
Materials and artificial intelligence

Outline

- What is Artificial Intelligence (AI) vs Machine learning?
- Examples of applications in materials science
- Local, national and International context : education and research

Scientific paradigms

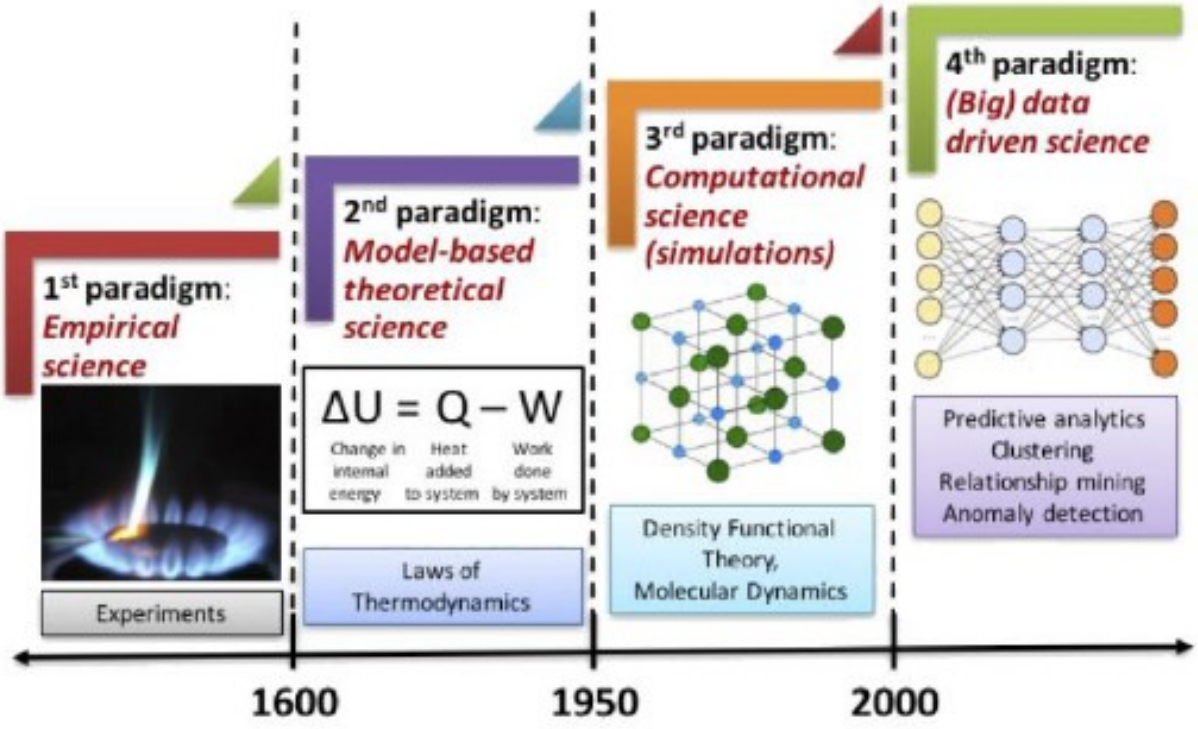
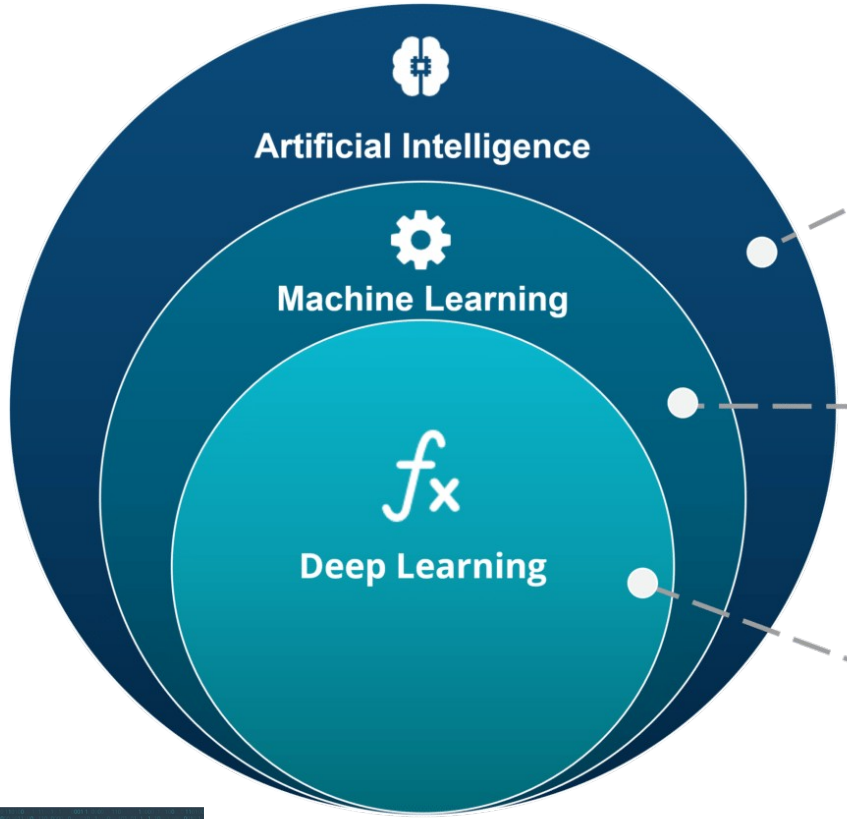


FIG. 1. The four paradigms of science: empirical, theoretical, computational, and data-driven.

A. Agrawal et A.Choudhray, Applied Materials, "Perspective: Material informatics and big data: realization of the 4th paradigm of science in materials science", 4 (2016)



ARTIFICIAL INTELLIGENCE

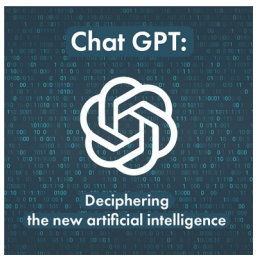
A technique which enables machines to mimic human behaviour

MACHINE LEARNING

Subset of AI technique which use statistical methods to enable machines to improve with experience

DEEP LEARNING

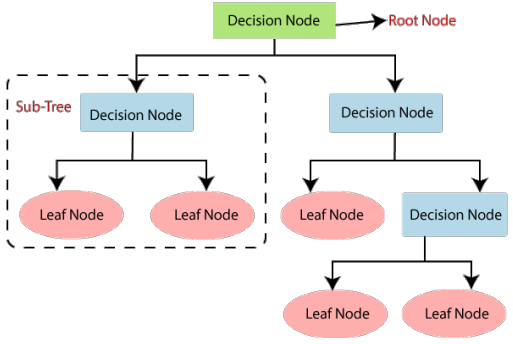
Subset of ML which make the computation of multi-layer neural network feasible



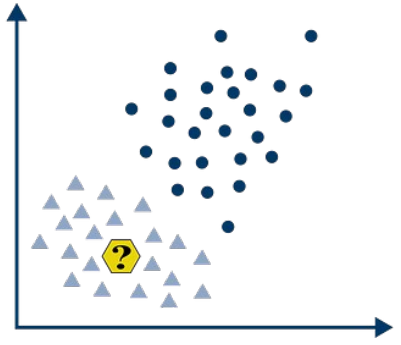
https://www.edureka.co/

Machine Learning

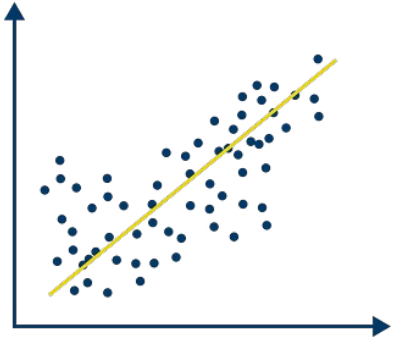
A collection of computational methods for using information in the data we have to make predictions about data we currently do not have.



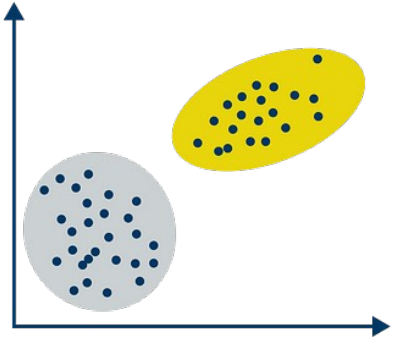
Decision Trees



Classification



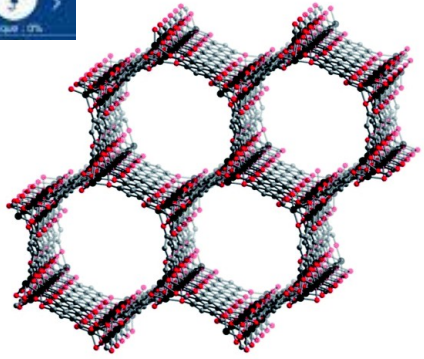
Regression



Clustering

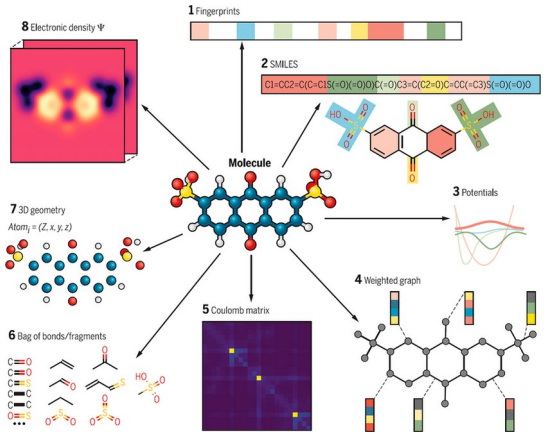
Do you need machine learning?

- When fundamental laws underlying a process are unknown or don’t exist (social sciences).
- *When fundamental laws exist but are extremely **complex** (e.g. weather forcast).*
- *When we have a **lot of data** and we are looking for correlations and simple rules.*



M_2(dobdc) (M = Ni, Co, Mg)
MOF-74

General methodology



Experimental + Ab initio databases

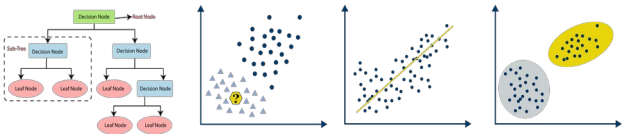
Datasets :
A resource of materials data

Human brain:
Descriptors :
A representation to describe each material quantitatively

Numerical brain
Intelligent search
(***Machine Learning tools***)

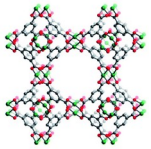
Lecture by Achile

Results (Predictions):
Guide towards new materials
or at least
Define candidates
to be tested in real experiments



Supervised Learning

Training : model set up



Inputs

$\{X_i\}$

ML model

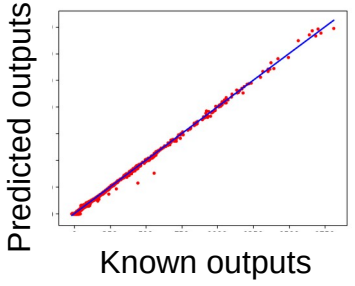
Known outputs

$\{Y_i\}$

Property of interest, e.g. Bandgap

Testing : model accuracy

Inputs → ML model → outputs



Prediction : generating new data

Inputs → ML model → outputs

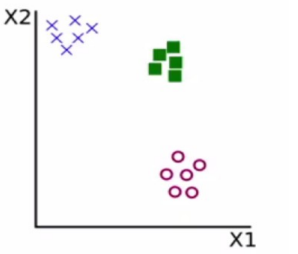
Unsupervised Learning

sample

Cluster/group

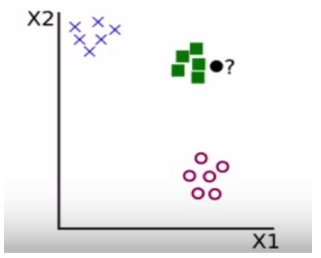
Training : model set up

Inputs → ML model



Prediction : generating new data

Inputs → ML model → Outputs

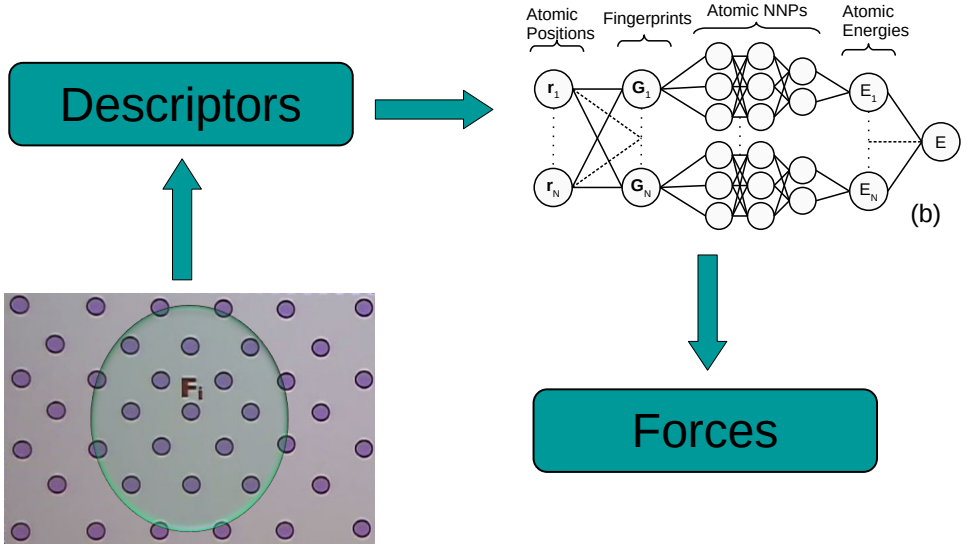


Semi-supervised Learning

- Harnessing the Power of Labeled and Unlabeled Data
- Combining supervised and unsupervised learning approach.
- Addressing the scarcity of labeled data in materials science.
- Reducing the need for expensive and time-consuming experiments.
- Exploiting the vast amount of available unlabeled data.
- Strongly developing field of **Active Learning**

ML Force Fields for Molecular Simulations

- Supervised Approach
- Dataset of Forces from QM simulations
  - Must be carefully constructed to contain relevant molecular structures
- Atomic Descriptors
  - Must have good way of summarizing the atomic positions



- Current Work
  - Feature Selection
  - Experimental data in training

Context of IA+Materials

- Course in phelma : SIM3A + FAME^{AIS} + AMIS
- UGA-INP: Multidisciplinary Institute of Artificial Intelligence (MIAI)
- PEPR initiatives:
  - DIADEM National Project : IA acceleration of research in materials sciences
  - IA
  - NUMPEX
- Many initiatives in Europe Matverk, Fairmat (Germany) Marvell (Switzerland), PDSI

Let’s get our hands dirty

https://jpalastus.github.io/


Thank You for Watching