Fundamentals of AI and ML

Lecture 1: Introduction

by

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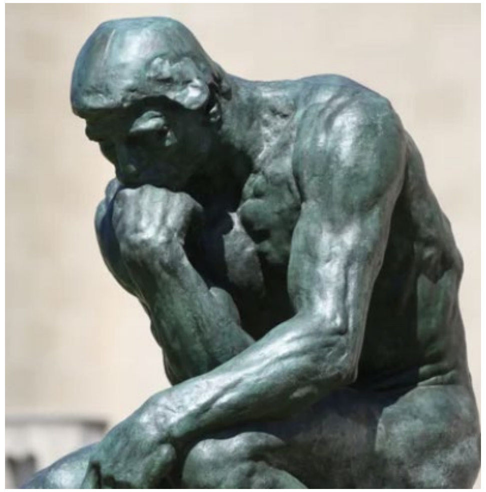
What is Artificial Intelligence?



Intelligence

- We call ourselves *Homo sapiens* meaning "man the wise" because we are "intelligent"
- For thousands of years, we have tried to understand how we think

But what features/abilities do humans have that are indicative or characteristic of intelligence?

Abstract concepts, mathematics, language, problem solving, memory, logical reasoning, emotions, morality, ability to learn/adapt, etc…

The field of artificial intelligence, or AI, goes further still: it attempts not just to understand but also to **build intelligent entities**

What is Artificial Intelligence?

How do make systems mimic human intelligence?

Four schools of thought

Systems that think like humans	Systems that think rationally
Systems that act like humans	Systems that act rationally

What is Artificial Intelligence?

Systems that think like humans

- Cognitive science (not a part of AI yet)

Systems that think rationally

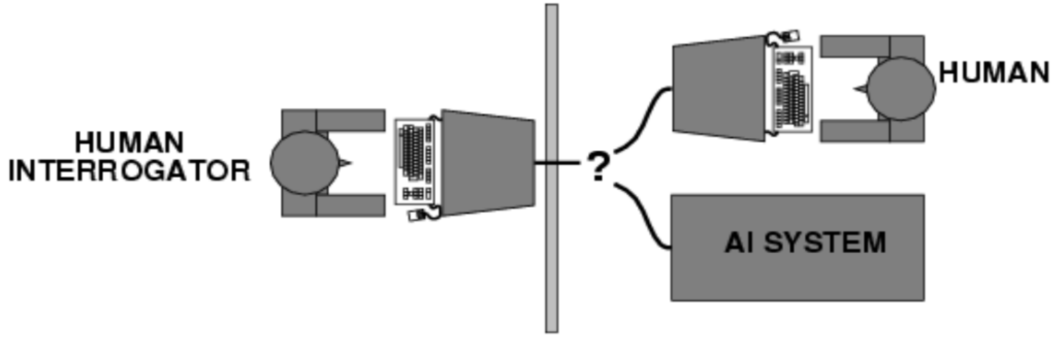
- **Aristotle**: What are the correct thought processes?
- Systems that reason in a logical manner
- Systems doing inference correctly

Systems that behave like humans

- Turing (1950) predicted that by 2000 a computer would have a 30% chance of fooling a lay person for 5 minutes

- Suggested major components of AI: **knowledge, reasoning, language understanding, learning**

  - **Knowledge representation:** to store what it knows or hears
  - **Automated reasoning:** to use the stored information to answer questions and to draw new conclusions
  - **NLP**: to enable it to communicate successfully (in English)
  - **Machine learning:** to adapt to new circumstances and to detect and extrapolate patterns
  - **Computer vision** to perceive objects
  - **Robotics:** to manipulate objects and move about



What is Artificial Intelligence?

Systems that behave rationally

- Rational behavior: “doing the right thing”
- Follow rational agent approach
- **Agent**: entity that perceives and acts
- **Rational agent**: acts so to achieve *best outcome*

A focus on rational AI requires learning

- General principles of rational agents
- Components for constructing rational agents

DeepBlue computer chess acting as an agent

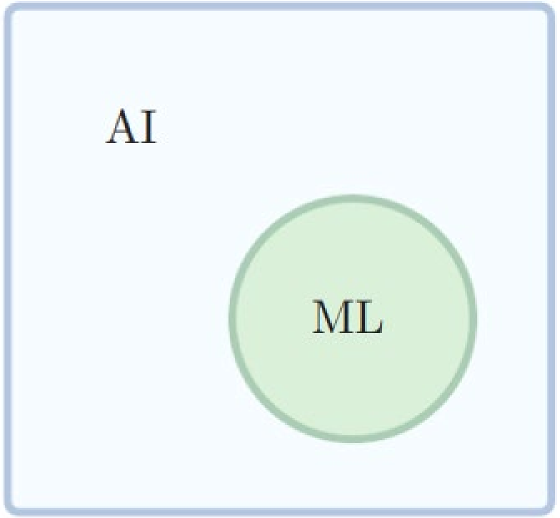
Machine Learning and Artificial Intelligence

- AI is the reproduction of an intelligent behavior by a machine: a combination of thinking and behaving rationally

- According to the **Turing test** (by Alan Turing), an AI agent must possess the following features:
  - Knowledge representation: to store what it knows or hears or sees
  - Automated reasoning: to use the stored information to answer questions
  - Natural language processing: to enable it to communicate successfully in a language
  - Machine learning: to detect patterns and extrapolate to unseen circumstances
  - Computer vision: to perceive objects
  - Robotics: to move and manipulate objects

- While AI and ML are very closely connected, they are not the same!

- **Machine learning is a part of AI**: It is the process of using mathematical models to help a computer learn without direct instruction (or hard-coding)



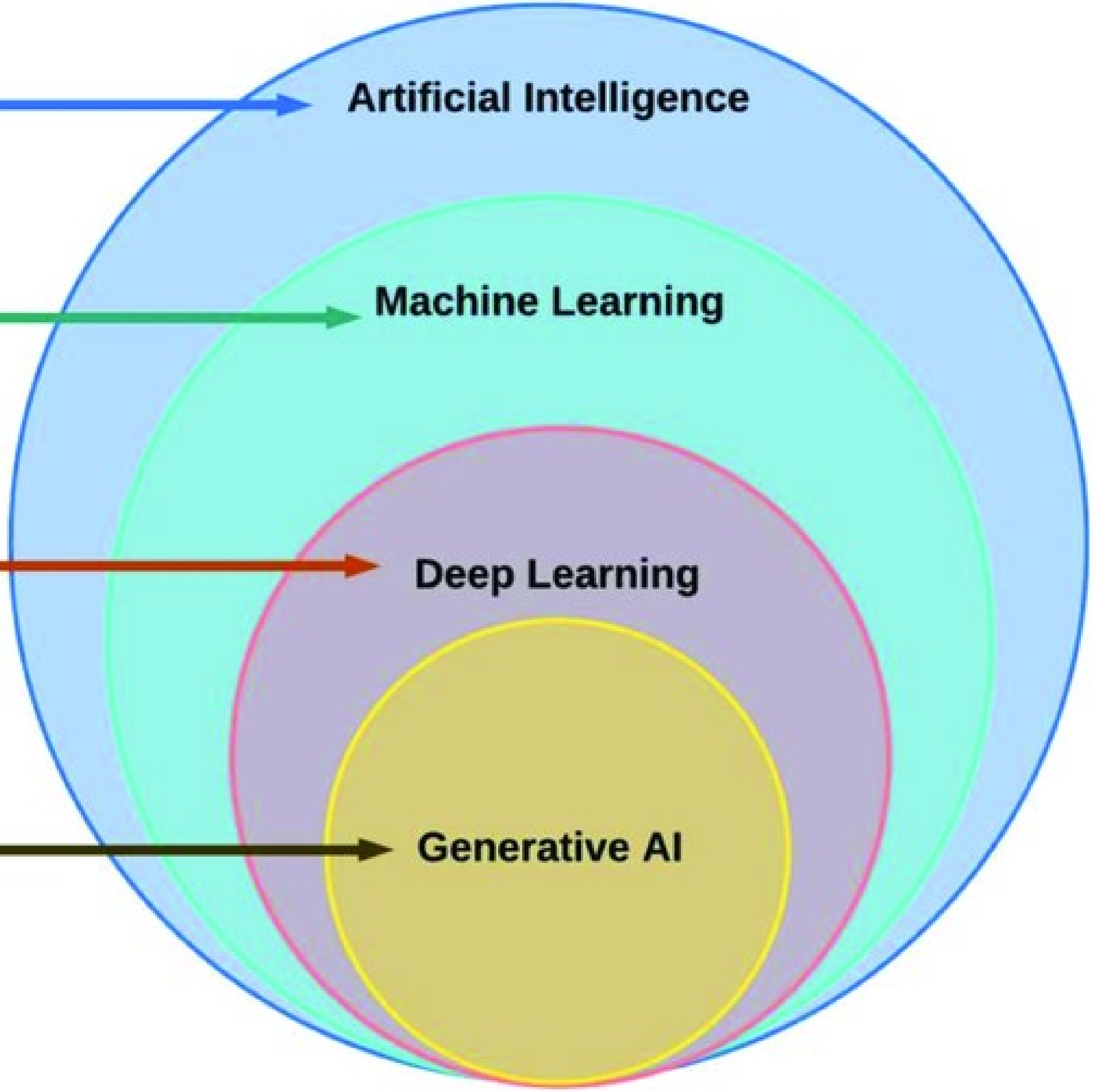
Different sub-components of AI

Artificial Intelligence
AI involves techniques that equip computers to emulate human behavior, enabling them to learn, make decisions, recognize patterns, and solve complex problems in a manner akin to human intelligence.

Machine Learning
ML is a subset of AI, uses advanced algorithms to detect patterns in large data sets, allowing machines to learn and adapt. ML algorithms use supervised or unsupervised learning methods.

Deep Learning
DL is a subset of ML which uses neural networks for in-depth data processing and analytical tasks. DL leverages multiple layers of artificial neural networks to extract high-level features from raw input data, simulating the way human brains perceive and understand the world.

Generative AI
Generative AI is a subset of DL models that generates content like text, images, or code based on provided input. Trained on vast data sets, these models detect patterns and create outputs without explicit instruction, using a mix of supervised and unsupervised learning.



What is machine learning?

Learning

"The activity or process of gaining knowledge or skill by studying, practicing, being taught, or experiencing something."

Merriam Webster dictionary

Machine Learning

"the field of study that gives computers the ability to learn without being explicitly programmed."

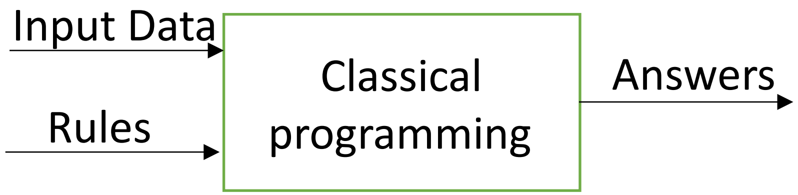
Arthur Samuel

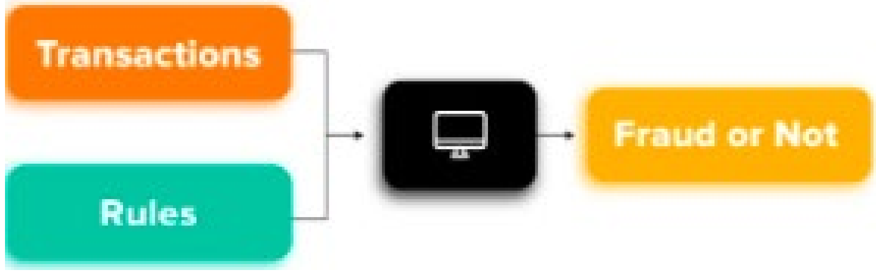
"A computer program is said to learn from *experience E* with respect to some class of *tasks T* and *performance measure P*, if its performance at tasks in *T*, as measured by *P*, improves with experience *E*."

Tom Mitchell

Classical programming vs machine learning

- **Classical programming**: Program/Hard-code the rules for every task



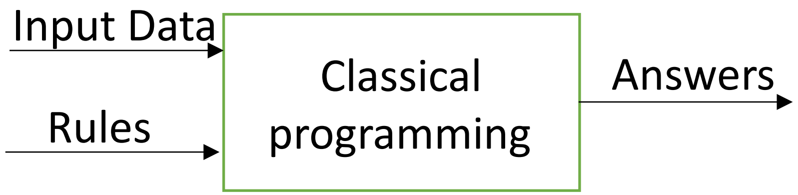


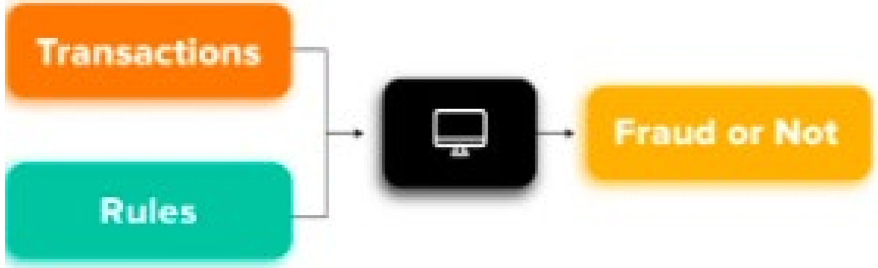
- In classical computer programming, a human designs the rules to figure out the relationship between the input data and answers and then build the rules

- However, for many tasks, it is difficult to manually design and hard-code correct rules
  - detecting spam, fraud transactions
  - recognizing people, objects
  - understanding human speech
  - detecting anomalous behaviors in systems

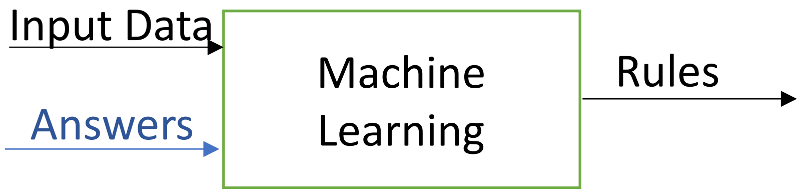
Classical programming vs machine learning

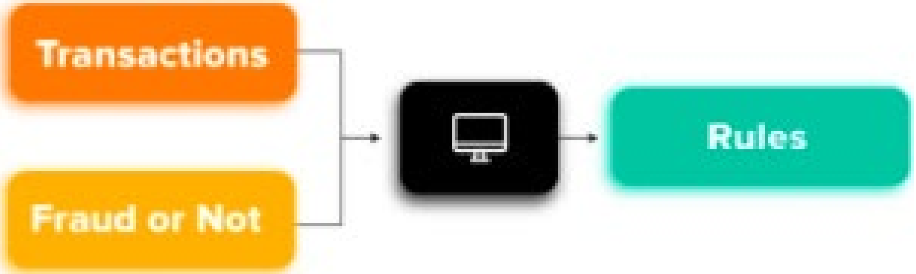
- **Classical programming**: Program/Hard-code the rules for every task





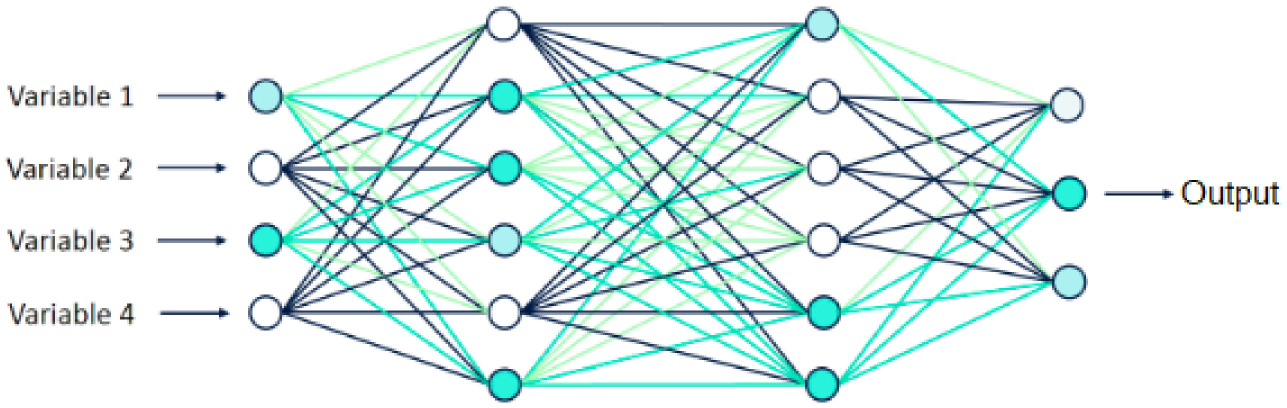
- **Machine learning approach**: An algorithm learn rules automatically from data or experience





What is machine learning?

- Machine learning is a way of generating *computer programs from examples for specific tasks*
- This generated computer program corresponds to a **mathematical model** of the data
  - It describes a relationship between *variables* (quantities involved), that correspond to the input data and the properties of interest (such as predictions, actions, etc.)
  - The model is a compact representation of the data that captures the key properties of the phenomenon we are studying



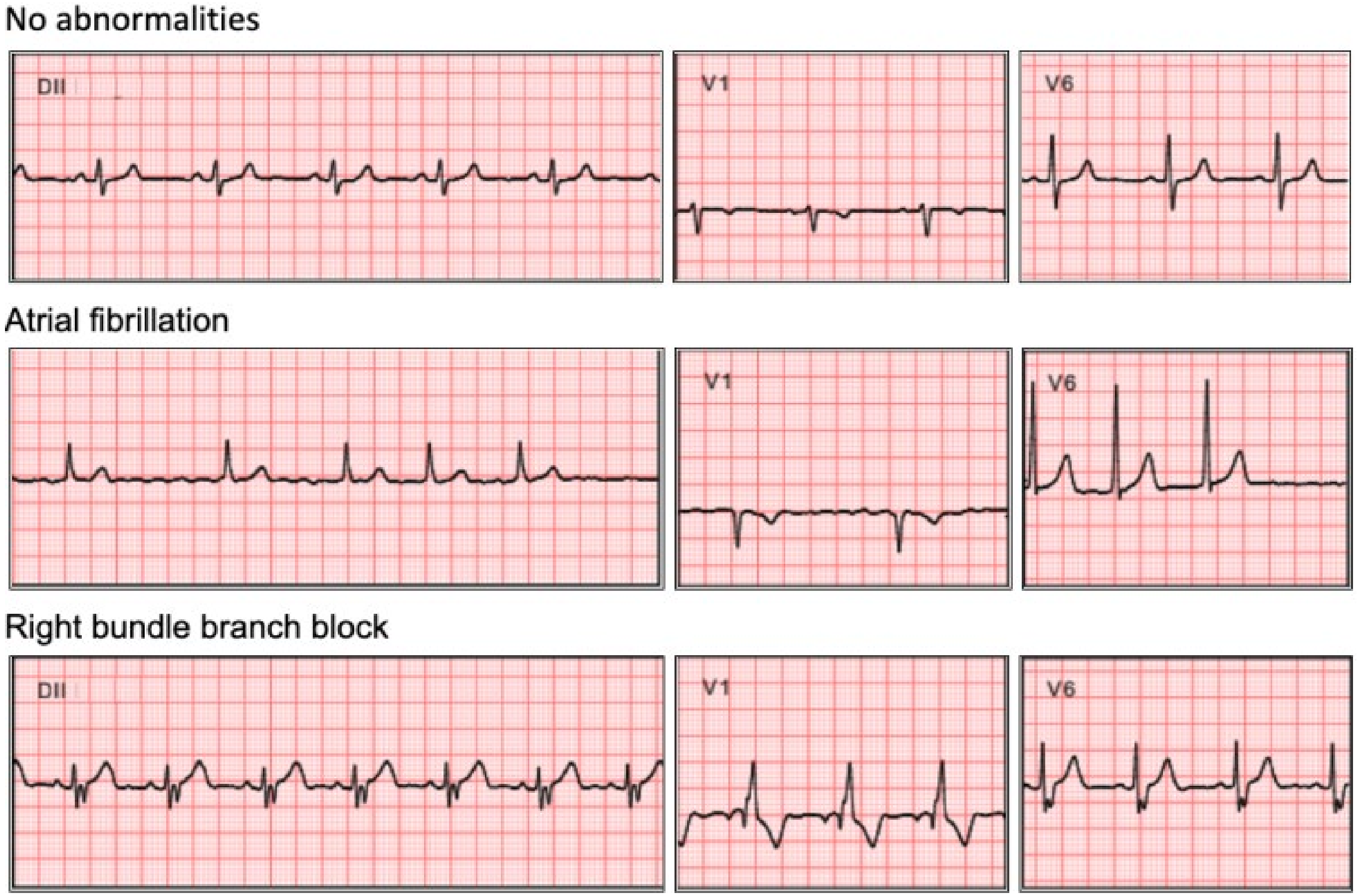
- Which model to use?
  - Guided by the machine learning engineer’s insights generated when looking at the available data and the practitioner’s general understanding of the problem

Examples of machine learning: Example 1

Automatically diagnosing heart abnormality

- Heart problems influence the electrical activity of the heart. These electrical signals can be measured using electrodes attached to the body (reported in ECG)

- ECG signal gives valuable information about the condition of the heart, which can be used to diagnose the patient and plan the treatment



Atrial fibrillation makes the heart beat without rhythm, making it hard for the heart to pump blood in a normal way

Right bundle branch block corresponds to a delay or blockage in the electrical pathways of the heart

Examples of machine learning: Example 1

Automatically diagnosing heart abnormality

- Can we construct a computer program that reads in the ECG signals, analyses the data, and returns a *prediction* regarding the normality or abnormality of the heart?

- **Challenge:** How to design a computer program that turns the raw ECG signal into a prediction about the heart condition?
  - An experienced cardiologist trying to explain his experience to a software developer (which patterns in the data to look for) would not be easy!

- **Machine learning approach:** Teach the computer program through *labelled examples*.
  - Ask the cardiologist (or a group of cardiologists) to *label* a large number of recorded ECG signals with labels corresponding to the underlying heart condition.

  - A machine learning algorithm can then learn to come up with its own rules based on these examples, so that the predictions agree with the cardiologists' labels on the "training" examples

  - The hope is that, if it succeeds on the training data (where we already know the answer), then it should be possible to use the predictions made the by program on previously unseen data (where we *do not* know the answer)

Examples of machine learning : Example 1

Automatically diagnosing heart abnormality

- Ribeiro et. al. developed a machine learning model for ECG prediction
- 23,00,000 ECG records (each of 7-10 s, sampled at 300-600Hz) were used evaluate the electrical activity of the heart of 17,00,000 patients
- The dataset comes with associated labels for **six different** classes according to the status of the heart, i.e., no abnormalities, atrial fibrillation, RBBB, etc.
- Based on this data, a machine learning model (specifically, a deep neural network) was trained to automatically classify a new ECG recording without requiring a human doctor to be involved
- To evaluate how the trained model performs in practice, cardiologists with experience in ECG examined and classified
- The average performance was then compared
- The result was that the algorithm achieved better or the same result when compared to the human performance on classifying six types of abnormalities

Ribeiro, Antônio H., et al. "Automatic diagnosis of the 12-lead ECG using a deep neural network." *Nature communications* 11.1 (2020): 1-9.

Examples of machine learning : Example 1

Various concepts central to machine learning can be understood from this ECG example

1. Data is an important ingredient in machine learning

2. In the ECG example, each data point consists of an **input** (e.g. ECG signal) and an associated **output** (e.g. label corresponding to the heart condition). Such type of data with both input and output is called *labelled* data

3. "Training" a model with labelled data (both inputs and outputs) points is referred to as ***supervised learning***
   - Think of the learning as being supervised by the domain expert, and the learning objective is to obtain a computer program that can mimic the labelling done by the expert

4. The ECG example represents a ***classification*** problem
   - Classification is a supervised machine learning task which amounts to predicting a certain class, for each data point
   - Another type of supervised learning problem is **regression**, where the output is a numerical value

5. In the first phase, a chunk of data is used to train the machine learning model → **Training** data

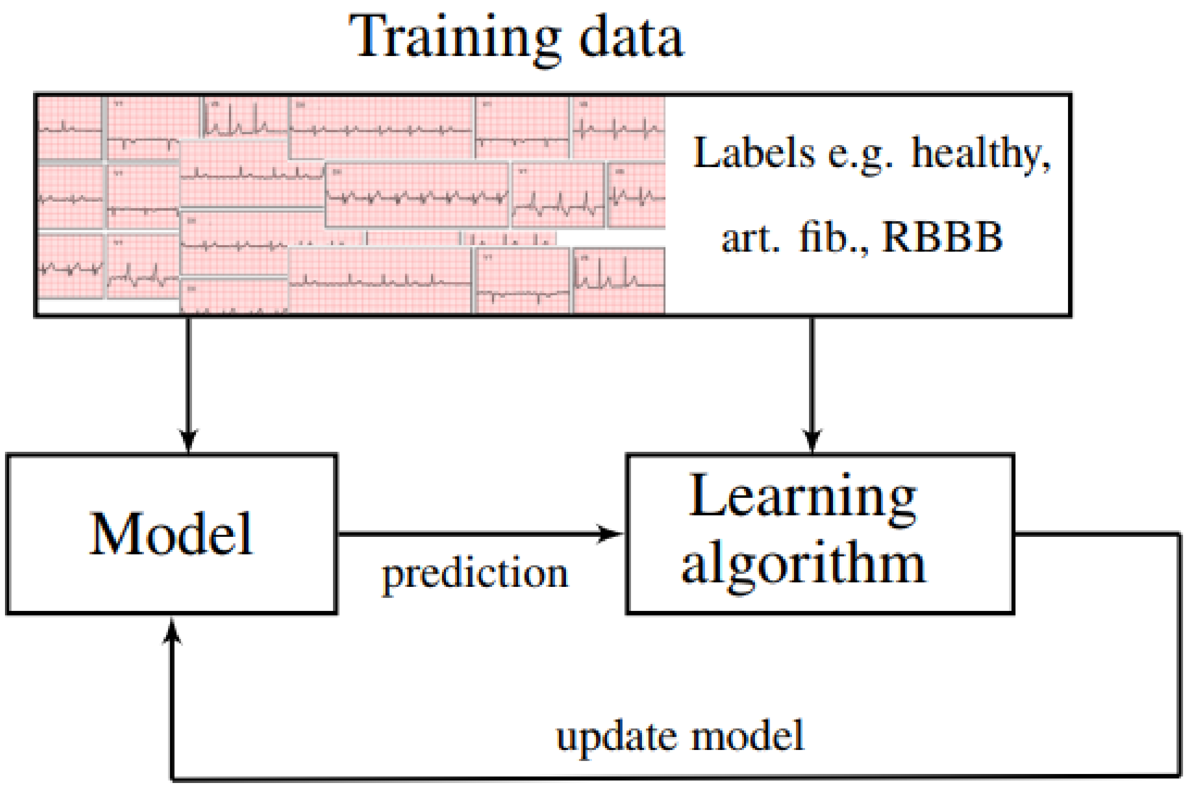
6. The ultimate goal of the trained ML model is to obtain accurate predictions in future. We say that the predictions made by the model must *generalise beyond the training data*

7. In 2nd phase, new unseen unlabelled data (only inputs) are fed to the computer program to predict the labels

Examples of machine learning : Example 1

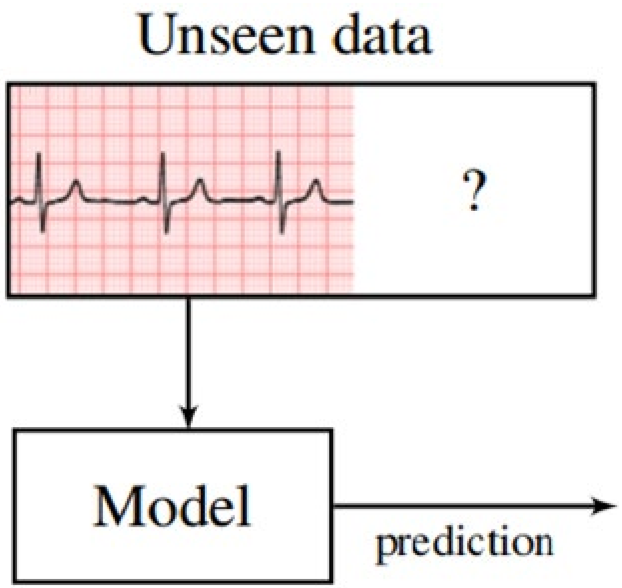
Automatically diagnosing heart abnormality

Training phase



The parameters of the model are tuned by the learning algorithm such that the model best describes the available training data

Testing phase



The learned model is used on new, previously unseen data (**test** data), where we hope to obtain a correct classification

Examples of supervised machine learning

- **Supervised learning - classification**: ECG ML model predicted a certain class

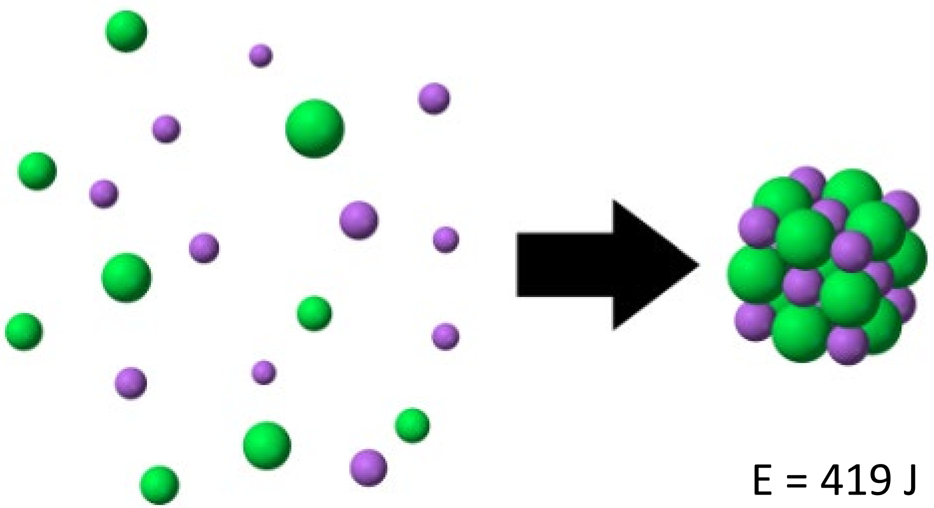
→ **Normal** or **Abnormal**?

Examples of machine learning : Example 2

Predicting formation energy of crystals

- **Motivation**:

  A basic property of interest when trying to discover or synthesize a hypothetical material is the *formation energy* of a crystal. The formation energy can be thought of as the energy that nature needs to spend to form the crystal from the individual elements. A crystal with lower formation energy is more stably synthesized



- **Challenge**: DFT is very accurate but computationally very expensive, even on modern supercomputers. Hence, only a small fraction of all potentially interesting materials can been analysed

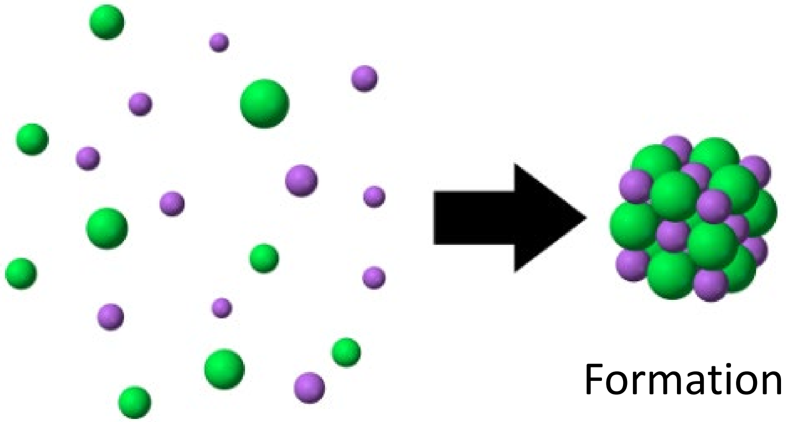
- **Machine learning approach:** Train an ML model that mimics the DFT but is computationally fast
  - Input → Description of the positions and atoms in the candidate crystal
  - Output → Formation energy of the candidate crystal computed using DFT
  - Faber et. al. (2016) used kernel ridge regression to predict the formation energy of 2 million crystals

Examples of supervised machine learning

- **Supervised learning - classification**: ECG ML model predicted a certain class

→ Normal or Abnormal?

- **Supervised learning - regression**: Material discovery model predicted a numerical value (formation energy of crystal)



Formation energy, E

Regression and classification are the two types of prediction problems that we will learn in this training

Different types of machine learning

Supervised

Teacher provides answer

- Labelled data
- Direct feedback
- Predict outcome

- Classification
- Regression

Unsupervised

No teacher, find patterns!

- No labels
- No feedback
- Find hidden structure

- Clustering
- Dimensionality reduction
- Outlier detection

Semi-supervised

- Some labelled data
- A lot of unlabeled data

Reinforcement

Teacher provides rewards

- Decision process
- Rewards
- Learn series of actions

- Gaming
- Control