Neural Networks

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What to expect?

In this session we will discuss:

- Neural networks
- Gradient Descent
- Backpropagation

Evolution of AI

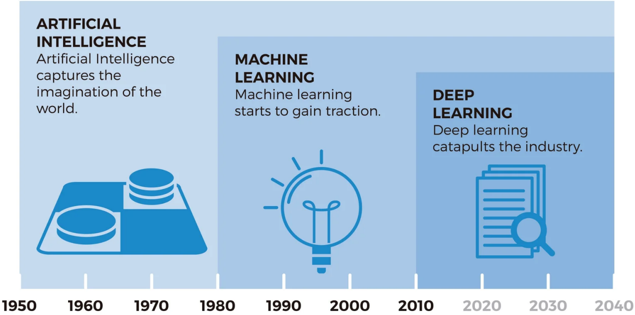

ARTIFICIAL INTELLIGENCE
Artificial Intelligence captures the imagination of the world.
MACHINE LEARNING
Machine learning starts to gain traction.
DEEP LEARNING
Deep learning catapults the industry.
1950
1960
1970
1980
1990
2000
2010
2020
2030
2040

Figure 1: Evolution of AI, ML and DL. Source BISMART.

Supervised ML

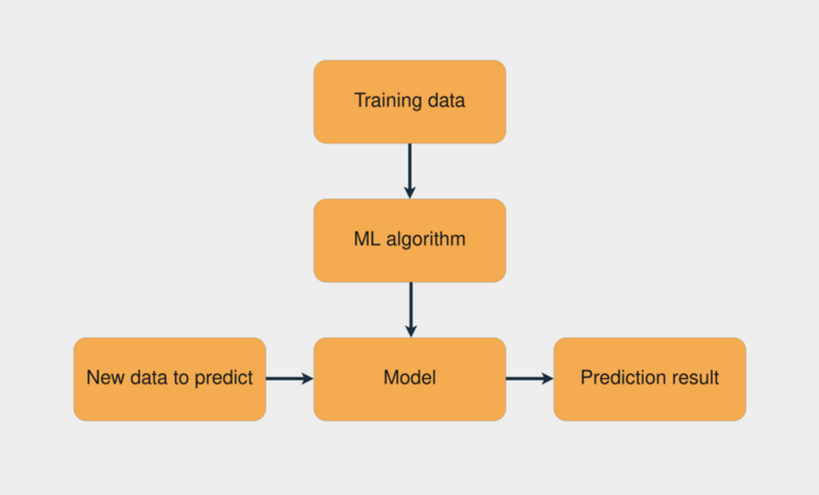


Figure 2: Workflow to train a model using supervised learning.

Supervised ML

- Build models capable of learning from a series of data (x)
- The learning process depends on the task we want to train the model:

Supervised the input data X is accompanied by the values y that we want the model to learn or also called targets (linear regression, decision trees, ...). The objective is that the prediction of the model given some data x is equal to the target.

Unsupervised the task to be learned is some type of association of the input data X with each other (i.e clustering).

Feature engineering

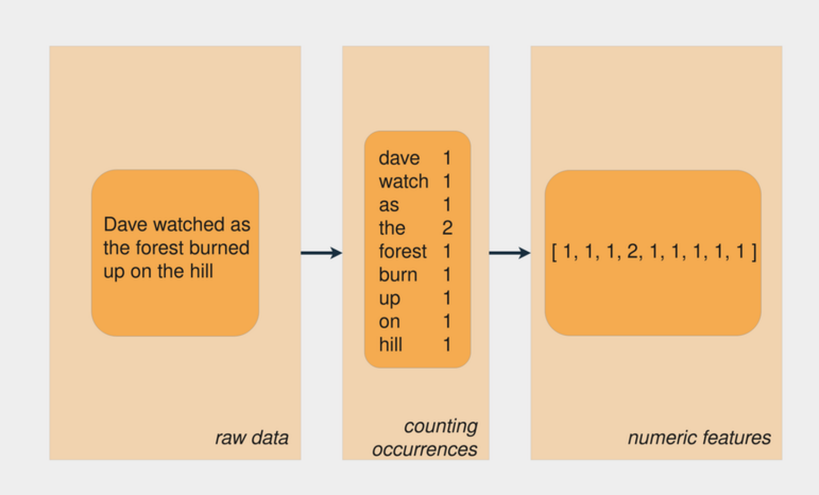


Figure 3: Feature engineering example.

Neural networks

- In the ML example above, we use lemmatization to eliminate inflection from words, generating a simpler model.
- In neural networks, **we leave the network itself** to find out the most important features in the data, without relying on feature engineering techniques.

Neural Networks are based on a collection of connected units (neurons), which, just like the synapses in a brain, can transmit a signal to other neurons, so that, acting like interconnected brain cells, they can learn and make decisions in a more human-like manner.

ML vs DL

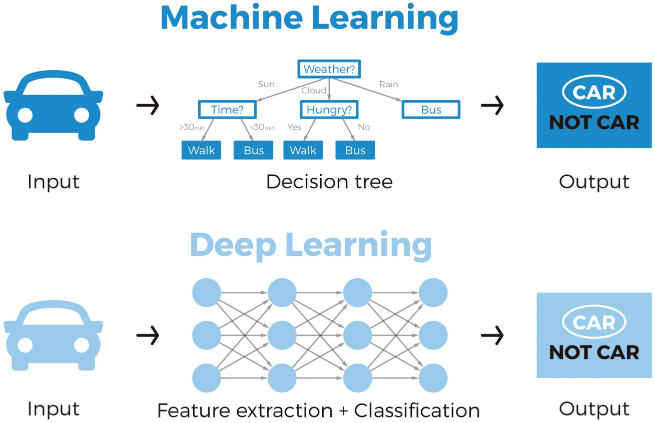


Figure 4: ML vs DL. Source BISMART

Neural networks

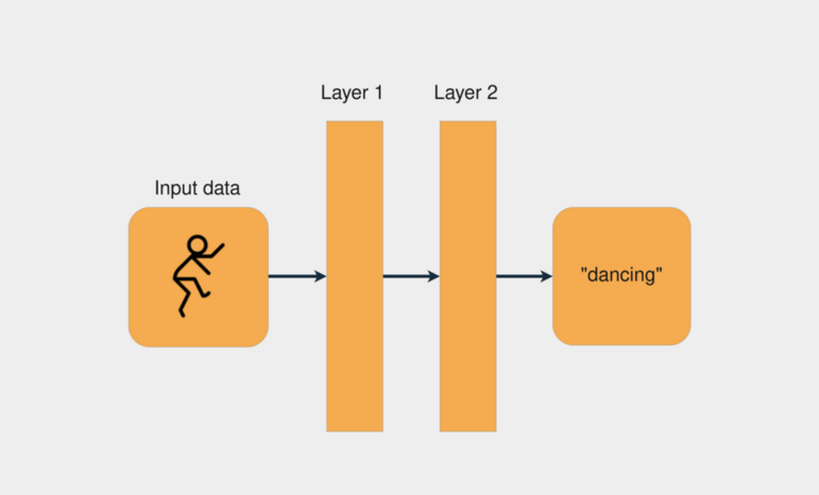
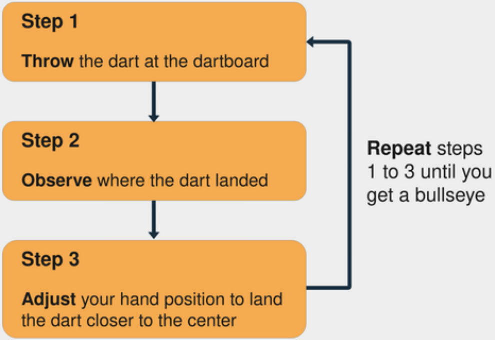


Figure 5: Schema of a 2 layer neural network.

Throwing darts and improving by learning



Step 1

Throw the dart at the dartboard

Step 2

Observe where the dart landed

Step 3

Adjust your hand position to land the dart closer to the center

Repeat steps 1 to 3 until you get a bullseye

Figure 6: Steps for trying to hit the center of a dartboard.

Artificial Neural Networks (ANN)

- ANN are formed by layers of neurons.
- Each layer has a certain number of neurons.
- The input data X enters through the first layer and through mathematical operations the input values are transformed into output values y'.
- The goal of the network is to modify the mathematical operations through some parameters (weights and biases, W and b) to minimize the difference bewteen y and y'.
- Deep Learning refers to all those models that use ANN of any type with multiple layers.

Perceptron

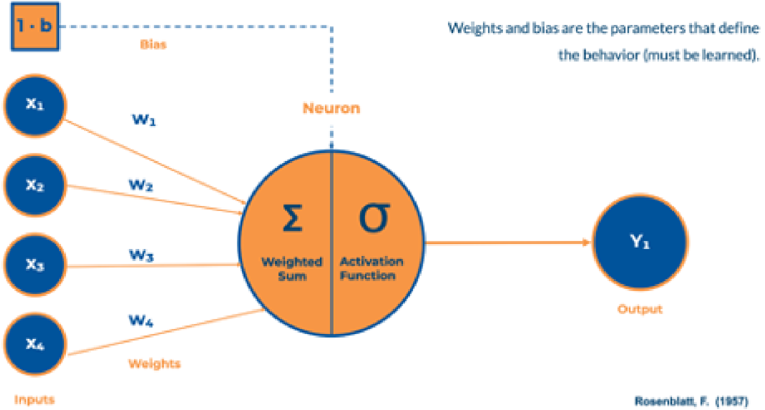


Figure 7: $w_1x_1 + w_2x_2 + w_3x_3 + w_4x_4 \leq \text{threshold} \Rightarrow Y = 0$. We can introduce bias and a given function: $\sigma(\mathbf{w} \cdot \mathbf{x} + b) = y'$. Adpated from [1].

Multilayer perceptron

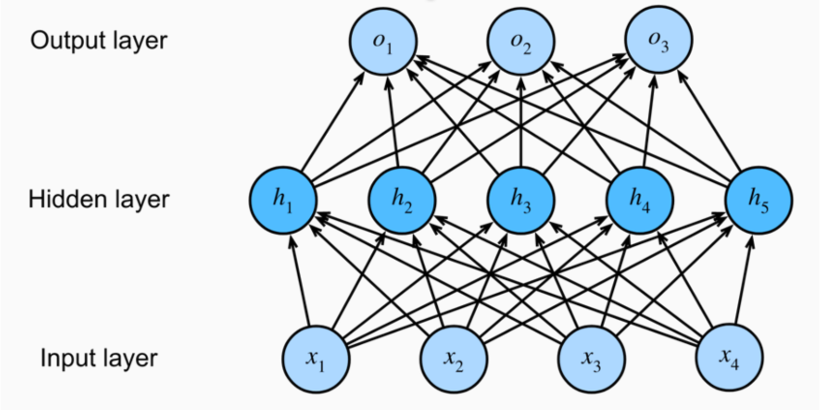


Figure 8: A multilayer perceptron with 5 hidden units.

Multilayer perceptron: some maths

$$w_{ij}^{L}, \begin{cases} L = \text{layer number} \\ i = \text{neuron from previous layer} \\ j = \text{neuron from following layer} \end{cases}$$

$$\sigma_1\left(\mathbf{W}^{(1)^T}\cdot\mathbf{X}+\mathbf{b}^{(1)}\right)=\sigma_1\left(\begin{bmatrix} w_{11}^{(1)} & w_{12}^{(1)} & w_{13}^{(1)} & w_{14}^{(1)} \\ w_{21}^{(1)} & w_{22}^{(1)} & w_{23}^{(1)} & w_{24}^{(1)} \\ w_{31}^{(1)} & w_{32}^{(1)} & w_{33}^{(1)} & w_{34}^{(1)} \\ w_{41}^{(1)} & w_{42}^{(1)} & w_{43}^{(1)} & w_{44}^{(1)} \\ w_{51}^{(1)} & w_{52}^{(1)} & w_{53}^{(1)} & w_{54}^{(1)} \end{bmatrix}\cdot\begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{bmatrix}+\begin{bmatrix} b_1^{(1)} \\ b_2^{(1)} \\ b_3^{(1)} \\ b_4^{(1)} \\ b_5^{(1)} \end{bmatrix}\right)=\mathbf{H}^{(1)}$$

$$\sigma_2\left(\mathbf{W}^{(2)^T}\cdot\mathbf{H}^{(1)}+\mathbf{b}^{(2)}\right)=\sigma_2\left(\begin{bmatrix} w_{11}^{(2)} & w_{12}^{(2)} & w_{13}^{(2)} & w_{14}^{(2)} & w_{15}^{(2)} \\ w_{21}^{(2)} & w_{22}^{(2)} & w_{23}^{(2)} & w_{24}^{(2)} & w_{25}^{(2)} \\ w_{31}^{(2)} & w_{32}^{(2)} & w_{33}^{(2)} & w_{34}^{(2)} & w_{35}^{(2)} \end{bmatrix}\cdot\begin{bmatrix} h_1 \\ h_2 \\ h_3 \\ h_4 \\ h_5 \end{bmatrix}+\begin{bmatrix} b_1^{(2)} \\ b_2^{(2)} \\ b_3^{(2)} \end{bmatrix}\right)=\mathbf{Y}^{\text{out}}$$

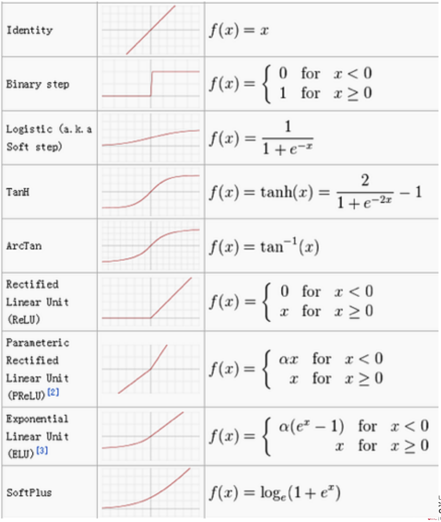
Multilayer perceptron: some details

- The MLP is the simplest neural network
- Weights connect neurons from an inner to an outer layer
- Operations in each layer are implemented using matrices and vectors
- The **forward pass** of the last layer produces the ouput.
- The MLP can be interpreted as a multivariant function with W and b as the parameters, X as input and Y^{out} as output.
- **Hiperparameters** are additional parameters that control other aspects: number of layers, number of neurons per layer, acivation functions, ...

Activation functions

Activation functions:

- The **sigmoid** function is used in the final layer in classification models.
- **ReLU** is used in inner layers, as they produce non-linerity.
- All are differentiable.



Identity		$f(x) = x$
Binary step		$f(x) = \begin{cases} 0 & \text{for} \quad x < 0 \\ 1 & \text{for} \quad x \geq 0 \end{cases}$
Logistic (a.k.a Soft step)		$f(x) = \dfrac{1}{1 + e^{-x}}$
TanH		$f(x) = \tanh(x) = \dfrac{2}{1 + e^{-2x}} - 1$
ArcTan		$f(x) = \tan^{-1}(x)$
Rectified Linear Unit (ReLU)		$f(x) = \begin{cases} 0 & \text{for} \quad x < 0 \\ x & \text{for} \quad x \geq 0 \end{cases}$
Parameteric Rectified Linear Unit (PReLU)[2]		$f(x) = \begin{cases} \alpha x & \text{for} \quad x < 0 \\ x & \text{for} \quad x \geq 0 \end{cases}$
Exponential Linear Unit (ELU)[3]		$f(x) = \begin{cases} \alpha(e^x - 1) & \text{for} \quad x < 0 \\ x & \text{for} \quad x \geq 0 \end{cases}$
SoftPlus		$f(x) = \log_e(1 + e^x)$

An example of a 2 layer Neural Network

Example of classification (for categories "1" and "0") with a 2 layers NN.

- In the first layer we use a linear regression approach.
- The second layer includes the non-linearity through the use of a sigmoid function that decides whether the prediction is 1 or 0, following the Bernouilli distribution.

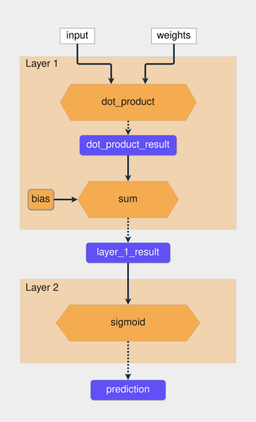


Figure 9: Training a two layer neural network.

The logistic function

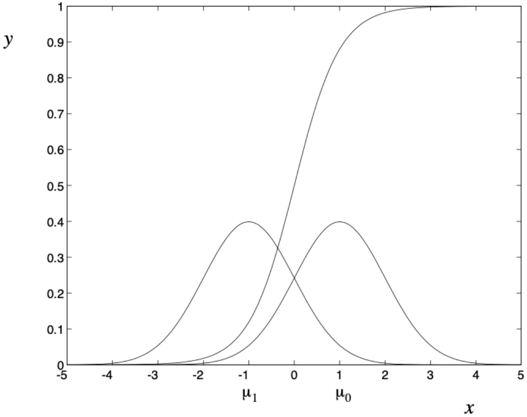


Figure 10: A binary classification problem. The class-conditional densities are Gaussians with unit σ^2. The posterior probability is the logistic function $y = 1/(1 + \exp\{(-2x)\})$[2].

Exercise 1

Loss/Cost function in a simple 2 layer NN Check the provided code for this session and expand it to:

1. Generate a collection of 100 synthetic data points from a two Gaussian distribution.
2. Assign the data points a category "0" or "1" depending on the Gaussian function they are obtained from.
3. Use the provided 2 layers NN to evaluate the expected value of the loss function with the provided weights.
4. Can you guess the weights that would improve the prediction (reducing the value of the error)?

Backpropagation: weights

Chain Rule in Backpropagation In each **backward pass**, you compute the partial derivatives of each function, substitute the variables by their values, and finally multiply everything.

Notice that, for the sigmoid function $f(x) = \frac{1}{1+e^{-x}}$, $f'(x) = 1 - f(x)$.

```
derror_dweights =
derror_dprediction
* dprediction_dlayer1
* dlayer1_dweights
```

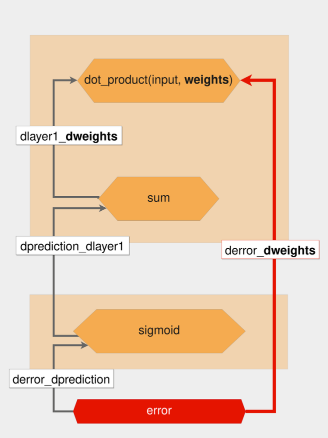


Figure 11: Chain rule: derivative of the error with respect to **weights**.

Backpropagation: bias

Chain rule applied to the derivative of the bias error in the 2 layer example.

```
derror_dbias =
derror_dprediction
* dprediction_dlayer1
* dlayer1_dbias
```

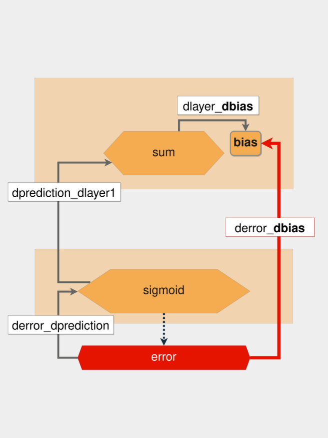


Figure 12: Chain rule: derivative of the error with respect to bias.

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