Fundaments of Machine learning for and with engineering applications

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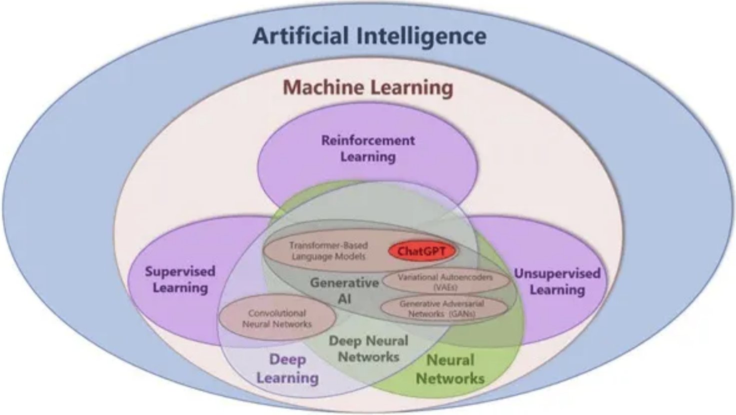
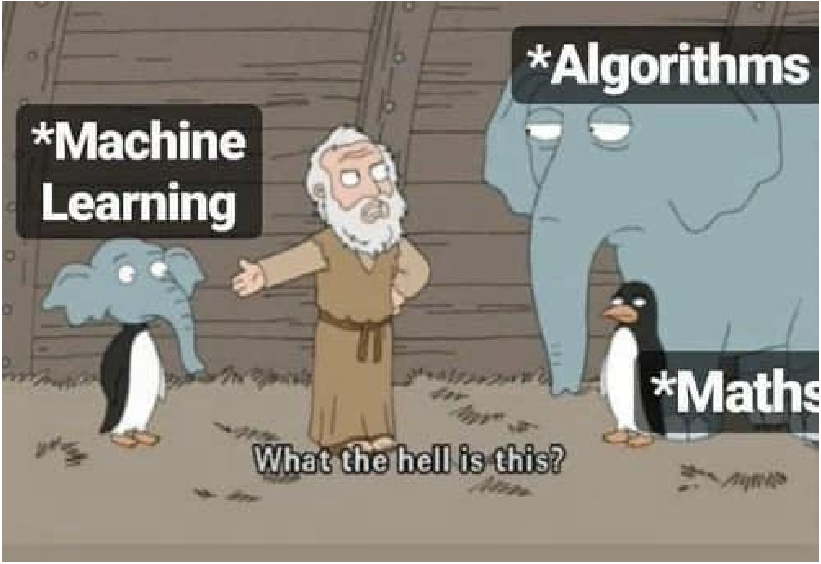
What is the main difference between the three fields?



How Machine Learning Started?



Let's start from the definition

- Statistics (origin "description of a state/country") is the discipline that concerns the collection, organization, analysis, interpretation, and presentation of data.
- It is conventional to begin with a statistical population or a statistical model to be studied. Populations can be diverse groups of people or objects such as "all people living in a country" or "every atom composing a crystal".
- Statistics deals with every aspect of data, including the planning of data collection in terms of the design of surveys and experiments.[Wikipedia]

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Machine learning

Definitions:

- Machine learning is a branch of artificial intelligence (AI) and computer science which focuses on the use of data and algorithms to imitate the way that humans learn, gradually improving its accuracy. [IBM]
- Machine learning (ML) is a field of study in artificial intelligence concerned with the development and study of statistical algorithms that can learn from data and generalize to unseen data, and thus perform tasks without explicit instructions. [WIKI]
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Machine learning is a set of computer based statistical approaches that aim to minimise the loss function to maximise inference accuracy. [Enrico, 5.2.2024]

The loss function is the actual engine in machine learning.

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It quantifies the difference between the predicted outputs of a machine learning algorithm and the actual target values.

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- Are there such things as good data and bad data?

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Data without metadata are just numbers (i.e. if they are integers, they are still good to play lottery)

Metadata can be pretty much anything. Depending on the application, we can distinguish between:

1. Descriptive : used for discovery and identification. It includes elements such as title, abstract, author, and keywords.
2. Structural : describe how compound objects are put together. It describes the types, versions, relationships, and other characteristics of digital materials.
3. Administrative : to help manage a resource, like resource type, permissions, and when and how it was created.
4. Reference : to indicate the information about the contents and quality of statistical data.
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MetaData aim

These characteristics shall all be considered when constructing data repositories.

They are a must for:

- Code repositories
- Data repositories

Please click on the link and explore. Those are just some of the open (scientific) repositories. The aim/hope is to allow people to extract information. How to make value from that information... is another story.

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MetaData for sharing and re-use

More considerations:

- Metadata is more and more important in a digital open world.
- Researchers and automatic algorithms would benefit from importing data directly.
- FAIR research is an important part of Open Science revolution (Findable, Accessible, interoperable, Reusable)
- New applications, business, discoveries can be thus enabled.
- ChatGPT, Bard, Gemini, and all the LLMs are functional only thanks to this!

Super controversial

- Who would be responsible for them then?
- What is the advantage for who releases the data?
- Who gets the money for what?
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Good examples

- Norwegian offshore directorate
- Norway Statistics
- World statistics
- Code repositories
- Data repositories

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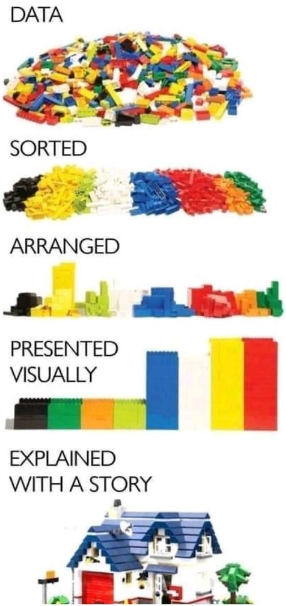
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Representation

A representation should **capture** the nature of the subject being studied.

Example: If you want to evaluate the 3D structure of a wind turbine, a set of descriptors an be:

1. Blade length
2. Turbine height
3. Geographical position
4. Output power
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which are two decimal numbers, a 2d tuple, a 1D time series and a 2D time series (or 3D even).

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Same meaning **represenations** for different objects (inputs).

Discussion point!

How do we compare two wind turbines accounting for the 5 variables previously introduced?

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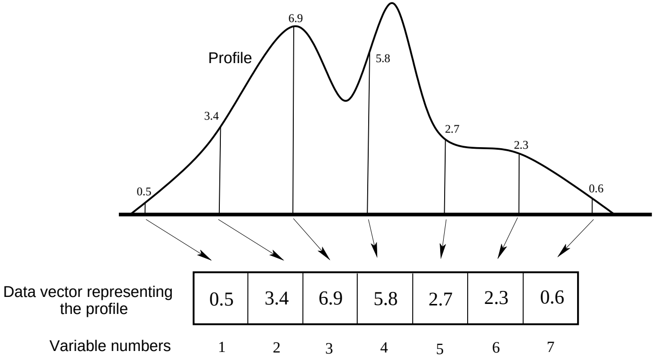
- We sample at regular intervals where each sample point is represented by a variable



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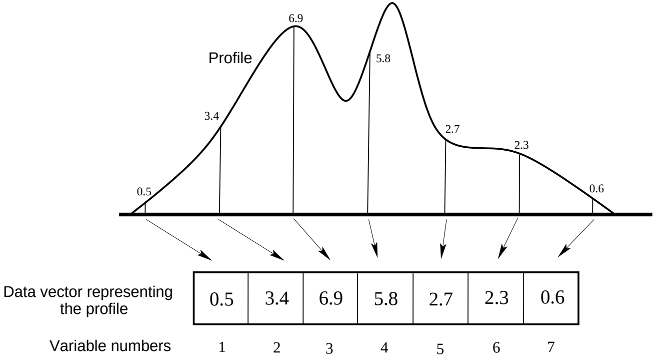

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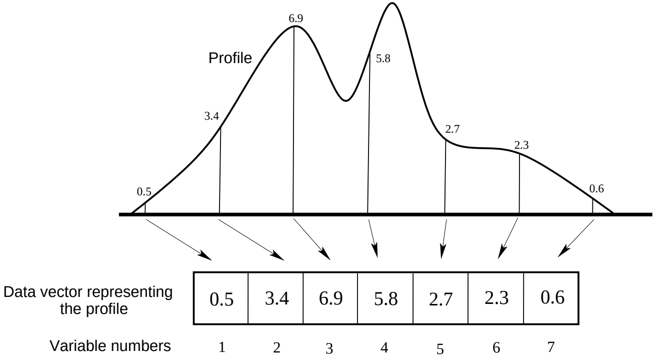

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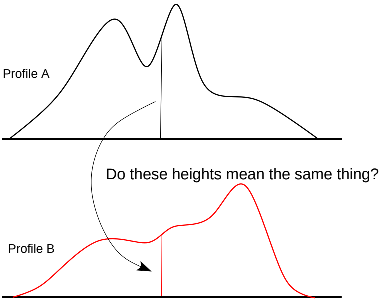

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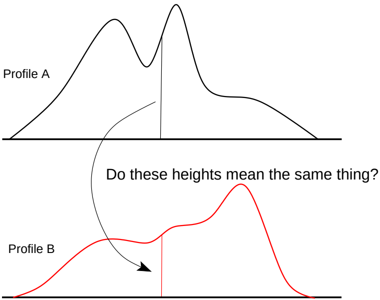

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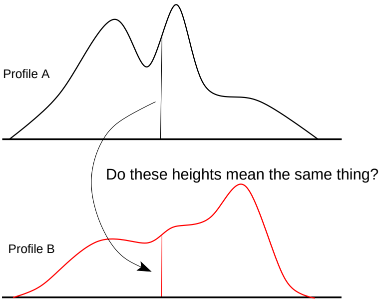

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Data structures

Given a representation, it is then needed to decide on a suitable **data structure** for the problem.

Definition

A data structure is a way of storing and organising data in a computer so that it can be used effectively.

Typical data structures used in data analysis are:

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A data structure is a way of storing and organising data in a computer so that it can be used effectively.

Typical data structures used in data analysis are:

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- Arrays (vectors, matrices, N-mode (way) arrays)
- Graphs (trees)
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Workflow

Data has to be prepared with these steps in mind

1. Plan experiments: Use experimental design to set up experiments in a *systematic* way
2. Pre-processing: Is there systematic variation in the data which should be removed Can cross-checking/validation procedures be designed?
3. Examine the data: Look at data (tables and plots). Strange behaviours? Smooth behaviour? WARNING!
4. Define desired model outcomes (speed, accuracy, false positive/negatives rate)
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Spatial and Temporal Data

Statistics is collecting, organising, and interpreting data

Spatial and temporal statistics is a branch of applied statistics that emphasises:

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Actual data

The data matrix is an extremely common data structure.

$$X = \begin{bmatrix} 95 & 89 & 82 \\ 23 & 76 & 44 \\ 61 & 46 & 62 \\ 49 & 2 & 79 \end{bmatrix}$$

In python these can be saved as

- lists (vanilla python)
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There are different conventions. Commonly we will construct data matrix such that:

- Rows are called instances, objects or samples.
- Columns are called features, variables.

One can think of each row to be an experiment, and the rows its properties. Each row (experiment, object, sample, ...) is thus a list of values, one for property.

Note

Mathematically speaking, this is just a notation. As long as one keeps track and is consistent, columns can be used as rows and vice versa.

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A quick example

Environmental measurements of rivers. The features (properties) can be:

- pH
- Temperature
- Concentration of pollutants
- Flow rate
- water speed

The experiments/observations/sample can be:

- Po
- Danube
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Hard and soft modelling

Models allow us to predict 'the future', or describe the past and present (what is the present...?)

Last life lesson for today

Models are always wrong, but some are useful. (George Box)

Three main families:

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- Based on an accurate physical description of the system and mathematical modelling (e.g. differential equations).

Hard models are often deterministic.

- Hard-modelling methods usually use optimization methods to find out the best values for the parameters of the model.
- Hard-modelling is preferable in laboratory experiments, where all the variables are controlled and the physicochemical nature of the dynamic model is known and can be fully described using a known mathematical model.
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Soft modelling

Characteristics:

- Soft-modelling describes systems without the need of an *a priori* physical or (bio)chemical model postulation. They are **data driven** models.
- Soft models are much easier to make than hard models.
- Soft modelling can be used to understand complex relationships.
- Soft modelling needs (much) more data than hard-modelling.
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After understanding the problem to be solved we need to:

1. Link mathematics to physics.
2. Define boundary conditions and constitutive equations.
3. Make tons of assumptions.
4. Solve the constitutive equation in space and time.
5. CHeck solution stability and sensitivity analysis.
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7. It is hard (but we are engineers!).
8. Get quite some money for the awesome job.

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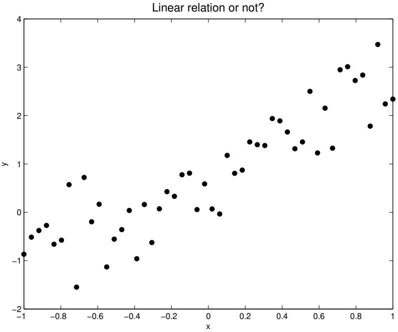
Finding a suitable model

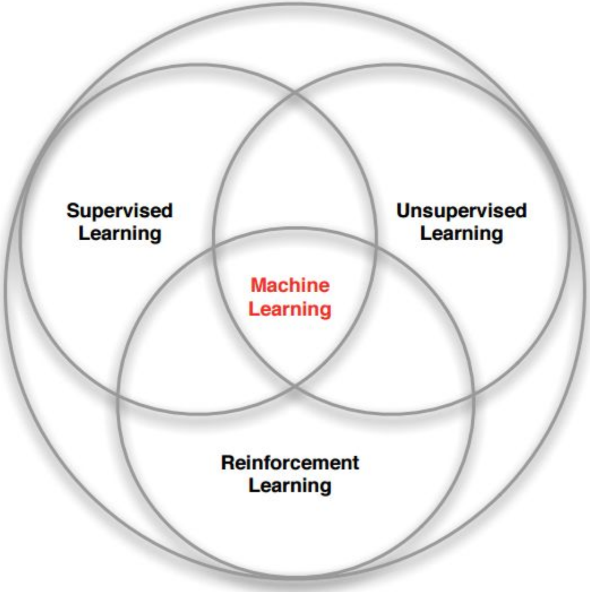
Soft modeling is in most cases based on **multivariate statistical methods**. Many of these methods may be viewed as sophisticated ways of performing curve fitting to data.



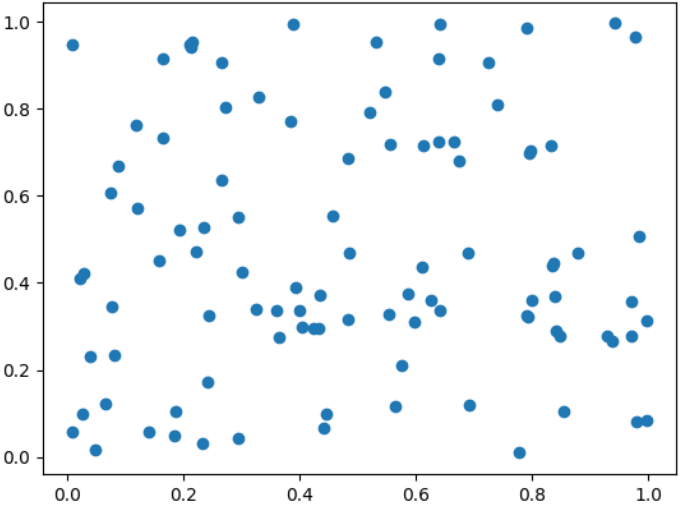
What would be the best model?

- Straight?: $y(x) = ax + b$
- Parabolic?: $y(x) = ax^2 + bx + c$
- Trigonometric?: $y(x) = asin(x) + bcos(x)$

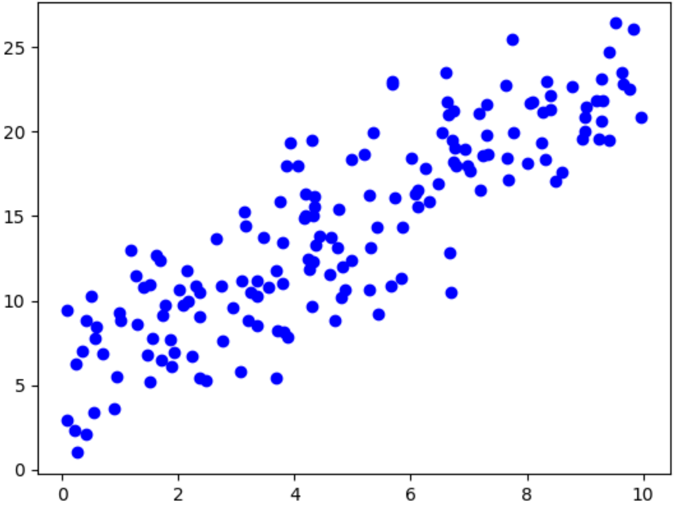
Families of Machine learning



What can we do with that?



What about in this case?



Python Source code 1

```python
import numpy as np
import matplotlib.pyplot as plt

# Generate some sample data
data = np.random.rand(100, 2)  # 100 data points with 2 features

plt.scatter(data[:, 0], data[:, 1])
plt.show()
```

Python Source code 2

```python
import numpy as np
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def generate_linear_data(n_random_points, noise=16):
    x = np.random.rand(n_random_points) * 10

    # Make 'perfect' data
    true_slope,  true_intercept = 2, 5
    y = true_slope * x + true_intercept

    # Add noise
    y += np.random.randn(n_random_points)*noise

    return x, y, true_slope, true_intercept

# Use the function to generate data
x, y, true_slope, true_intercept = generate_linear_data(
        n_random_points=166,
        noise=3)

# Plot all
plt.scatter(x, y, color='blue', label='Data Points')
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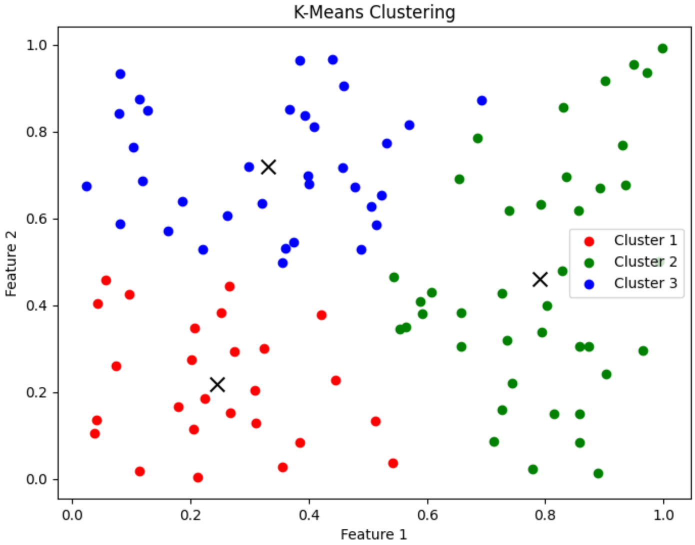
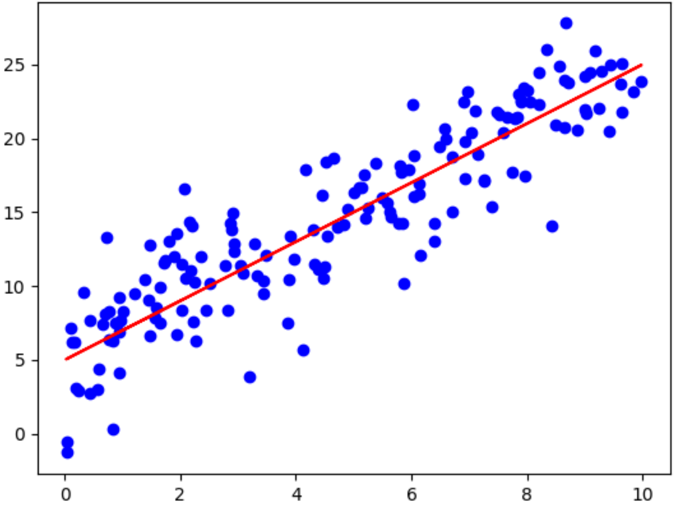
Unsupervised learning



Supervised learning



The data decides

This is why we focus so much on the data type.

The data properties dictate what statistical model can be adopted.

An statistical model has leverages our understanding of the data structure to improve its **predictions** (inference).

The numerical recipe that we used to generate the data is defined the **truth**

Psychology or data science?

Most Machine learning tools are aimed to find the truth. In most cases, we are happy to not find lies.

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Unsupervised learning

Unsupervised learning, a term that resonates with the autonomy of machine intelligence, operates on the principle of identifying patterns and structures in datasets without labelled responses.

This branch of machine learning is distinguished by its lack of explicit guidance, where algorithms are tasked with uncovering hidden structures from unlabeled data.

The most common clustering strategies are :

- filtering
- clustering
- dimensionality reduction
- association learning

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Application of unsupervised learning

It is a bit of a holy grail: a computer that finds patterns without guidance. (Yes, it doesn't work, most of the time)

Still, it has been shown efficient for:

- Computer vision
- Anomaly detection
- Exploratory data analysis

Main challenge

The right result is quite undefined, Uncertain goal.

We will demonstrate it with a famous problem.

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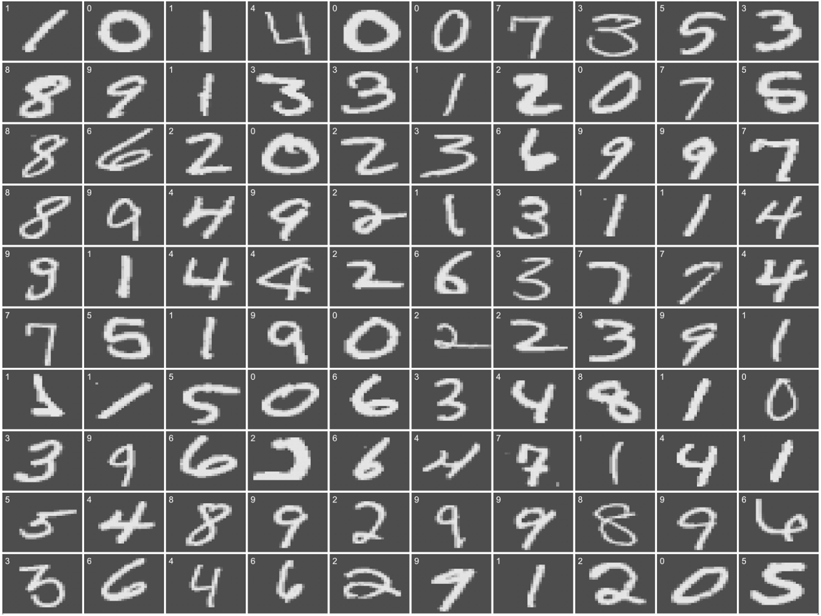

Wak supervised learning

A less popular type of machine learning problem is when labels are assigned to groups of instances.

The group of instances is called **bag**.

The question is, what is the level of a previously unforeseen bag?

This data structure and question type request a hybrid treatment between supervised and supervised learning.

Multiple instance learing

Multiple instances are needed to learn (quite clear name)

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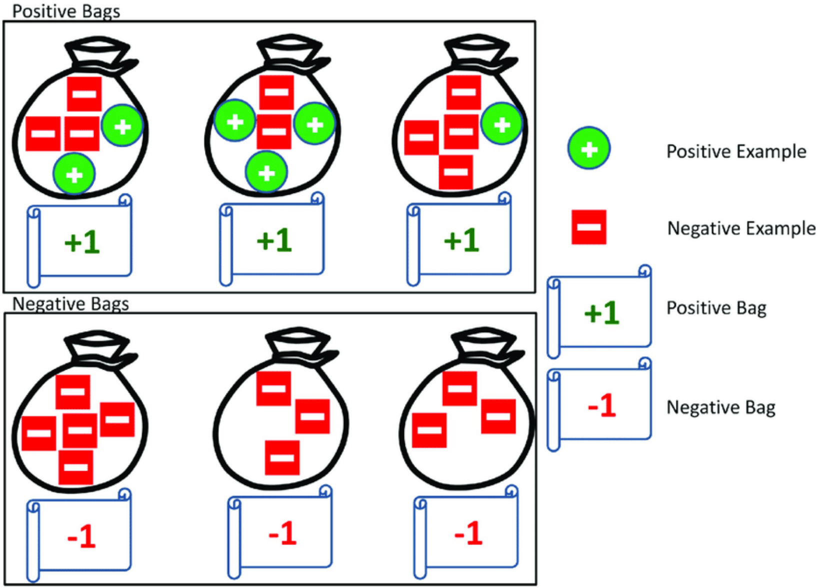

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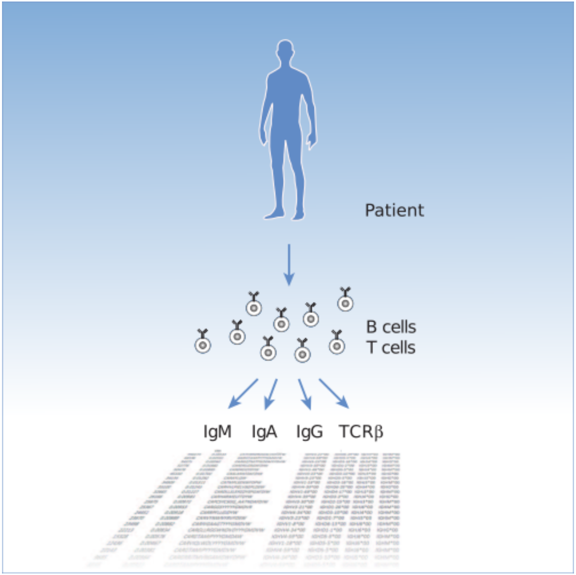

Reinforcement learning

Finally, there is a further approach.

Reinforcement learning (RL)

It aims to train an intelligent agent to take actions in a dynamic environment in order to maximise the cumulative reward.

It learns from outcomes and decides which action to take next. After each action, the algorithm receives feedback that helps it determine whether the choice it made was correct, neutral or incorrect.

It is a self-teaching system that essentially learns by trial and error.

It is a dependable tool for automated decision making.

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Generative AI

A generative AI model is a type of artificial intelligence that is designed to generate new content, based on the data it has been trained on.

It started in 1932, with the **mechanical brain** by Georges Artsrouni that was suppoused to translate automatically between languages,

Here a nice recaps of Generative AI and its storyline

Key characteristics of generative AI models include:

1. Learning from Data: They are trained on large datasets, enabling them to learn patterns, styles, or features inherent in the data.
2. Generating New Content: Generative models can create new data instances. For example, a model trained on a dataset of paintings can generate new images in the style of those paintings.

Trained generative models are thus able to input information at a low resolution/dimension and give output with a much greater dimensionality.

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Applications

Here a list of possible applications:

- Images/video: Image generation, Super-resolution, Deep fakes.
- Music: noise filter, voice and music generation, voice deep fake.
- Text(LLM): chatGPT, bard, Gemini, etc.
- Chemistry: DeepMind (Alphafold).
- Coding (co-pilot)
- Speech
- Attacks and Hacking (Security testing)
- Generating training sets
- And many more

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Science fiction?

This is scary:

1. Virtual best friends
2. Medical images to show diseases consequences
3. Synthetic data for digital twins
4. Preemptive suggestions (e.g. driving)
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Problems (currently)

New possibilities do not come with side effects.

1. Lack of transparency: how the output is generated, and why?
2. Accuracy: a lot of hallucinations
3. Bias: human biases are kept, supported and eventually increased
4. Intellectual properties (IP): who owns what is produced=
5. Cybersecutiry and frauds: mass cyber attacks can be created
6. Sustainability: massive quantity of electricity is used
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Where generative AI is ?

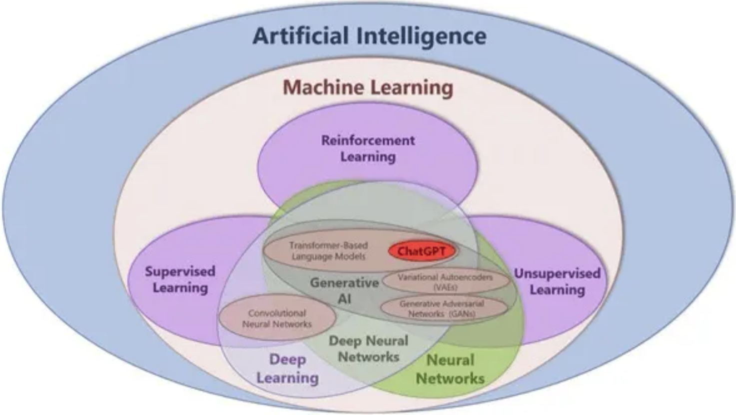

Image: https://iot-analytics.com

Structure of generative AI

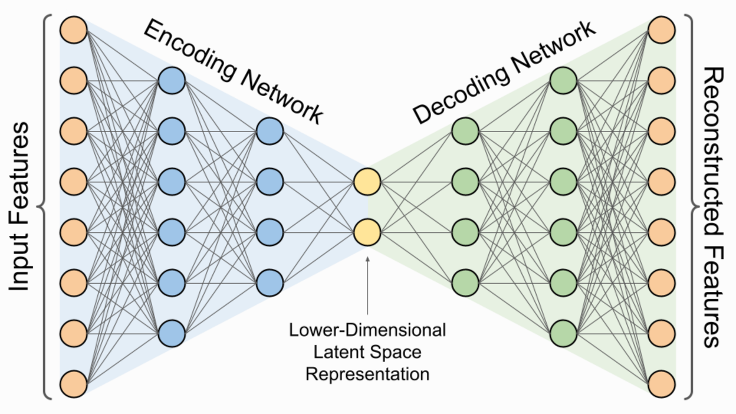

Image: https://www.rapidops.com

A new field?

Generative AI is actually a new evolution.

It is based on Neural Network, and in comprises a set of advanced tools (numerical recepites):

1. Generative Adversarial Networks
2. Generative Pre-trained Transformers
3. Variational Autoencoders
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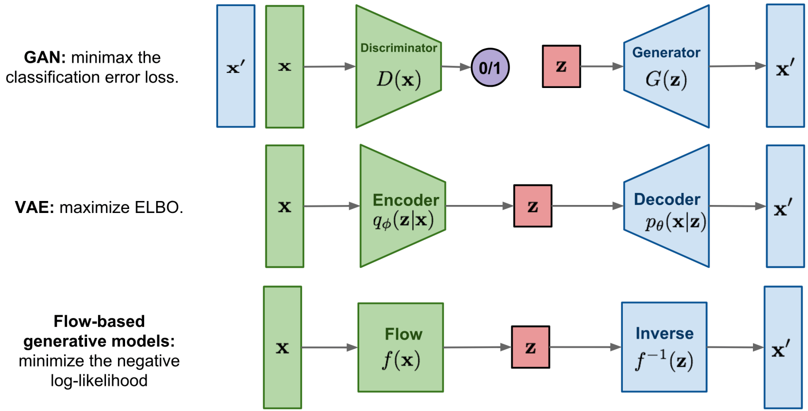
Types of generative AI

It is quite an advanced technique



Source: Lilian Weng

A **linear model**

Considering a univariate case, we have:

$$q = f(x)$$

which relates the **independent variable** x to the **true dependent variable** q.

!vspace1em

Assuming a linear model

$$q = \beta_0 + \beta_1 x$$

where β_i are the arbitrary selected coefficients.

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Model set-up

For a given x we do not know the true response q, only the measurementa y_i for experiment i.

We have that:

$$y_i = q_i + \epsilon_i$$

NOTE: do not proceed if you do not fully understand this equation.

which is

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Discussion point

Does ϵ_i matter? And why so?

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Estimated model paramters

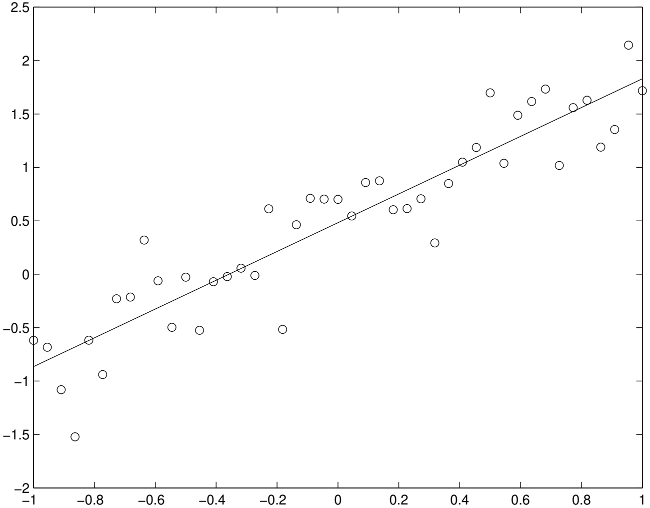
The model parameters β_0, β_1 are unknown, but they can be **estimated**. To distinguish estimates from true model parameters we call them b_0, b_1. These estimates are calculated such that the model

$$\hat{y} = b_0 + b_1 x$$

fits the n different experimental observations as well as possible.

Linear model example

We would like to find the TRUTH (What it it?)



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    # Add noise
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# Plot all
plt.plot(x, true_slope*x + true_intercept,
         color='red', label='Truth Line')
plt.scatter(x, y, color='blue', label='Data Points')
plt.show()
```

Linear model(s)

Does a linear model mean only straight lines (or hyperplanes in general)?

That answer to this is *no*. different. In general for a model f to be defined linear, it has to be linear with respect to the unknown parameters $\beta_0, \cdots, \beta_n$. The general linear model is

$$q = \beta_0 + \beta_1 f_1(x_1) + \beta_2 f_2(x_2) + \cdots + \beta_n f_n(x_n)$$

where $f_i(x_i)$ may be non-linear functions. It is the **form** of the equation which makes it linear, i.e. that $f_i(x_i)$ does not depend on the parameters β_i.

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$$q = \beta_0 + \beta_1 x_1^2 + \beta_2 x_2^{-1} + \beta_3 \log x_3$$

The answer is *yes* because by simple substitution it is possible to convert this formula into a linear form.

With $h_1 = x_1^2$, $h_2 = x_2^{-1}$ and $h_3 = \log x_3$, then we can formulate the new model:

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The answer is *yes* because by simple substitution it is possible to convert this formula into a linear form.

With $h_1 = x_1^2$, $h_2 = x_2^{-1}$ and $h_3 = \log x_3$, then we can formulate the new model:

$$q = \beta_0 + \beta_1 h_1 + \beta_2 h_2 + \beta_3 h_3$$

which is in the standard linear form.

Curvilinear models

A special class of linear models which we will investigate later are those which are expressed in terms of *polynomials* (here in only 1D):

$$q = \beta_0 + \beta_1 x + \beta_2 x^2 + \cdots + \beta_m x^m = \sum_{i=0}^{n} \beta_i x^i$$

For n-D case there are a wide range of interaction terms and combinations, that can still be converted to standard linear form.

Such models are sometimes referred to as **curvilinear** instead of non-linear

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Nonlinear models

But there are many other models that cannot be substituted to such a form. For instance:

$$q = \beta_0 + \log(x - \beta_1)$$

No substitution can transform this equation to the linear form.

That is the case for all the model that:

$$q \sim f(x, \beta)$$

Another example is:

$$f(x, \beta) = \frac{x\beta}{x + \beta}$$

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Estimation of linear regression parameters

For the 1-dimensional problem, we have

$$\hat{y} = b_0 + b_1 x$$

where $\hat{y}$ is the estimated y-value from the approximate model that has been generated from a set of measurements (x_i, y_i). We aim to find the b_i parameters such that the regression line fits the observed data as well as possible.

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$$e_i = y_i - \hat{y}_i$$

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- Cannot sum e_i values since they might be positive and negative and thus cancel
- Could use e.g. $\sum_{i=1}^{n} |e_i|$, but is mathematically more difficult to handle
- Residual"smallness" measured by $\sum_{i=1}^{n} e_i^2$.

Thus, we find the linear regression coefficients by *minimising*

$$R = \sum_{i=1}^{n} e_i^2 = \sum_{i=1}^{n} (y_i - \hat{y}_i)^2$$

How?

Regression!

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Before to continue, let's make sure to have all the main elements clear:

1. Splitting the data in dependent and independent variables
2. Assumption of a linear model between them
3. Recognise the difference between the truth and the estimation
4. Aiming to *minimize* the residuals

Discussion

What happen when the sun of residual is 0 ?

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Regression

To minimize the sum of the square residuals, we can try to solve the following equations:

$$\frac{\partial R}{\partial b_0} = 0$$
$$\frac{\partial R}{\partial b_1} = 0$$

where:

$$R = \sum_{i=1}^{n} (y_i - \hat{y}_i)^2 =$$

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Skipping the math (but you are more than welcome to try), here are the results:

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\begin{aligned}
b_0 &= \bar{y} - b_1\bar{x} \\
b_1 &= \frac{\sum_{i=1}^{n}(x_i - \bar{x})(y_i - \bar{y})}{\sum_{i=1}^{n}(x_i - \bar{x})^2}
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Straightforward derivation becomes very cumbersome for multiple variables. Thus, a different approach must be used. Yet, it is important to understand that there is an analytical solution (even if not all the time).

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Many variable equation

The general equation would look like:

$$\hat{y} = b_0 + b_1 x_1 + b_2 x_2 + \cdots + b_n x_n = \sum_{j=0}^{m} x_{ij} b_j$$

where we will have to solve all the $n + 1$ equations (called the **normal equations**) of the form:

$$\frac{\partial R}{\partial b_j} = 0 \quad \forall j \in [0, n]$$

Is there a way for us to simplify this?

We can use vector and matrix algebra.

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Regression via Matrix operation

Remember that

$$R = \sum_{i=1}^{N} (y_i - \hat{y}_i)^2$$

then we can define the vector $\mathbf{e}$:

$$\boldsymbol{e} = \boldsymbol{y} - \hat{\boldsymbol{y}}$$

thus

$$\boldsymbol{e}^T = [(y_1 - \hat{y}_1)\ (y_2 - \hat{y}_2) \cdots\ (y_N - \hat{y}_N)]$$

and can then write

$$R = \boldsymbol{e}^T \boldsymbol{e}$$

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From the following equation:

$$\hat{y}_i = b_0 + \sum_{j=1}^{m} x_{ij} b_j = \sum_{j=0}^{m} x_{ij} b_j$$

where $x_{i0} = 1$
we make the matrix equation:

$$\hat{\boldsymbol{y}} = \boldsymbol{X}\boldsymbol{b}$$

where the first column in **X** consists of ones only.

Residual

$$
\begin{aligned}
R &= \boldsymbol{e}^T\boldsymbol{e} \\
&= (\boldsymbol{y}-\hat{\boldsymbol{y}})^T(\boldsymbol{y}-\hat{\boldsymbol{y}}) \\
&= (\boldsymbol{y}-\boldsymbol{Xb})^T(\boldsymbol{y}-\boldsymbol{Xb}) \\
&= (\boldsymbol{y}^T-\boldsymbol{b}^T\boldsymbol{X}^T)(\boldsymbol{y}-\boldsymbol{Xb}) \\
&= \boldsymbol{y}^T\boldsymbol{y}-\boldsymbol{y}^T\boldsymbol{Xb}-\boldsymbol{b}^T\boldsymbol{X}^T\boldsymbol{y} \\
&+ \boldsymbol{b}^T\boldsymbol{X}^T\boldsymbol{Xb}
\end{aligned}
$$

All the parts of this equation are scalar values. This means e.g. that

$$\boldsymbol{y}^T\boldsymbol{Xb} = \boldsymbol{b}^T\boldsymbol{X}^T\boldsymbol{y}$$

This gives

$$R = \boldsymbol{y}^T\boldsymbol{y} - 2\boldsymbol{y}^T\boldsymbol{Xb} + \boldsymbol{b}^T\boldsymbol{X}^T\boldsymbol{Xb}$$

Residual

But how can we now compute $\frac{\partial R}{\partial b_j}$ more efficiently in matrix form?

Vector differentiation ! Let

$$y = \boldsymbol{a}^T \boldsymbol{x} = a_1 x_1 + \cdots + a_n x_n$$

If

$$\frac{\partial y}{\partial \boldsymbol{x}} = \begin{bmatrix} \frac{\partial y}{\partial x_1} \\ \frac{\partial y}{\partial x_2} \\ \vdots \\ \frac{\partial y}{\partial x_n} \end{bmatrix} = \begin{bmatrix} a_1 \\ \vdots \\ a_n \end{bmatrix} = \boldsymbol{a}$$

and $y = \boldsymbol{x}^T \boldsymbol{a}$, then:

$$\frac{\partial y}{\partial \boldsymbol{x}} = \boldsymbol{a}$$

General solution

In general, when $y = \boldsymbol{x}^T \boldsymbol{A}\boldsymbol{x}$, then

$$\frac{\partial y}{\partial \boldsymbol{x}} = 2\boldsymbol{A}\boldsymbol{x}$$

if $\mathbf{A}$ is symmetric
(check *Matrix calculus* for more properties)

We can use this to compute

$$\frac{\partial R}{\partial \boldsymbol{b}}$$

General solution

We have from above:

$$\begin{aligned} R &= \boldsymbol{y}^T\boldsymbol{y} - 2\boldsymbol{y}^T\boldsymbol{X}\boldsymbol{b} \\ &+ \boldsymbol{b}^T\boldsymbol{X}^T\boldsymbol{X}\boldsymbol{b} \end{aligned}$$

Vector differentiation gives

$$\frac{\partial R}{\partial \boldsymbol{b}} = 0 - 2\boldsymbol{X}^T\boldsymbol{y} + 2\boldsymbol{X}^T\boldsymbol{X}\boldsymbol{b} = 0$$

Solving this for $\boldsymbol{b}$ we get:

$$\begin{aligned} \boldsymbol{X}^T\boldsymbol{X}\boldsymbol{b} &= \boldsymbol{X}^T\boldsymbol{y} \\ (\boldsymbol{X}^T\boldsymbol{X})^{-1}\boldsymbol{X}^T\boldsymbol{X}\boldsymbol{b} &= (\boldsymbol{X}^T\boldsymbol{X})^{-1}\boldsymbol{X}^T\boldsymbol{y} \\ \boldsymbol{b} &= (\boldsymbol{X}^T\boldsymbol{X})^{-1}\boldsymbol{X}^T\boldsymbol{y} \end{aligned}$$

Multiple linear regression

Previous equation make the solution of MLR rather obvious!

When we have a matrix of y-variables **Y**:

$$\boldsymbol{B} = (\boldsymbol{X}^T\boldsymbol{X})^{-1}\boldsymbol{X}^T\boldsymbol{Y}$$

in the equation:

$$\boldsymbol{Y} = \boldsymbol{XB}.$$

These equations give us the **multiple linear regression** (MLR) solution.

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