Fundaments of Machine learning for and with engineering applications

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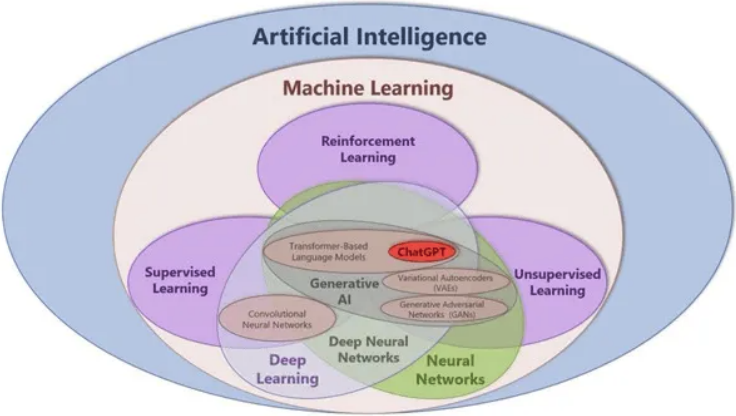
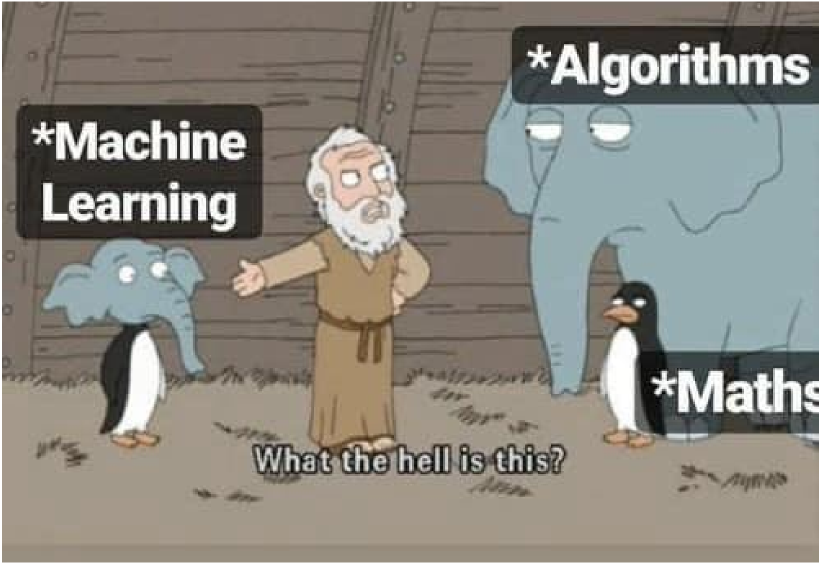
Feb 6, 2024

Statistics, Machine learning or Artificial intelligence?

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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One technical definition

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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MetaData properties

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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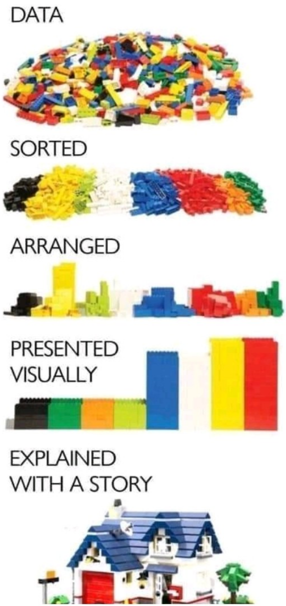
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Representation

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
5. Wind direction

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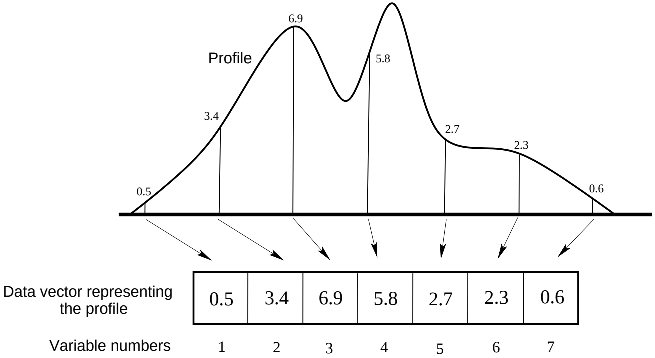
- We sample at regular intervals where each sample point is represented by a variable



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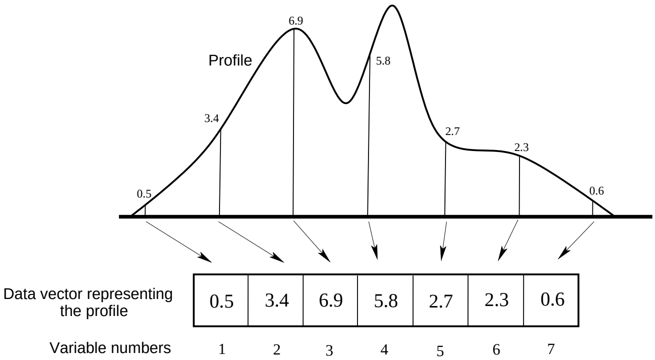

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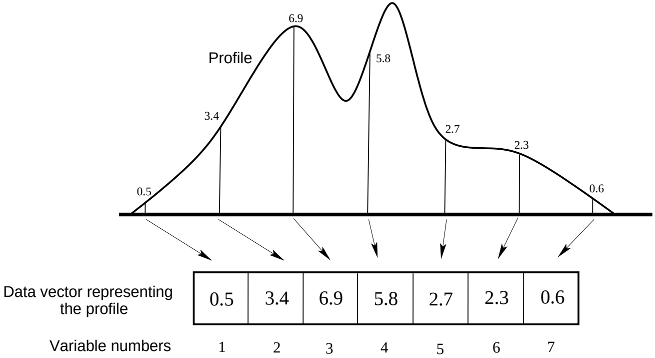

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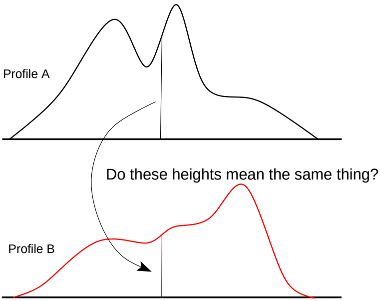

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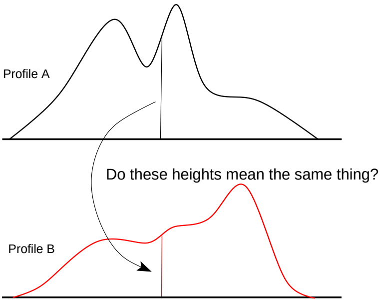

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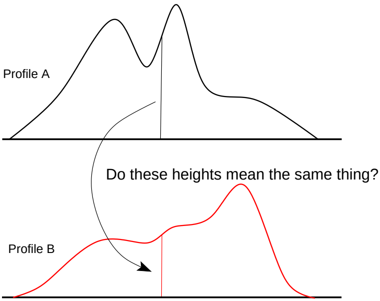

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Data structures

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

- Data points
- 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)
5. Estimate and validate model: What do the results tell us? Is the generated model general (valid for future sampling)?
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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

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- 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

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A quick example

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

- pH
- Temperature
- Concentration of pollutants
- Flow rate
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The experiments/observations/sample can be:

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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).

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- 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:

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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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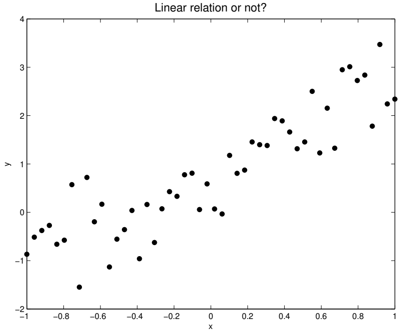
Finding a suitable model

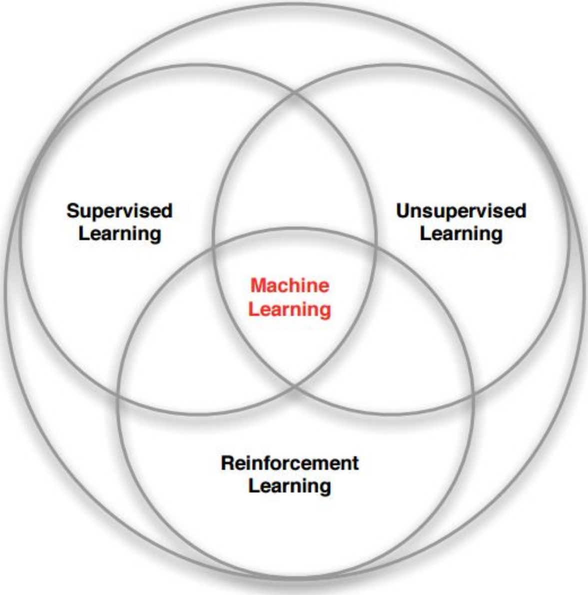
Soft modeling is in most cases based on **multivariate statistical methods**. Many of these methods may be viewed as sophisticated ways of performing curve fitting to data.



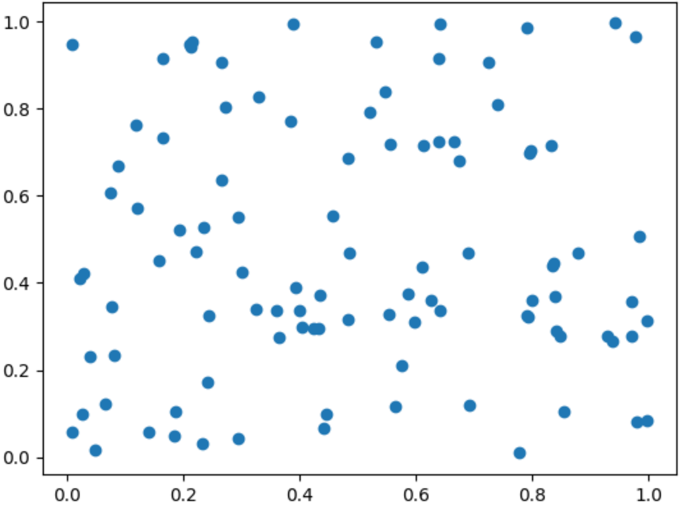
What would be the best model?

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

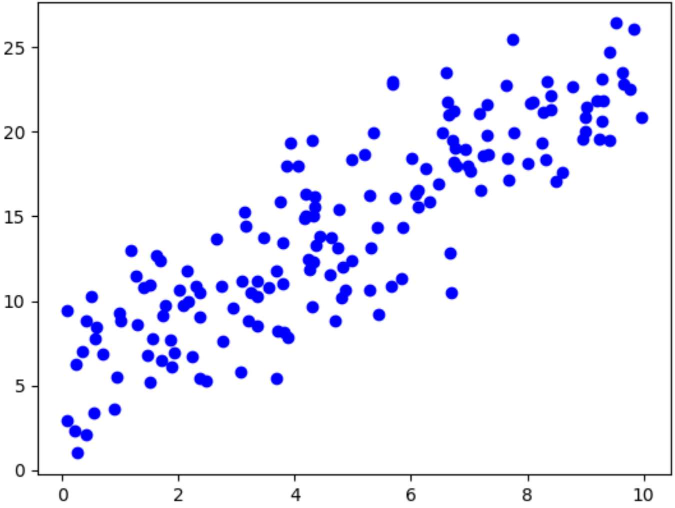
Families of Machine learning



What can we do with that?



What about in this case?



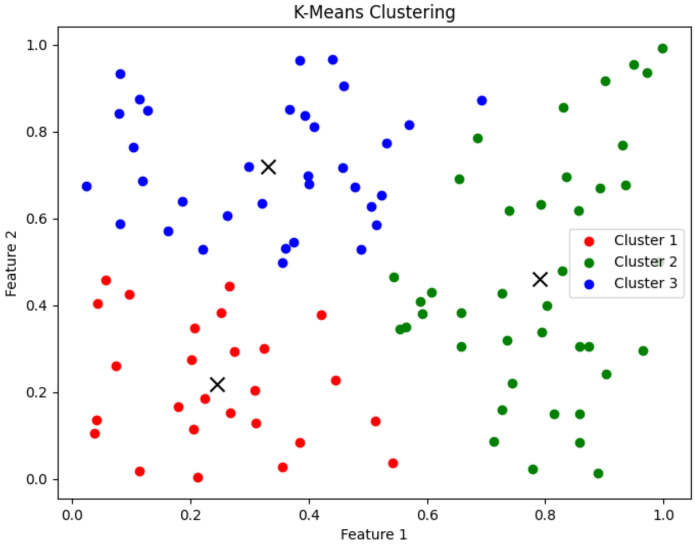
Python Source code 1

```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()
```

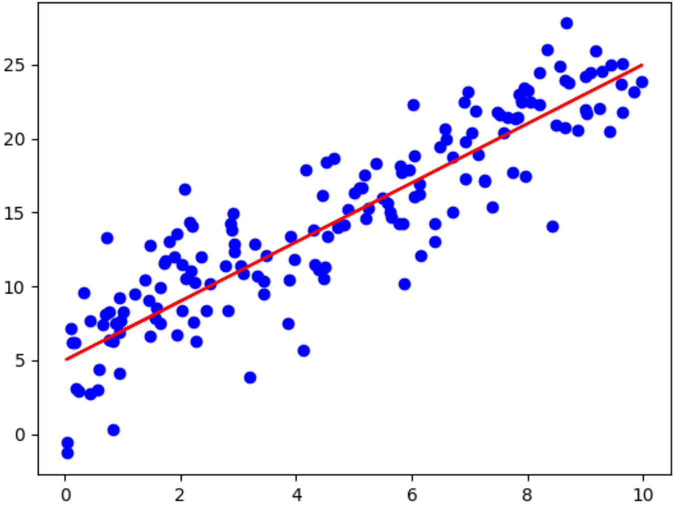
Python Source code 2

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

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')
plt.show()
```

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, 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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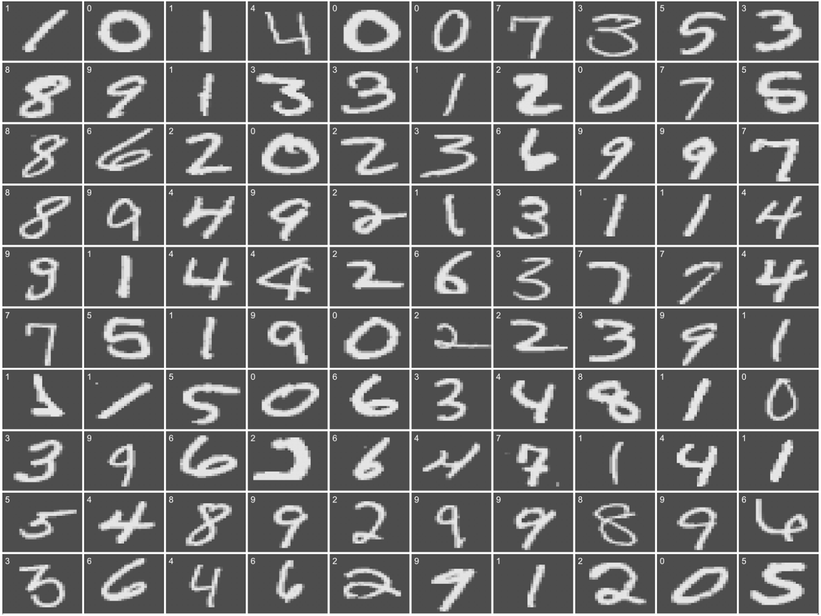

Wak supervised learning

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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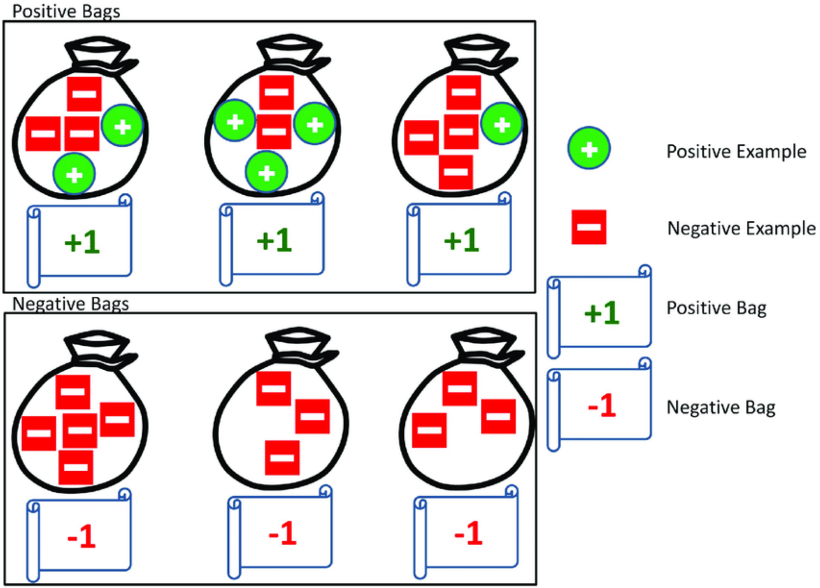

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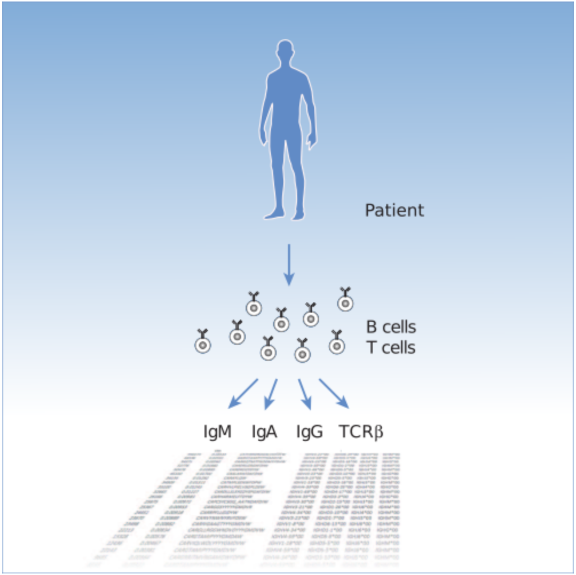

Reinforcement learning

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.

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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

Generative AI

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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- Images/video: Image generation, Super-resolution, Deep fakes.
- Music: noise filter, voice and music generation, voice deep fake.
- Text(LLM): chatGPT, bard, Gemini, etc.
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3. Bias: human biases are kept, supported and eventually increased
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Where generative AI is ?

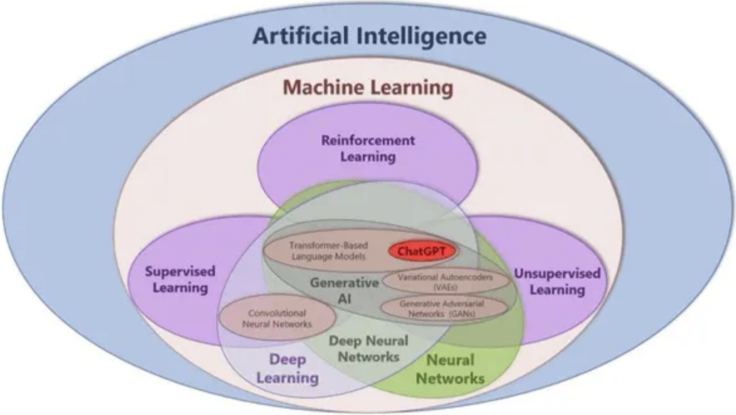

Image: https://iot-analytics.com

Structure of generative AI

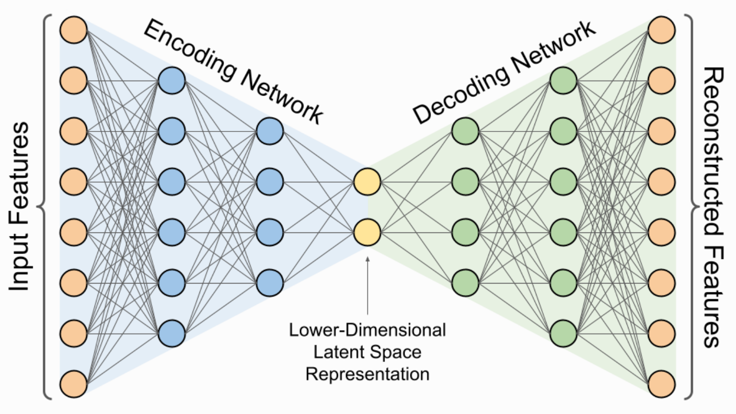

Image: https://www.rapidops.com

A new field?

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

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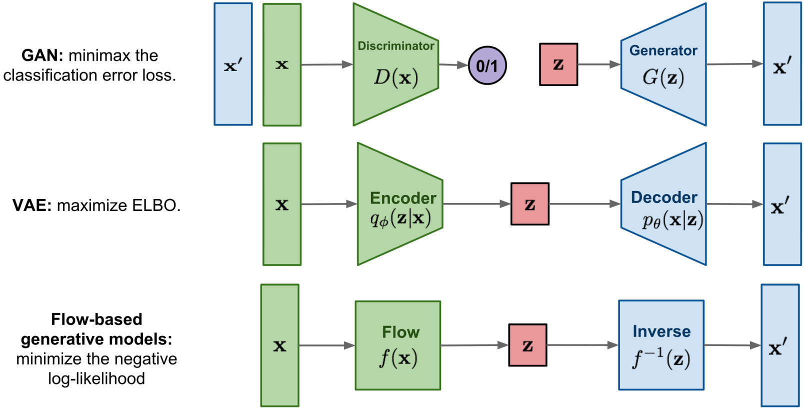
Types of generative AI

It is quite an advanced technique



Source: Lilian Weng