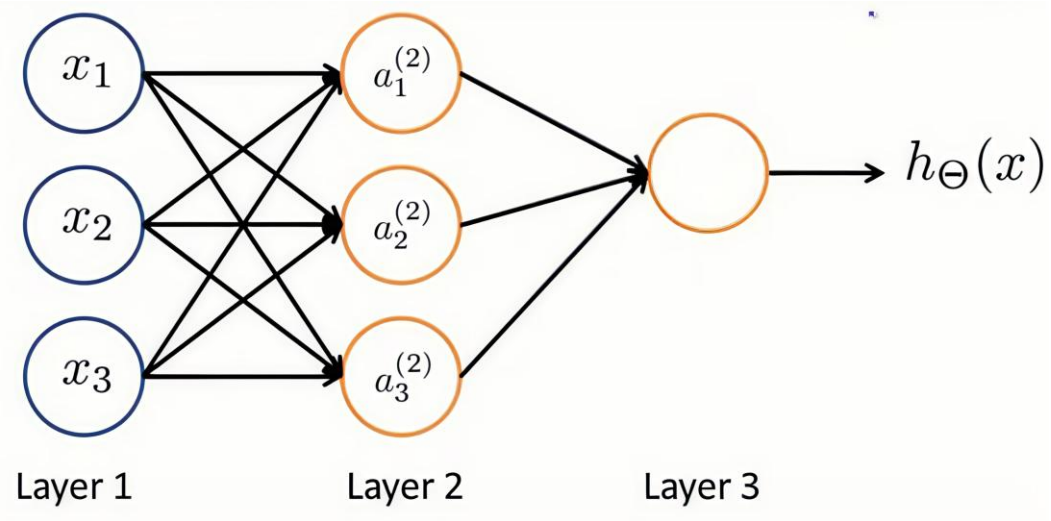
Goal: the network transforms the data until it is able to classify the data into an output.

How:

1. Each neuron multiplies an initial value by some weight
2. The results are summed with other values coming into the same neuron
3. The resulting number is adjusted by the neuron's bias
4. The output is normalized with an activation function.

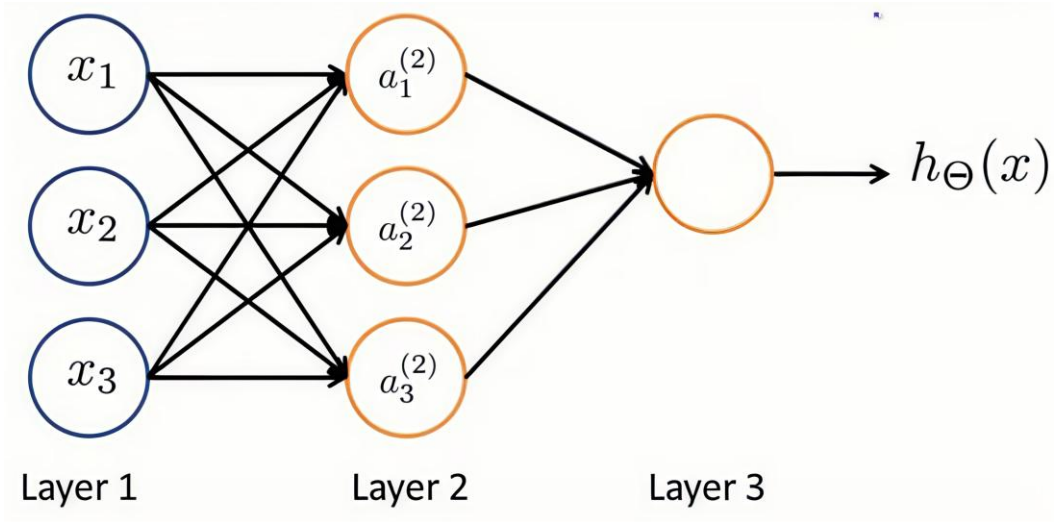
NN are composed of layers of computational units (neurons), with connections in different layers.

NN



Input layer hidden layer output layer

NN



Input layer hidden layer output layer

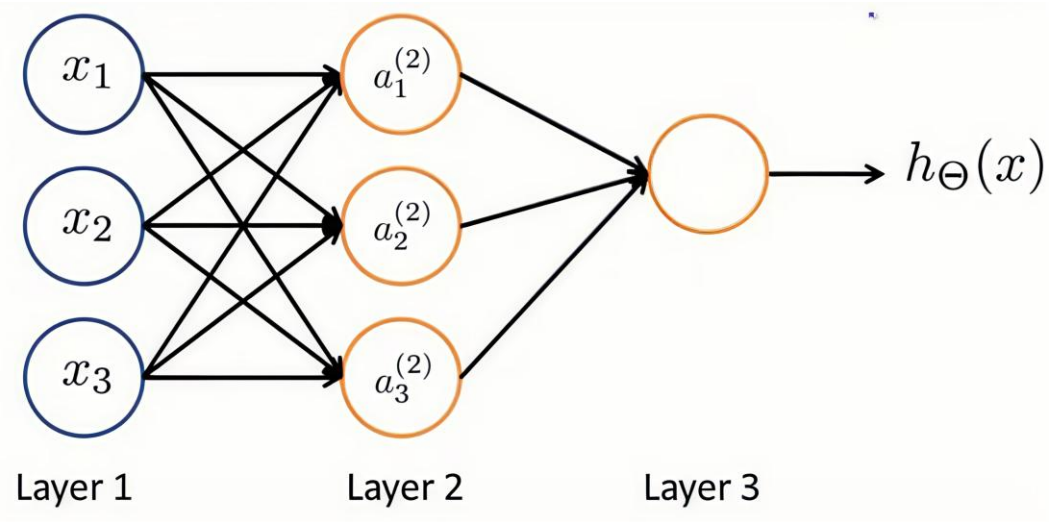
$a_i^{(j)}$ = "activation" of unit i in layer j

$\Theta^{(j)}$ = matrix of weights controlling function mapping from layer j to layer $j+1$

$$a_1^{(2)} = g(\Theta_{10}^{(1)}x_0 + \Theta_{11}^{(1)}x_1 + \Theta_{12}^{(1)}x_2 + \Theta_{13}^{(1)}x_3)$$
$$a_2^{(2)} = g(\Theta_{20}^{(1)}x_0 + \Theta_{21}^{(1)}x_1 + \Theta_{22}^{(1)}x_2 + \Theta_{23}^{(1)}x_3)$$
$$a_3^{(2)} = g(\Theta_{30}^{(1)}x_0 + \Theta_{31}^{(1)}x_1 + \Theta_{32}^{(1)}x_2 + \Theta_{33}^{(1)}x_3)$$
$$h_\Theta(x) = a_1^{(3)} = g(\Theta_{10}^{(2)}a_0^{(2)} + \Theta_{11}^{(2)}a_1^{(2)} + \Theta_{12}^{(2)}a_2^{(2)} + \Theta_{13}^{(2)}a_3^{(2)})$$

If network has s_j units in layer j, s_{j+1} units in layer $j+1$, then $\Theta^{(j)}$ will be of dimension $s_{j+1} \times (s_j + 1)$.

NN - vectorized implementation



$$x = \begin{bmatrix} x_0 \\ x_1 \\ x_2 \\ x_3 \end{bmatrix} \qquad z^{(2)} = \begin{bmatrix} z_1^{(2)} \\ z_2^{(2)} \\ z_3^{(2)} \end{bmatrix}$$

$$z^{(2)} = \Theta^{(1)} x$$
$$a^{(2)} = g(z^{(2)})$$

$$a_1^{(2)} = g(\Theta_{10}^{(1)} x_0 + \Theta_{11}^{(1)} x_1 + \Theta_{12}^{(1)} x_2 + \Theta_{13}^{(1)} x_3)$$
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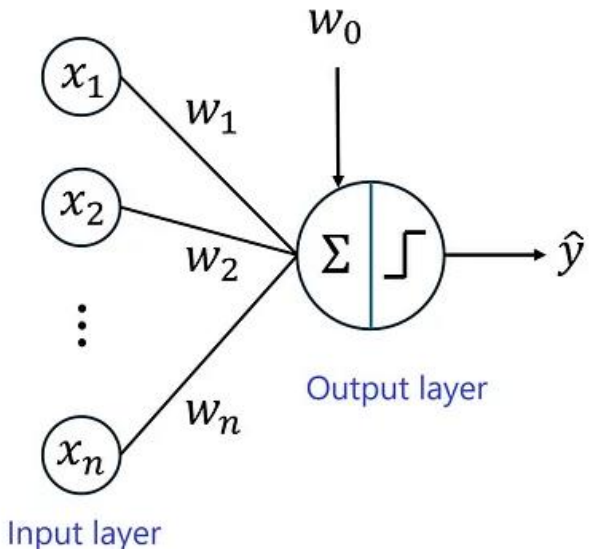
NN - Base



NN are composed of a collection of nodes.
Usually, the nodes are spread out across at least three layers.

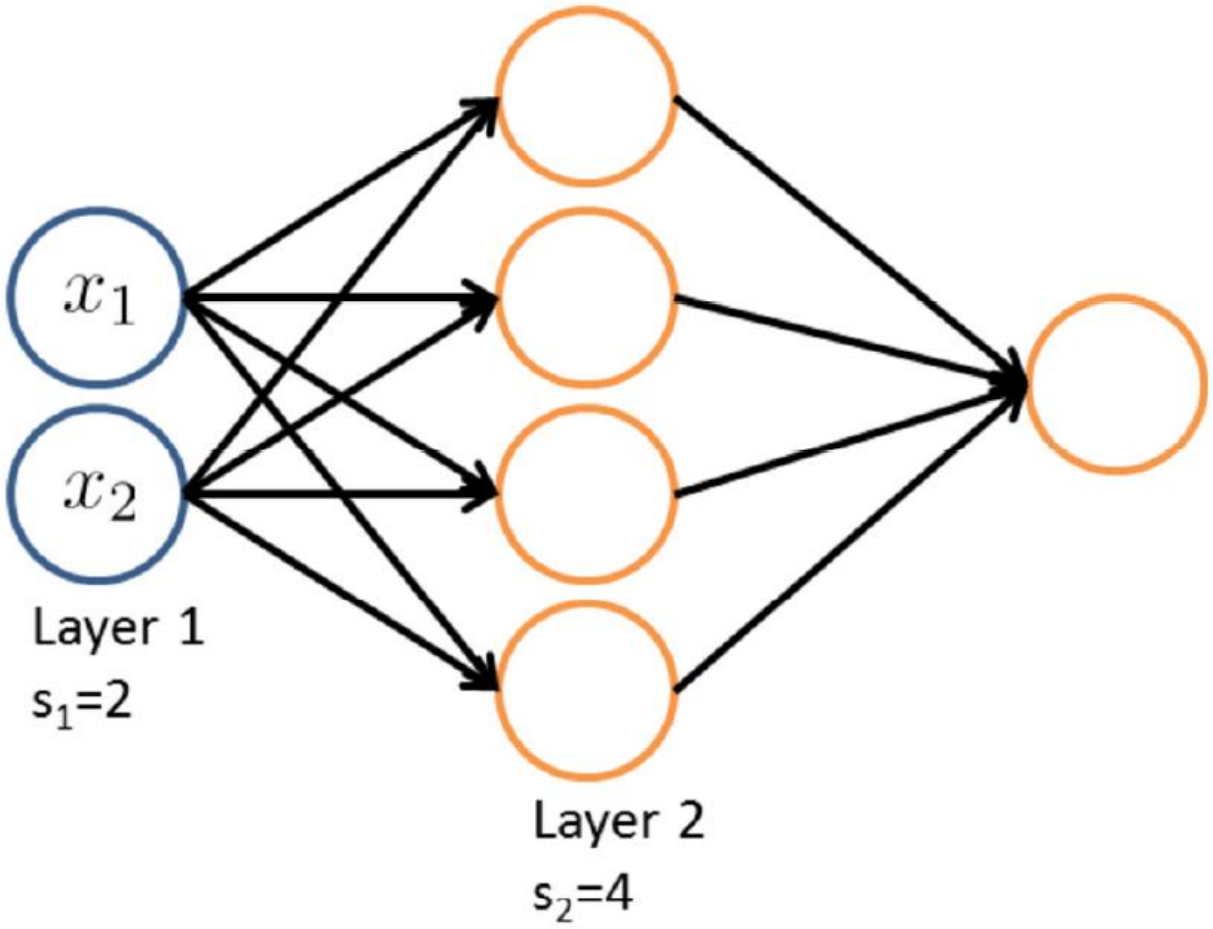
- input layer
- hidden layer
- output layer

NN can have more than one hidden layer, in addition to the input layer and output layer.

Node operation (independently of the layer)

- information processing task
- each node contains a mathematical formula, with each variable within the formula weighted differently
- (**activation function**) the output of applying that mathematical formula to the input:
  - If exceeds a certain threshold the node passes data to the next layer
  - if the output is below the threshold, no data is passed to the next layer.

How many weight matrices does the NN have? What is the dimension of each matrix?



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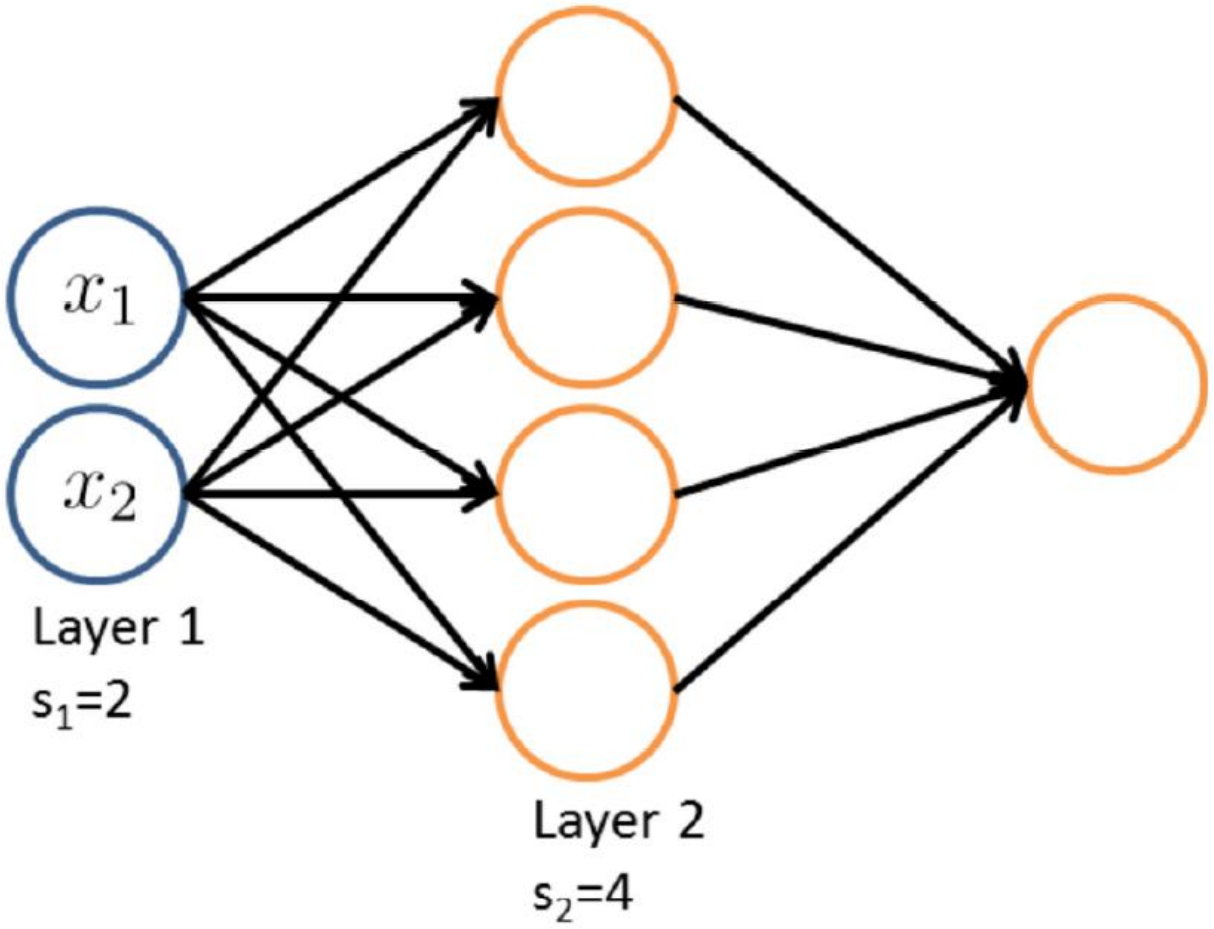
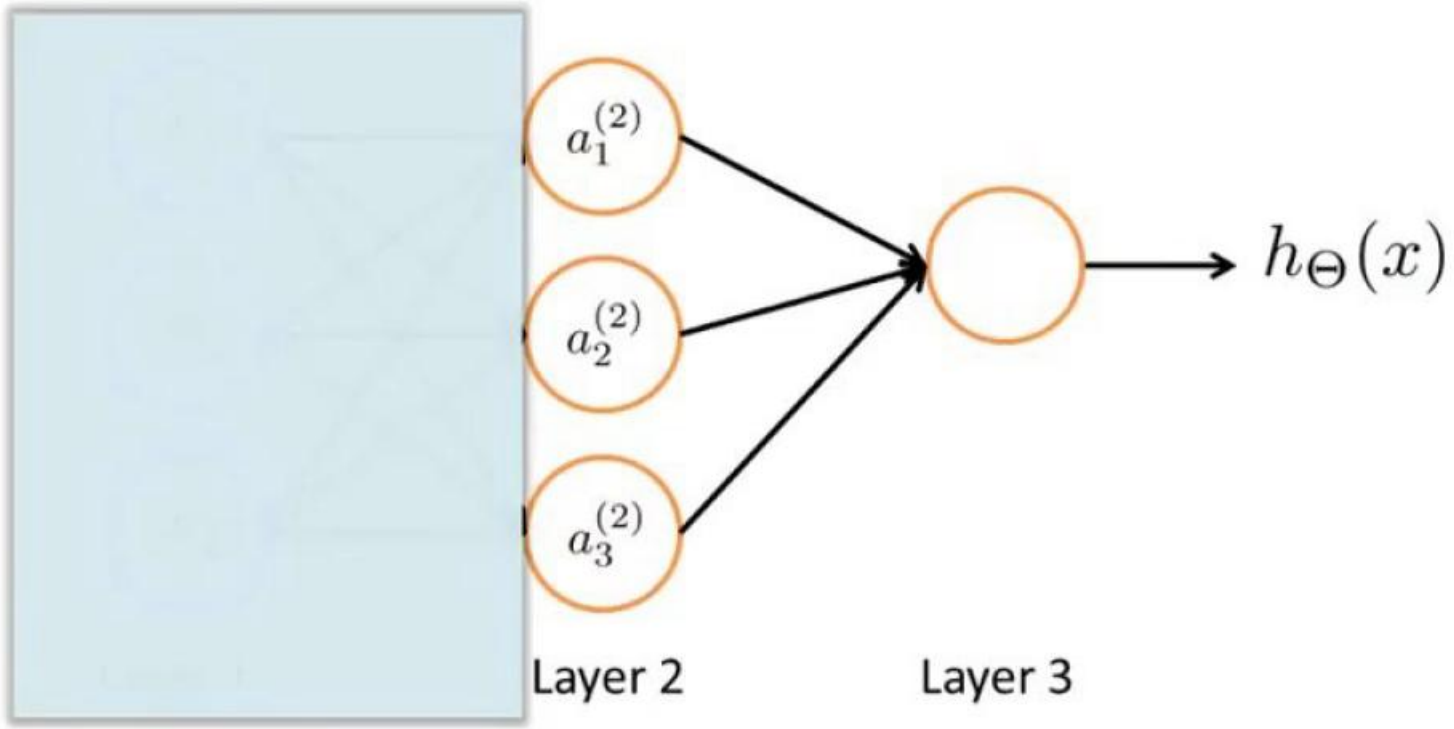


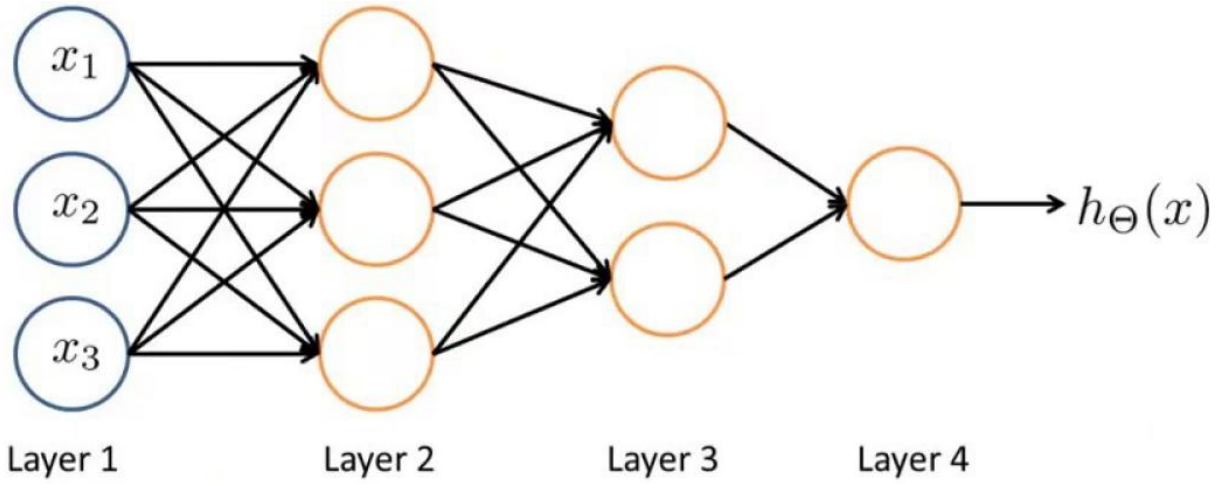
Q1=> 4x3

Q2=> 1x5

NN is learning its own features



NN - Other Architectures



Many hidden layers can built more complex functions of the inputs (the data) → NN can learn complex functions → **deep learning**

Neuron model: logistic unit

Typical Activation functions

Properties of an activation function that should be evaluated in its selection:

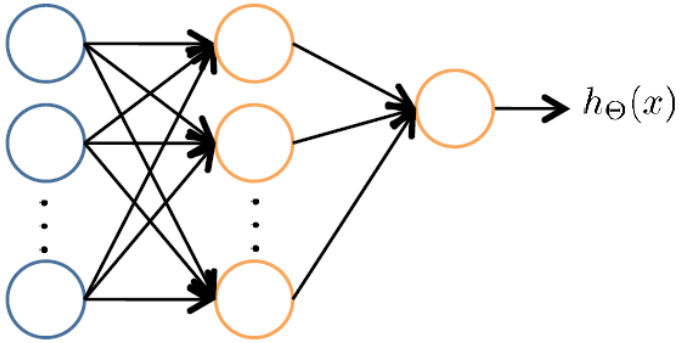
- ✓ **Nonlinearity**: The main property is nonlinearity. It is well-known that compared to a linear function, nonlinearity improves the training of ANN. Since the ANN can separate high-dimensional nonlinear data, instead of being restricted to linear space.

- ✓ **Computational cost**: The activation function is being used at every timestep during the simulations, in particular with backpropagation during training, becoming essential to validate if the activation function is trackable in terms of computation.

- ✓ **The gradient**: When training ANN, the gradient can be subject to vanishing or exploding gradient problems. This is a consequence of the activation functions contracting the variables after every step. The logistic function is contracting towards [0,1]. This can lead the network to have no gradients left to propagate back after a few iterations. A solution to this is to use non-saturating activation functions.

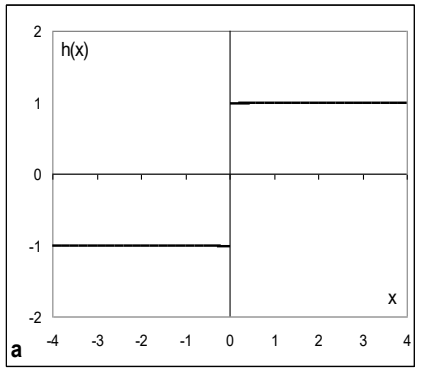
- ✓ **Differentiability**: Considering the training algorithms (e.g. backpropagation algorithm), it is necessary to ensure the differentiability of the activation function to make sure the algorithm works properly.

Typical Activation functions

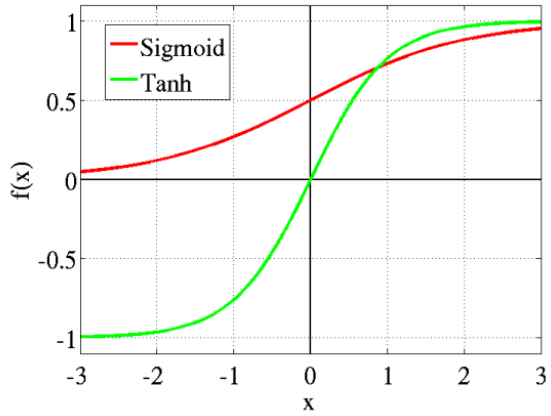


What is an Activation function in Neural networks?

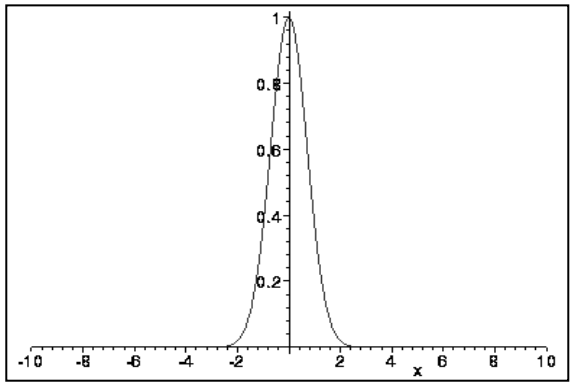
Activation function **helps decide if we need to fire a neuron or not**. If we need to fire a neuron, then what will be the strength of the signal.



Step (heaviside)



Sigmoid (logistic) vs.
Hyperbolic tangent (Tanh)



Radial Basis Function (RBF)

Typical Activation functions

RELU:

+ Computationally efficient— the network training can converge faster

+ Non-linear (though it looks like a linear function), it is easy to compute the ReLU derivative => suitable to be used for backpropagation.

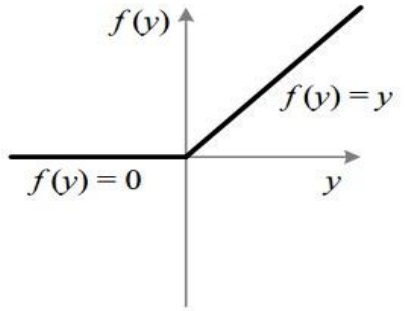
- Dying ReLU problem—when inputs approach zero, or are negative, ReLu gradient = 0, the network cannot perform backpropagation and cannot learn.

Leaky ReLU:

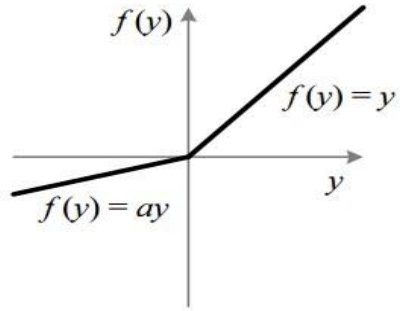
+ Prevents dying ReLU problem—this variation of ReLU has a small positive slope in the negative area, so it does enable backpropagation, even for negative input values.

Softmax:

handles multiple classes, has as many outputs as classes. The value of each output is the probability of the class. The sum of all softmax outputs = 1.



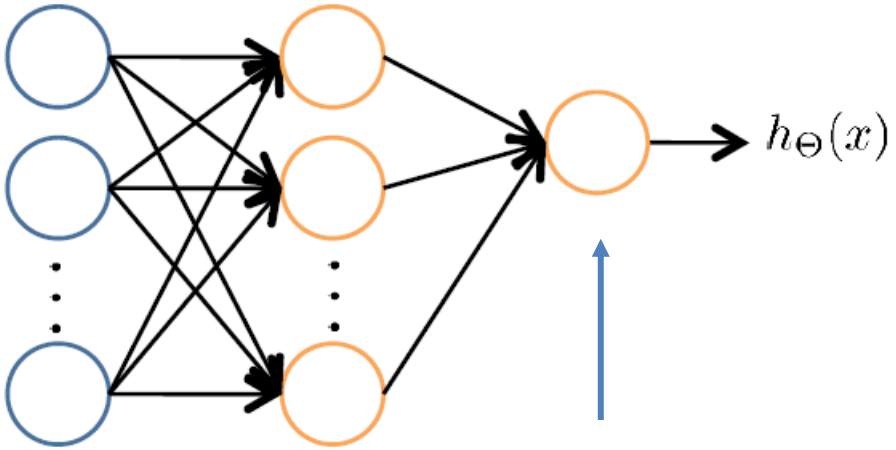
ReLU (Rectified Linear Unit)



Leaky ReLU

NN - binary versus multi-class classification

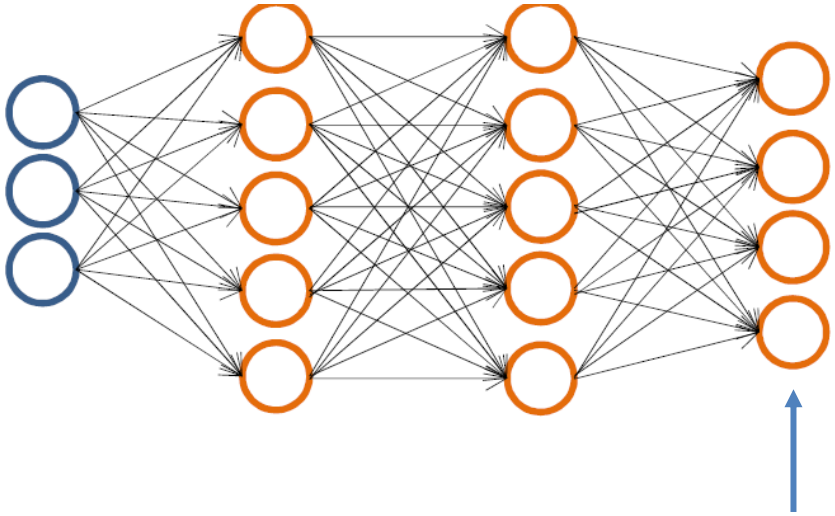
NN – Binary Classification



2 classes { 0,1 } => one output unit

Training set: $(x^{(1)}, y^{(1)}), (x^{(2)}, y^{(2)}), \ldots, (x^{(m)}, y^{(m)})$

NN – Multi-class Classification



$$h_\Theta(x) \in \mathbb{R}^4$$

K classes {1,2, K} => K output units

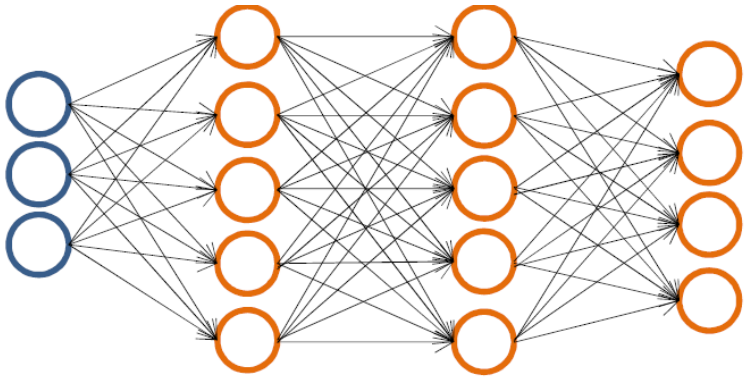
Pedestrian

Car

Motorcycle

Truck

Multiple output units: One versus all



$h_\Theta(x) \in \mathbb{R}^4$

Want $h_\Theta(x) \approx \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \end{bmatrix}$, $h_\Theta(x) \approx \begin{bmatrix} 0 \\ 1 \\ 0 \\ 0 \end{bmatrix}$, $h_\Theta(x) \approx \begin{bmatrix} 0 \\ 0 \\ 1 \\ 0 \end{bmatrix}$, etc.

when pedestrian when car when motorcycle

Training set: $(x^{(1)}, y^{(1)}), (x^{(2)}, y^{(2)}), \ldots, (x^{(m)}, y^{(m)})$

$y^{(i)}$ one of $\begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \end{bmatrix}$, $\begin{bmatrix} 0 \\ 1 \\ 0 \\ 0 \end{bmatrix}$, $\begin{bmatrix} 0 \\ 0 \\ 1 \\ 0 \end{bmatrix}$, $\begin{bmatrix} 0 \\ 0 \\ 0 \\ 1 \end{bmatrix}$

Cost function

NN Cost Functions (without regularization)

Logistic Regression
(Binary cross-entropy loss function)

$$J(\theta) = \frac{1}{m} \sum_{i=1}^{m} \left[-y^{(i)} \log(h_\theta(x^{(i)})) - (1 - y^{(i)}) \log(1 - h_\theta(x^{(i)})) \right]$$

NN with 1 output (logistic) unit
(suitable for binary classification)

$$J(\theta) = \frac{1}{m} \sum_{i=1}^{m} \left[-y^{(i)} \log(h_\theta(x^{(i)})) - (1 - y^{(i)}) \log(1 - h_\theta(x^{(i)})) \right]$$

NN with K output (logistic) units
(suitable for multiclass problems)

$$J(\theta) = \frac{1}{m} \sum_{i=1}^{m} \sum_{k=1}^{K} \left[-y_k^{(i)} \log((h_\theta(x^{(i)}))_k) - (1 - y_k^{(i)}) \log(1 - (h_\theta(x^{(i)}))_k) \right]$$

NN with 1 output (**not** logistic)
(suitable for nonlinear regression problems)

$$J(\theta) = \frac{1}{2m} \sum_{i=1}^{m} \left(h_\theta(x^{(i)}) - y^{(i)} \right)^2$$

NN Cost Functions (with regularization)

Regularized Logistic Regression

$$J(\theta) = -\frac{1}{m}\left[\sum_{i=1}^{m} y^{(i)} \log h_\theta(x^{(i)}) + (1-y^{(i)}) \log(1 - h_\theta(x^{(i)}))\right] + \frac{\lambda}{2m}\sum_{j=1}^{n} \theta_j^2$$

Regularization term

NN with K output (logistic) units

$$h_\Theta(x) \in \mathbb{R}^K \quad (h_\Theta(x))_i = i^{th} \text{ output}$$

$$J(\Theta) = -\frac{1}{m}\left[\sum_{i=1}^{m}\sum_{k=1}^{K} y_k^{(i)} \log(h_\Theta(x^{(i)}))_k + (1-y_k^{(i)}) \log(1 - (h_\Theta(x^{(i)}))_k)\right]$$

$$+\frac{\lambda}{2m}\sum_{l=1}^{L-1}\sum_{i=1}^{s_l}\sum_{j=1}^{s_{l+1}} (\Theta_{ji}^{(l)})^2$$

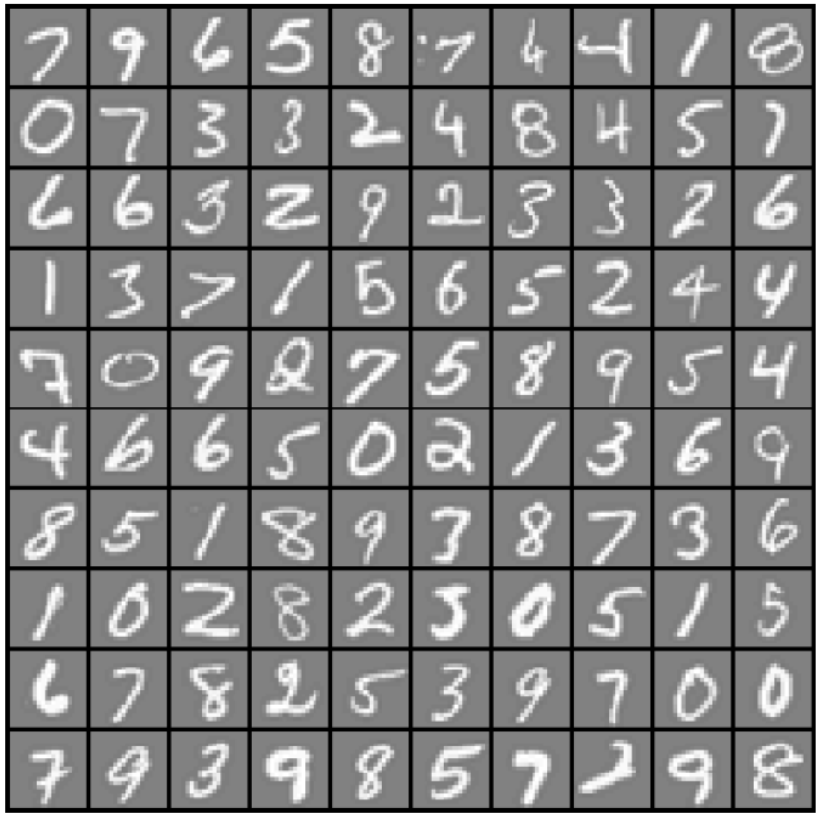
Regularization term

$L =$ total no. of layers in network

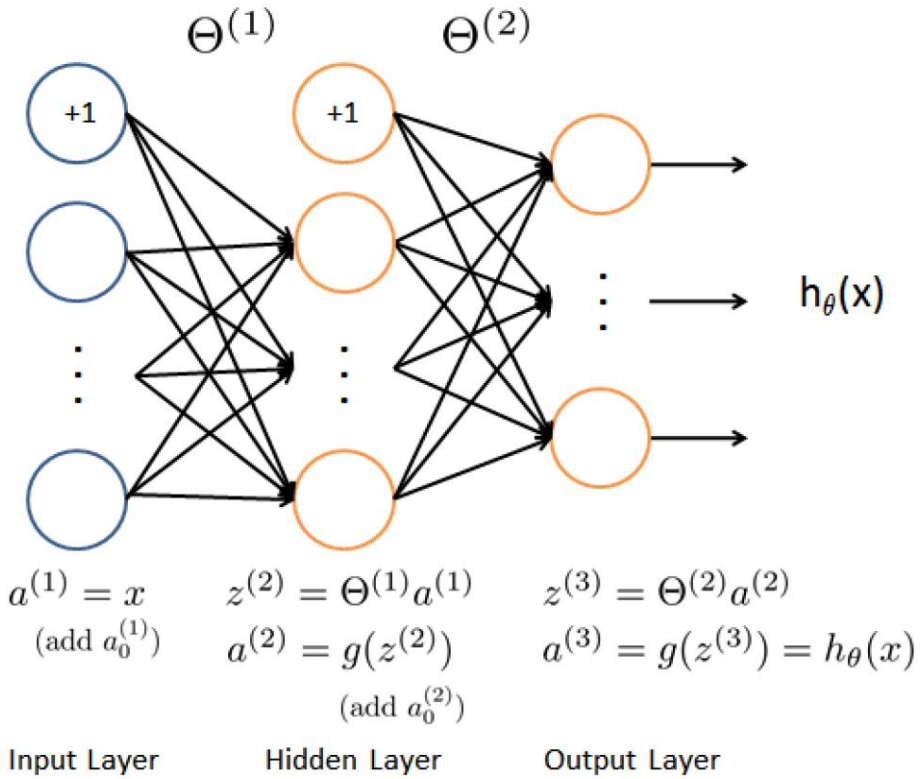
$s_l =$ no. of units (not counting bias unit) in layer l

NN classification - example

- MNIST handwritten digit dataset (http://yann.lecun.com/exdb/mnist/).
- 5000 training examples (20x20 pixels image, indicating the grayscale color intensity).
- The image is transformed into a row vector (with 400 elements).
- This gives 5000 x 400 data matrix X (every row is a training example).



NN classification - example

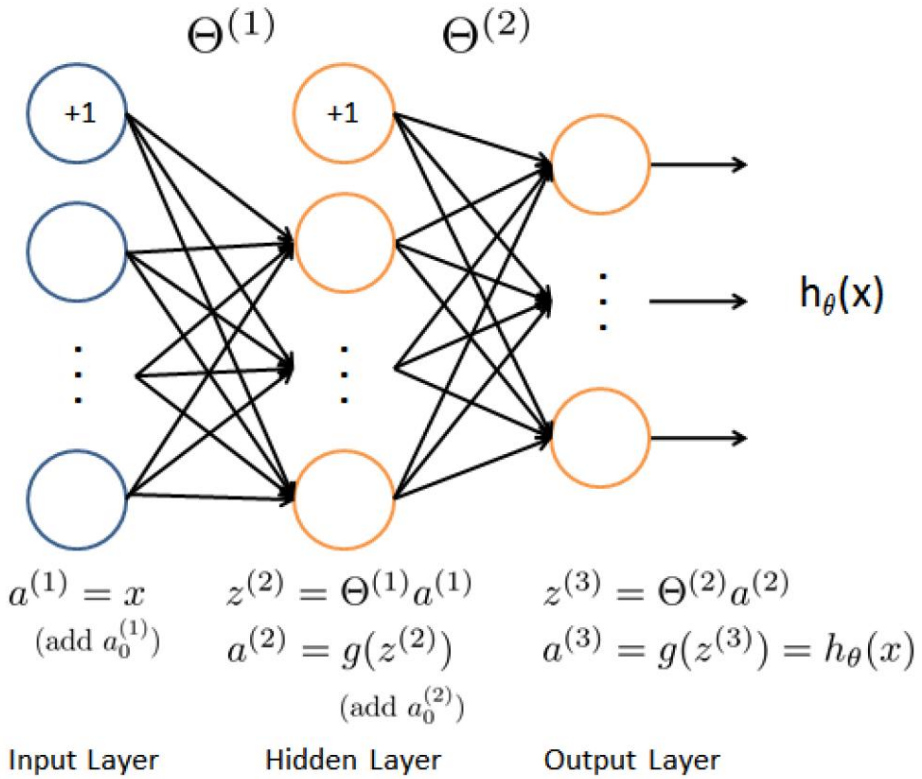


$$y = \begin{bmatrix} 1 \\ 0 \\ 0 \\ \vdots \\ 0 \end{bmatrix}, \begin{bmatrix} 0 \\ 1 \\ 0 \\ \vdots \\ 0 \end{bmatrix}, \quad \dots \quad \text{or} \quad \begin{bmatrix} 0 \\ 0 \\ 0 \\ \vdots \\ 1 \end{bmatrix}$$

- input layer:
  - 400 units = 20x20 pixels (input features) + 1 unit (the bias)
- hidden layer:
  - 25 units + 1 unit (the bias)
- output layer:
  - 10 output units (corresponding to 10-digit classes 0,1,2….9).

Matrix parameters: Θ_1 has size 25x401; Θ_2 has size 10x26.

NN model learning – forward pass



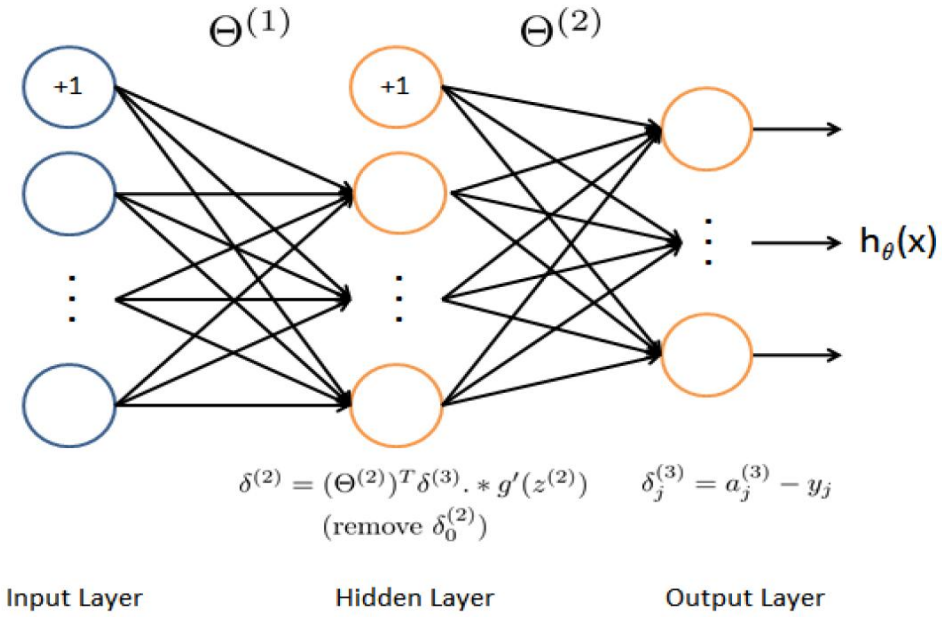
- Randomly initialize the NN parameters (matrices Q_1 and Q_2).
- Provide features as inputs to the NN, make a forward pass to compute all activations through the NN and the NN outputs.
- Repeat for all examples (batch training)

Feedforward Neural Networks

Feedforward neural networks are the simplest type of neural network. Information flows in one direction, from the input layer to the output layer, without any loops or feedback connections. These networks are commonly used for classification and regression tasks.

Backpropagation

NN model learning -Error Backpropagation



- ✓ Compute the **output error** (the difference between the NN output value and the true target value).
- ✓ For **all hidden layer nodes** compute an “error term" that measures how much that node was “**responsible**" for the NN output error.
- ✓ Compute the **gradient** as sum of the accumulated errors for all examples.
- ✓ **Update** the weights.

After each forward pass through a network, backpropagation performs a backward pass while adjusting the model’s parameters (weights and biases).

Error Backpropagation

0) Randomly initialize the parameters (matrices Θ_1 and Θ_2)
1) For ii =1:number of examples (m)
2) Provide training example *ii* at the NN input.
3) Perform a feedforward pass to compute z2, a2 (for the hidden layer) and z3, a3 (for the output layer)

4) For each unit k in the output layer compute:

$$\delta_k^{(3)} = (a_k^{(3)} - y_k)$$

5) For the hidden layer, compute:
(***error backpropagation***)

$$\delta^{(2)} = \left(\Theta^{(2)}\right)^T \delta^{(3)} .* g'(z^{(2)})$$

6) Accumulate the gradient from this example:

$$\Delta^{(l)} = \Delta^{(l)} + \delta^{(l+1)}(a^{(l)})^T$$

7) NN gradient (no regularization)

$$\frac{\partial J(\Theta)}{\partial \Theta_{ij}^{(l)}} = \frac{1}{m}\Delta_{ij}^{(l)}$$

8) Update NN parameters:

$$\Theta_{ij}^{(l)} = \Theta_{ij}^{(l)} - \alpha \frac{\partial J(\Theta)}{\partial \Theta_{ij}^{(l)}}$$

Regularized Cost Function

Cost function

$$J(\theta) = \frac{1}{m}\sum_{i=1}^{m}\sum_{k=1}^{K}\left[-y_k^{(i)}\log((h_\theta(x^{(i)}))_k) - (1-y_k^{(i)})\log(1-(h_\theta(x^{(i)}))_k)\right] +$$

$$\frac{\lambda}{2m}\left[\sum_{j=1}^{25}\sum_{k=1}^{400}(\Theta_{j,k}^{(1)})^2 + \sum_{j=1}^{10}\sum_{k=1}^{25}(\Theta_{j,k}^{(2)})^2\right]$$

Regularization term

After computing the gradient by backpropagation, add the regularization term

$$\frac{\partial}{\partial\Theta_{ij}^{(l)}}J(\Theta) = D_{ij}^{(l)} = \frac{1}{m}\Delta_{ij}^{(l)} \qquad \text{for } j = 0$$

$$\frac{\partial}{\partial\Theta_{ij}^{(l)}}J(\Theta) = D_{ij}^{(l)} = \frac{1}{m}\Delta_{ij}^{(l)} + \frac{\lambda}{m}\Theta_{ij}^{(l)} \qquad \text{for } j \geq 1$$

Parameters Update

Learning rate

$$\theta_j = \theta_j - \alpha \frac{\partial J}{\partial \theta_j}$$

Learning rate:

- Fixed
- Adaptive

$$\alpha^{(r+1)} = \begin{cases} b\alpha^{(r)} & if \quad J^{(r+1)} \le J^{(r)}, \quad b \ge 1 \, (\text{ex. } b = 1.2) \\ b\alpha^{(r)} & if \quad J^{(r+1)} > J^{(r)}, \quad b < 1 \, (\text{ex. } b = 0.2) \end{cases} \qquad \alpha^{(0)} = 0.01$$

Gradient Descent with momentum
(extra term - momentum)

$$\theta_j^{(r)} = \theta_j^{(r-1)} - \alpha \frac{\partial J}{\partial \theta_j} + \beta\left(\theta_j^{(r-1)} - \theta_j^{(r-2)}\right)$$

Coefficient of momentum:

- Increase convergence rate far from minima
- Slow down near minima

Gradient Descent with momentum is analogous to a ball moving on a surface with multiple valleys, accelerating on steep slides and decelerating when it reaches a valley.
The intuition behind is to add inertia to the gradient descent so that it smooth's the overall trajectory, in order to find better convergence points.

NN Parameters (weights) Initialization

Setting the weights to zero (Simplest approach)
However, by initializing every weight to zero, every neuron will have the same activations, all the calculated gradients will be the same, and consequently, each parameter will suffer the same update. Therefore, the initialization of the weights must break the symmetry between different units.

Drawn from a random Gaussian distribution with mean 0 & deviation 1
This may lead to vanishing gradients

Empirical initializations:
Xavier/ Glorot's initialization
It is drawn from uniform distribution near zero.

$$\sim U(-\frac{\sqrt{6}}{\sqrt{m}}, \frac{\sqrt{6}}{\sqrt{m}})$$

LeCun initialization:

$$\sim U(-\frac{\sqrt{3}}{\sqrt{m}}, \frac{\sqrt{3}}{\sqrt{m}})$$

Advantages

- ✓ **Ability to Learn Complex Patterns**: Neural networks can discover intricate patterns and relationships within data, even when they are not explicitly defined.
- ✓ **Adaptability**: They can adapt to changing conditions by adjusting their internal parameters, making them flexible and robust.
- ✓ **Parallel Processing**: Neural networks can process multiple inputs simultaneously, enabling fast and efficient computations.
- ✓ **Non-linear Transformations**: Activation functions introduce non-linearities, allowing neural networks to model complex non-linear relationships.

Limitations

- ✓ **Computational Requirements**: Training and evaluating large neural networks can be computationally intensive, requiring substantial computing resources.
- ✓ **Data Dependency**: Neural networks heavily rely on large, high-quality datasets for effective training and generalization. Insufficient or biased data can impact their performance.
- ✓ **Lack of Explainability**: Neural networks are often referred to as “black boxes” since it can be challenging to understand their decision-making process. Interpreting their inner workings and providing explanations for their predictions can be difficult.

Examples of NN algorithms

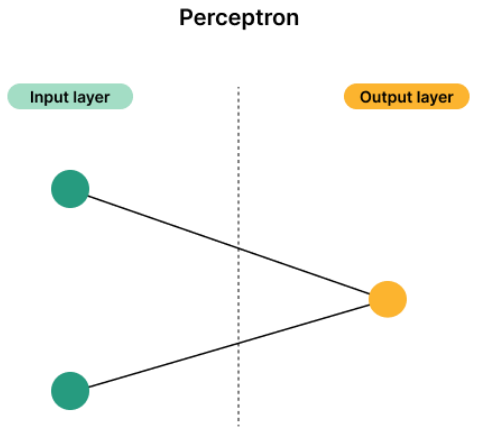
There is no limit on how many nodes and layers a neural network can have, and these nodes can interact in almost any way. Because of this, the list of types of neural networks is ever-expanding.

But, they can roughly be sorted into these categories:

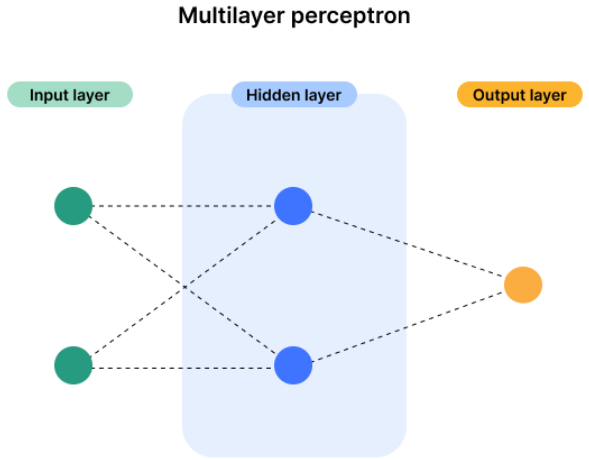
- **Shallow neural networks** usually have only one hidden layer
- **Deep neural networks** have multiple hidden layers

Shallow neural networks are fast and require less processing power than deep neural networks, but they cannot perform as many complex tasks as deep neural networks.

Examples of NN algorithms

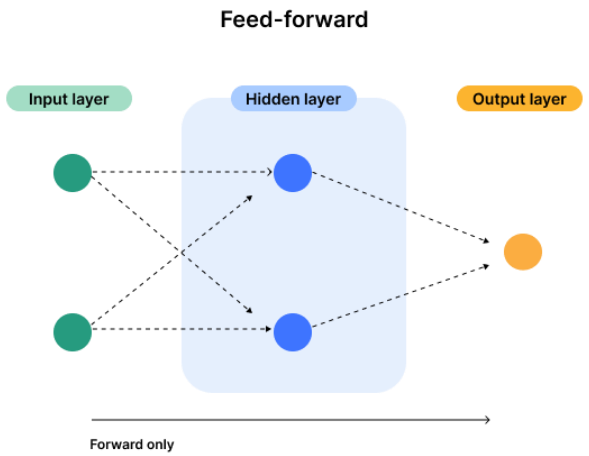


Perceptron neural networks are simple, shallow networks with an input layer and an output layer.

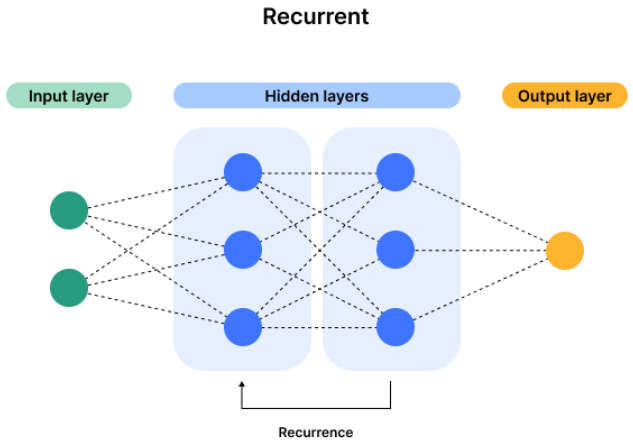


Multilayer perceptron neural networks add complexity to perceptron networks, and include a hidden layer.

Examples of NN algorithms

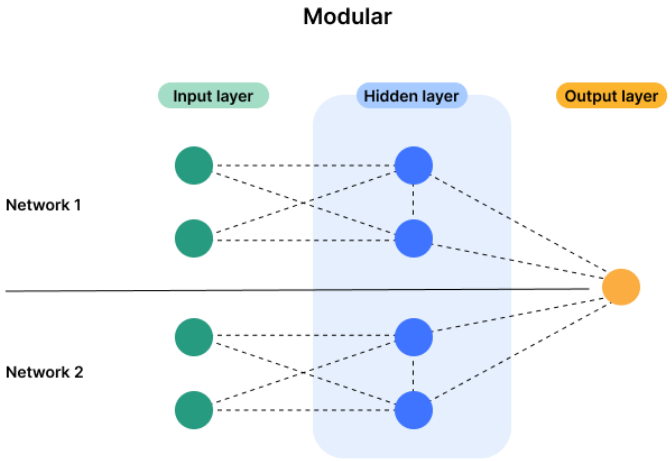


Feed-forward neural networks only allow their nodes to pass information to a forward node.

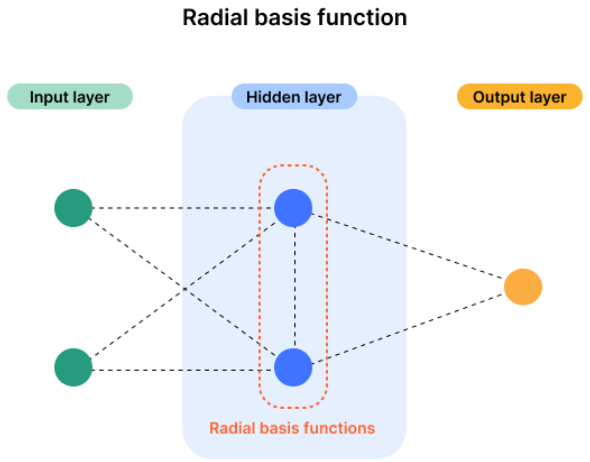


Recurrent neural networks (RNN) can go backwards, allowing the output from some nodes to impact the input of preceding nodes. These learning algorithms are primarily leveraged when using time-series data to make predictions about future outcomes, such as stock market predictions or sales forecasting.

Examples of NN algorithms

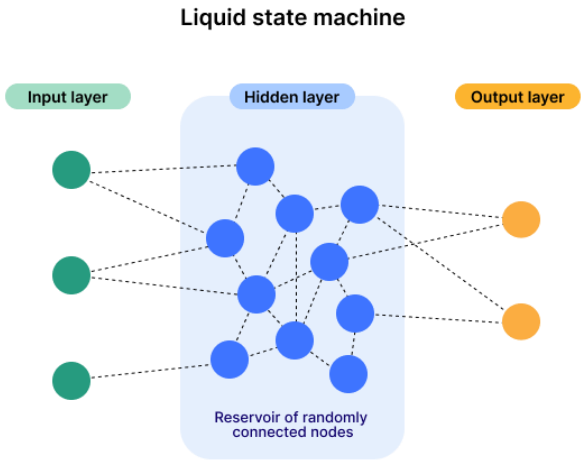


Modular neural networks combine two or more neural networks to arrive at the output.

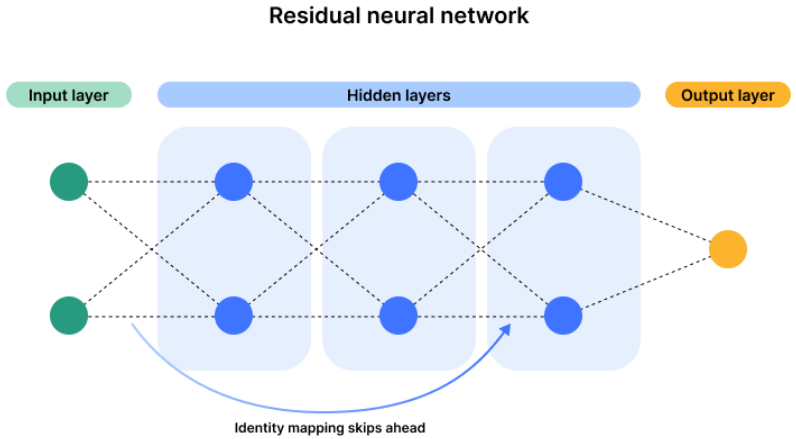


Radial basis function neural network nodes use a specific kind of mathematical function called a radial basis function.

Examples of NN algorithms

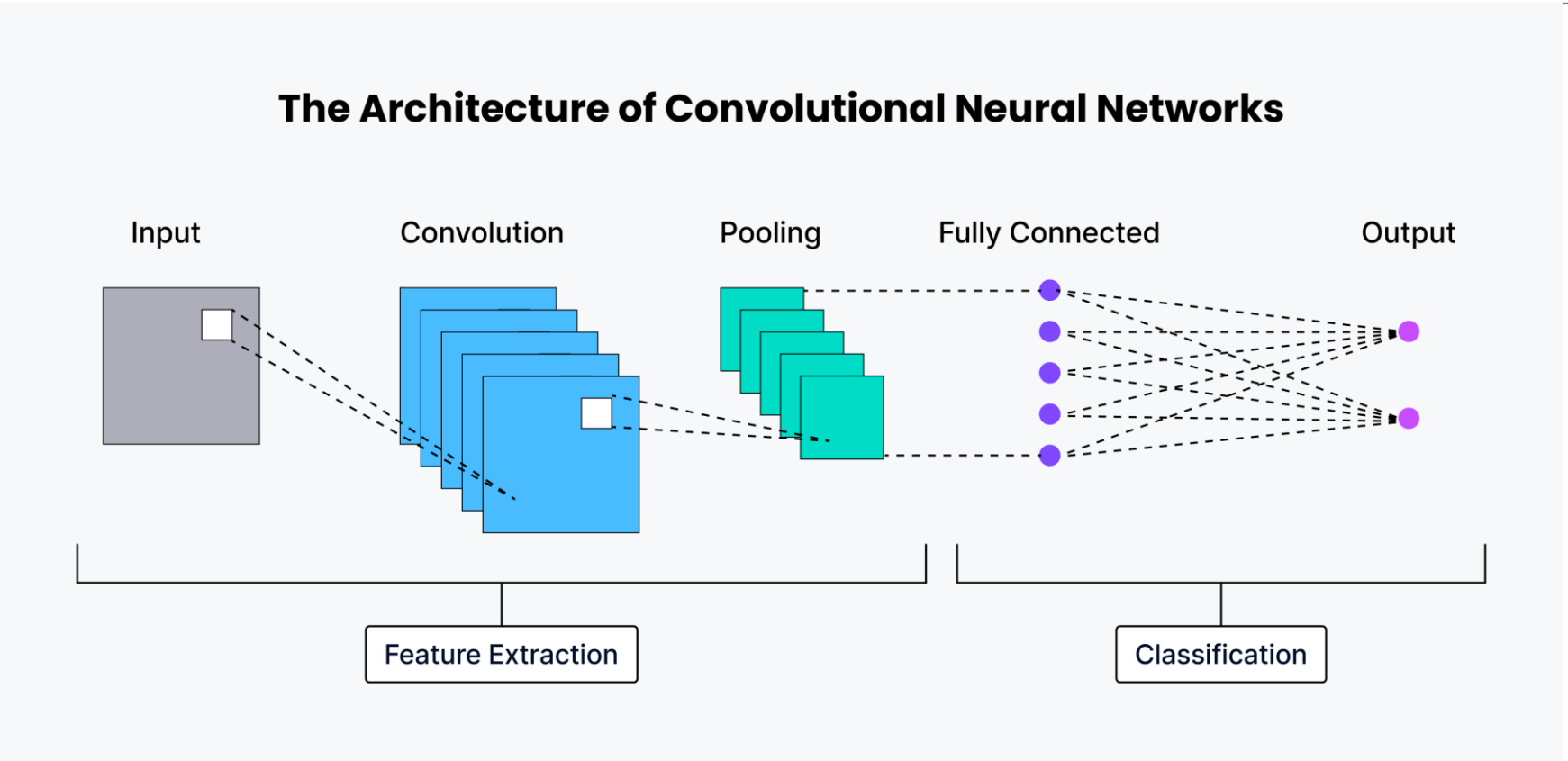


Liquid state machine neural networks feature nodes that are randomly connected to each other.



Residual neural networks allow data to skip ahead via a process called identity mapping, combining the output from early layers with the output of later layers.

Examples of NN algorithms



Convolutional neural networks (CNNs) are similar to feedforward networks, but they're usually utilized for image recognition, pattern recognition, and/or computer vision. These networks harness principles from linear algebra, particularly matrix multiplication, to identify patterns within an image.
They preserve image structure, such as local connectivity and content of the pixels of the image data, making them efficient at pattern recognition.

Deep Learning

Specifically, neural networks are used in deep learning — an advanced type of machine learning that can draw conclusions from unlabeled data without human intervention. For instance, a deep learning model built on a neural network and fed sufficient training data could be able to identify items in a photo it has never seen before.

Neural networks make many types of artificial intelligence (AI) possible. Large language models (LLMs) such as ChatGPT, AI image generators like DALL-E, and predictive AI models all rely to some extent on neural networks.

Transformer neural networks assumed a place of outsized importance in the AI models in widespread use today. First proposed in 2017, transformer models are neural networks that use a technique called "self-attention" to take into account the context of elements in a sequence, not just the elements themselves. Via self-attention, they can detect even subtle ways that parts of a data set relate to each other.

Transformer models are an integral component of generative AI, in particular LLMs that can produce text in response to arbitrary human prompts.