MARTA

Machine le**AR**ning **T**utori**A**l

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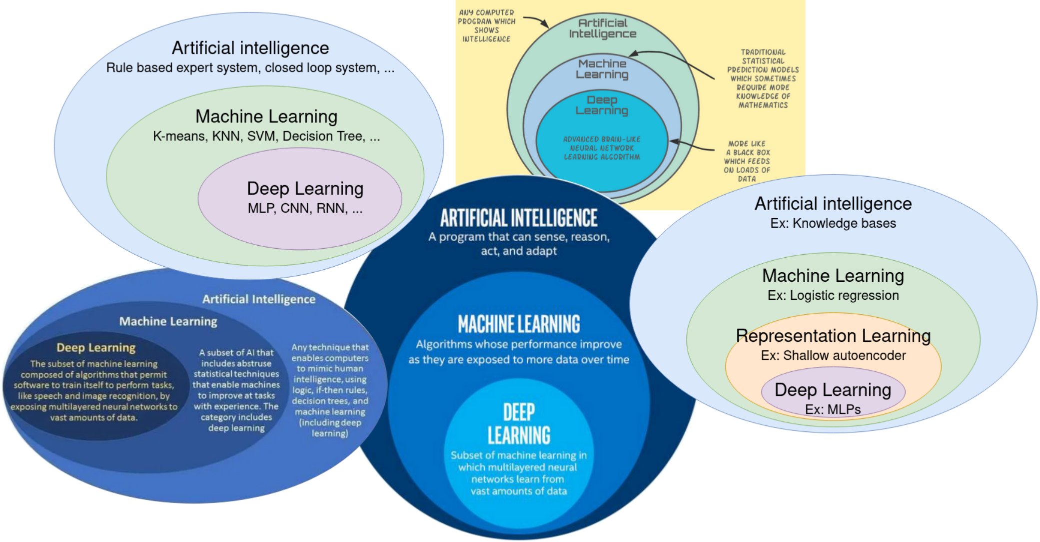
What is Machine Learning ?



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Images extracted from [1, 2, 4, 5, 6]

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What is Machine Learning ?

Machine Learning can be further classified in **three** categories:

Supervised | **Semi-supervised** | **Unsupervised**

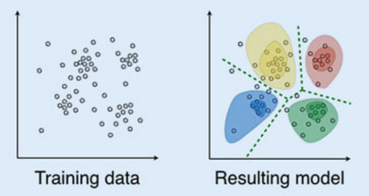
= Lion

= Cow

= Dog

= Labels

Uses a small set of **labeled** data and a larger set of **unlabeled** data, happy compromise between the two previous categories.



PCA and **POD** are also examples of unsupervised learning (=dimensionality reduction) and can also be performed with neural networks

What is Machine Learning ?

Examples of common Machine Learning algorithms:

- **Linear regression** is now part of ML techniques, even if it is used for many decades now
- **Logistic regression** is a supervised learning used to make predictions for categorical response variables
- **Clustering** is an unsupervised learning that identifies patterns in data to group them
- **Decision trees** are used both for regression problems (prediction of numerical values) and for classification (branching sequence of linked decisions)
- **Random forests**, the machine learning algorithm predicts a value or category by combining the results from several decision trees.
- **Neural networks** can be seen as "*the way the human brain works*"

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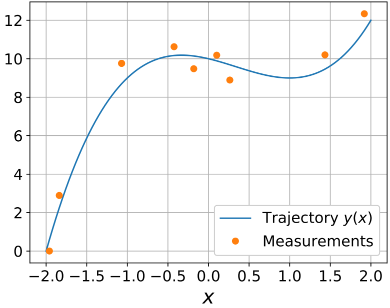
- **Speech recognition**
  - to conduct voice search (e.g., Siri)
  - to translate human speech into a written format
- **Computer vision**
  - facial recognition,
  - radiology imaging in healthcare, and
  - self-driving cars in the automotive industry.
- Applications into **Physics**
  - Space ablation model (**Tool**: LSTM)
  - Wall models and improvement of RANS models based on Direct Numerical Simulations (DNS) and Large Eddy Simulations (LES) data (**Tool**: CNN, MDN, MLP, ...)
  - Ice accretion model (**Tool**: well-chosen combination of MLP)
  - Prediction of the temperature evolution in additive manufacturing (**Tool**: Graph Neural Network)
  - ...

Let's start with a basic example of machine learning

Database

Assuming a phenomena y that is controlled by a single variable x (e.g. the trajectory a moving object with $y(x)$ the instantaneous position at time x). Let us construct a database of n pairs of values $\{(x_i, y(x_i)), i = 0, \ldots, n\}$, being a set of y measurements for different values of x.



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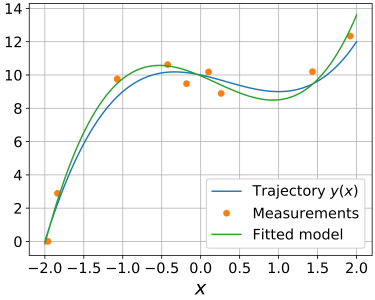
Let's start with a basic example of machine learning

Model

The database on itself is not useful. However, as an engineer, we are interested to predict the value of the phenomena y at any value of the control parameter x. We want to build a model $\hat{y}(x)$ that "*fits*" (i.e., according to a given risk) the values of the real phenomena $y(x_i)$ as recorded in the database but with generalization capabilities allowing to predict $\hat{y}$ for any x value.



Note: The model is here all polynomial functions of order 3 defined as

$$\hat{y} = p_3 x^3 + p_2 x^2 + p_1 x + p_0$$

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Let's start with a basic example of machine learning

Method

1. **Database creation:** build, clean, and organize the available data in an adapted format
2. **Model definition:** the example above uses a polynomial fitting of order 3 such that we try to fit the four coefficients in $\hat{y} = p_3x^3 + p_2x^2 + p_1x + p_0$ according to a given risk
3. **Training the model on the database:** an optimization method is used to adjust the values of the four model parameters p_i such that $\hat{y}(x)$ is "*close*" (according to a given *metric*) to the measured value $y(x)$ for each of the point $(x, y(x))$ in the database
   - Define a minimization function $\mathcal{L}$ (e.g., MSE)
   - Setup an optimization method to adapt the four parameters (e.g., gradient descent):

   $$p_{i,t+1} = p_{i,t} - \gamma \left(\frac{\partial \mathcal{L}}{\partial p_i}\right)_t \quad \text{where } \gamma \text{ is the learning rate}\,.$$

   - Loop over the database to reach the desired model accuracy
   - Save the '*trained model*' for future use
4. **Test** the '*trained model*' on unseen data

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More complicated example of machine learning

Remark

The previous example was an easy one-to-one relation. However, real-world problems are not as simple as that.

Question

How can an algorithm be implemented to recognise low-resolution handwritten digits (see figure on the right [3])?

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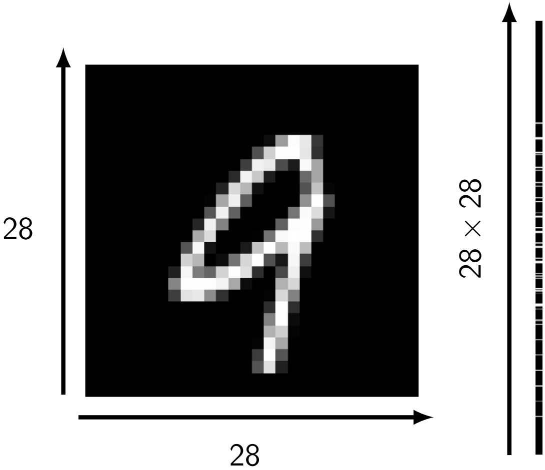
Digits classification using (deep) neural network

The human brain can quickly distinguish a three, a one, or a nine, but how can a machine make the same distinction as us? This is where deep learning appears as *almost miraculous*. Deep neural networks are large artificial neural networks (ANN) that claim to combine both

- automatic feature engineering, and,
- **universal approximation** capabilities.

Thanks to their hidden and activation layers, ANN are able to identify relevant features and their functional relationships with limited human intervention. However, the remaining **drawback** is the size of the database that needs to be large enough to capture the relevant phenomena. You will also have to deal with a list of **hyperparameters** to tune.

More complicated example of machine learning



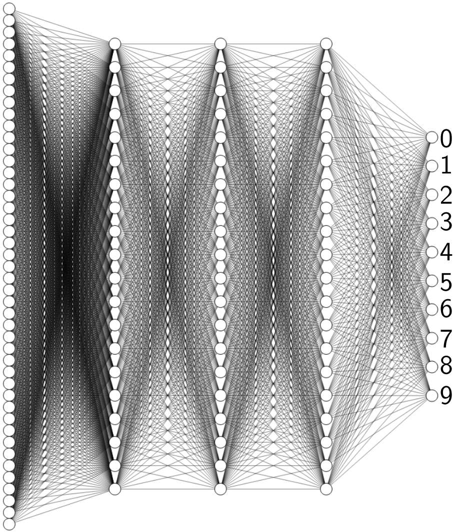


Image extracted from MNIST database and neural network generated on https://alexlenail.me/NN-SVG/

After this brief introduction about Machine Learning model, we can dive into the tutorial which is construct according to six sections:

1. The **first** section is dedicated to the `Pytorch` data structures. Through this section, we will see how to construct a tensor and how to perform operations on them.

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6. The **sixth** section ... it's your turn.

Nomenclature[1]

- **Input** is a p-dimensional vector of features or descriptors.
- **Output** is the prediction of a model (e.g., a scalar value, a label, an image, a signal, ...).
- **Target** is the feature of a dataset about which you want to gain a deeper underdstanding.
- **Epoch** is a N/batch size training iterations, where N is the size of training database (i.e., number of training samples). A full training pass over the entire training set such that each sample of the training database is visited.
- **Batch** is a set of samples used in one training iteration.
- **Batch size** corresponds to the number of samples contained in a batch.
- **Learning rate** is a floating point which is multiplied to the gradient to adjust the weights and biases on each iteration.
- **Layer** is a set of neurons in a neural network. There exists three common layers: the input layer, the hidden layer and the output layer. A model underfits the training data if it has poor prediction abilities because it has not fully captured the training data complexity.

[1] Inspired by `https://developers.google.com/machine-learning/glossary$#$h`

- **Backpropagation** is an algorithm that implements the gradient descent based on the chain rule for a neural network.
- **Neuron** is the basic unit of computation in a neural network, aslo called node or unit.
- **Weights and Biases** are parameters learned during the training.
- **Hyperparameter** is a parameter whose value is used to control the learning process (e.g. the learning rate).
- **Loss function** measures how far the model's prediction is from its target value (i.e., its label) according to a given metric (e.g. MSE, Cross Entropy, ...).
- **Activation function** is the key ingredient to help neural network to learn nonlinear (complex) relationship between the features (=inputs) and the label (=targets).
- **Overfitting** A model overfits the training data if the predictions on it are so closely that it fails to make correct predictions on unseen data.
- **Underfitting** A model underfits the training data if it has poor prediction abilities because it has not fully captured the training data complexity.

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AI vs ML vs DL Venn Diagram.
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