# APL 405: Machine Learning for Mechanics

# Lecture 1: Introduction

by

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# COURSE STRUCTURE

# Course Structure

Course website: https://coursesam.github.io/APL405/

**Class timings:** Mon, Thu & Fri (11:00 to 11:50 AM) at LHC517

**Practical Session:** Fri (3:15 to 5:15 PM) at two labs LH503 and LH502

## Practical Schedule

| Week# | Topics | Practical Questions |
|---|---|---|
| Week 1 | Probability refresher | Practical 1 |
| Week 2 | k-Nearest Neighbours | Practical 2 |
| Week 3 | Decision Trees | Practical 3 |

## Homework Schedule

A total of 4 homeworks would be given

| HW# | Questions |
|---|---|
| HW1 | Homework 1 |
| HW2 | Homework 2 |
| HW3 | Homework 3 |
| HW4 | Homework 4 |

# Course Grading Scheme

## Grading

| Component | Scores |
|---|---|
| Practical Exam | 10 |
| Practical Attendance | 5 |
| Homework | 10 |
| Project | 20 |
| Minor #1 | 15 |
| Minor #2 | 15 |
| Major | 25 |
| Total | 100 |

- Students are highly encouraged to attend all classes, but there is no marks on lecture attendance. **You still have to mark your attendance on Timble. If the combined lecture-plus-practical attendance is below 75% of the total, one grade would be lowered.**
- There would be a practical exam conducted towards the end of the semester.
- A penalty of 50% of the mark of the respective homework would be deducted if submitted after the deadline. Any submissions two days after the deadline would not be accepted.

# Course Project

A maximum of *two students per project* is allowed

Choose from any one of the catergory of projects you like. Each catergory has different maximum attainable marks.

- Option A (Literature survey) [**15/20 marks**]:
    - Pick a problem that interests you within the domain of civil and/or mechanical engineering
    - Search the literature for machine learning approaches to tackle this problem
    - Survey and discuss the relative strengths of each approach
- Option B (Empirical evaluation) [**17.5/20 marks**]:
    - Pick a problem that interests you within the domain of civil and/or mechanical engineering
    - Implement and experiment with several machine learning techniques to tackle this problem
- Option C (Algorithm design) [**20/20 marks**]:
    - Identify a problem within the domain of civil and/or mechanical engineering for which there are no satisfying approaches
    - Develop a new machine learning technique to tackle this problem
    - Analyze theoretically and/or empirically the performance of your technique
- Project proposal must be submitted by Feb 12th (11:59 pm) (**10% of total project marks**)
- Mid-semester project report must be submitted by Mar 26th (11:59 pm) (**25% of total project marks**)
- Final project report plus a link to a recorded video presentation must be submitted by Apr 27th (11:59 pm) (**(40% +25%) of total project marks**)
- Any delay in submission of the above will be penalized by 1 mark per hour after the deadline has passed!!

Please follow this link for more details on the project.

# Course References

This course is not based on any particular textbook. However, the course materials have been prepared using the following four references:

- Christopher Bishop, "*Pattern Recognition and Machine Learning*", Springer, 2006.
- Andriy Burkov, "*The Hundred Page Machine Learning Book*", 2019 [free pdf].
- Andreas Lindholm et. al., "*Machine Learning: A First Course for Engineers and Scientists*", Cambridge University Press, 2022 [free pdf]
- Brunton, Steven L., and J. Nathan Kutz. "*Data-driven science and engineering: Machine learning, dynamical systems, and control*". Cambridge University Press, 2022.

# Lecture 1

# 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."

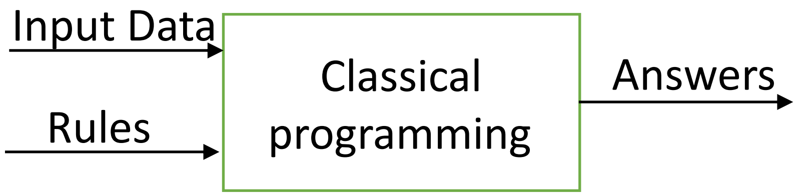
Arthur Samuel

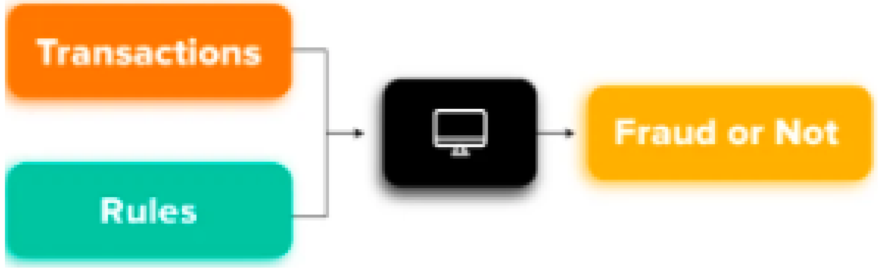
"A computer program is said to learn from *experience E* with respect to some class of *tasks T* and *performance measure P*, if its performance at tasks in T, as measured by P, improves with experience E."

Tom Mitchell

# What is machine learning?

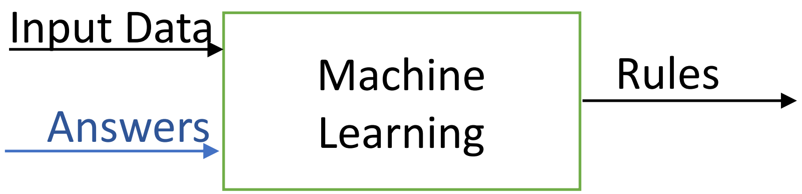
- Classical programming: Program/code the rules for every task

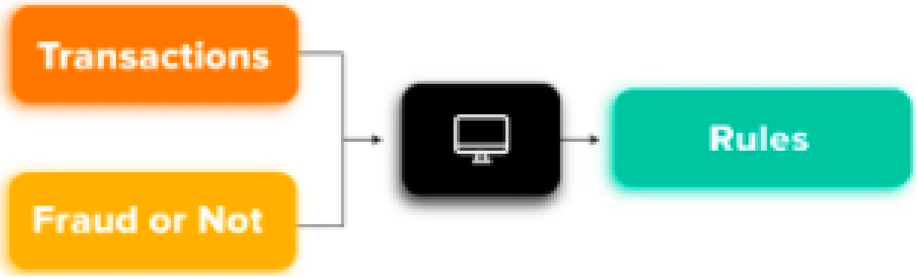



- For many problems, it is difficult to program the correct behaviour by hand
  - detecting spam, fraud transactions
  - recognizing people, objects
  - understanding human speech

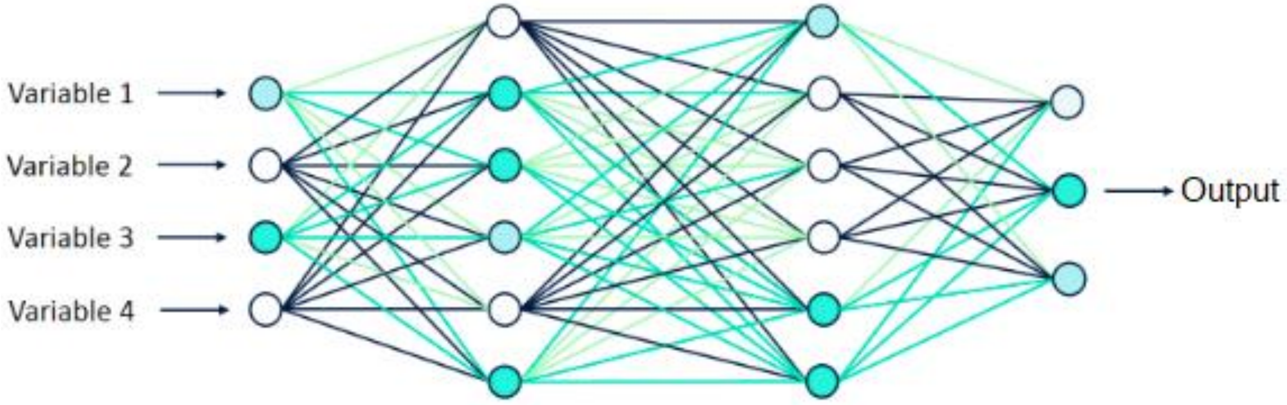
- Machine learning approach: an algorithm automatically learn rules from data, or from experience



# What is machine learning?

- Machine learning is a way of generating *computer programs by example*
- 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.)
  - It is a compact representation of the data that, in a precise mathematical form, captures the key properties of the phenomenon we are studying



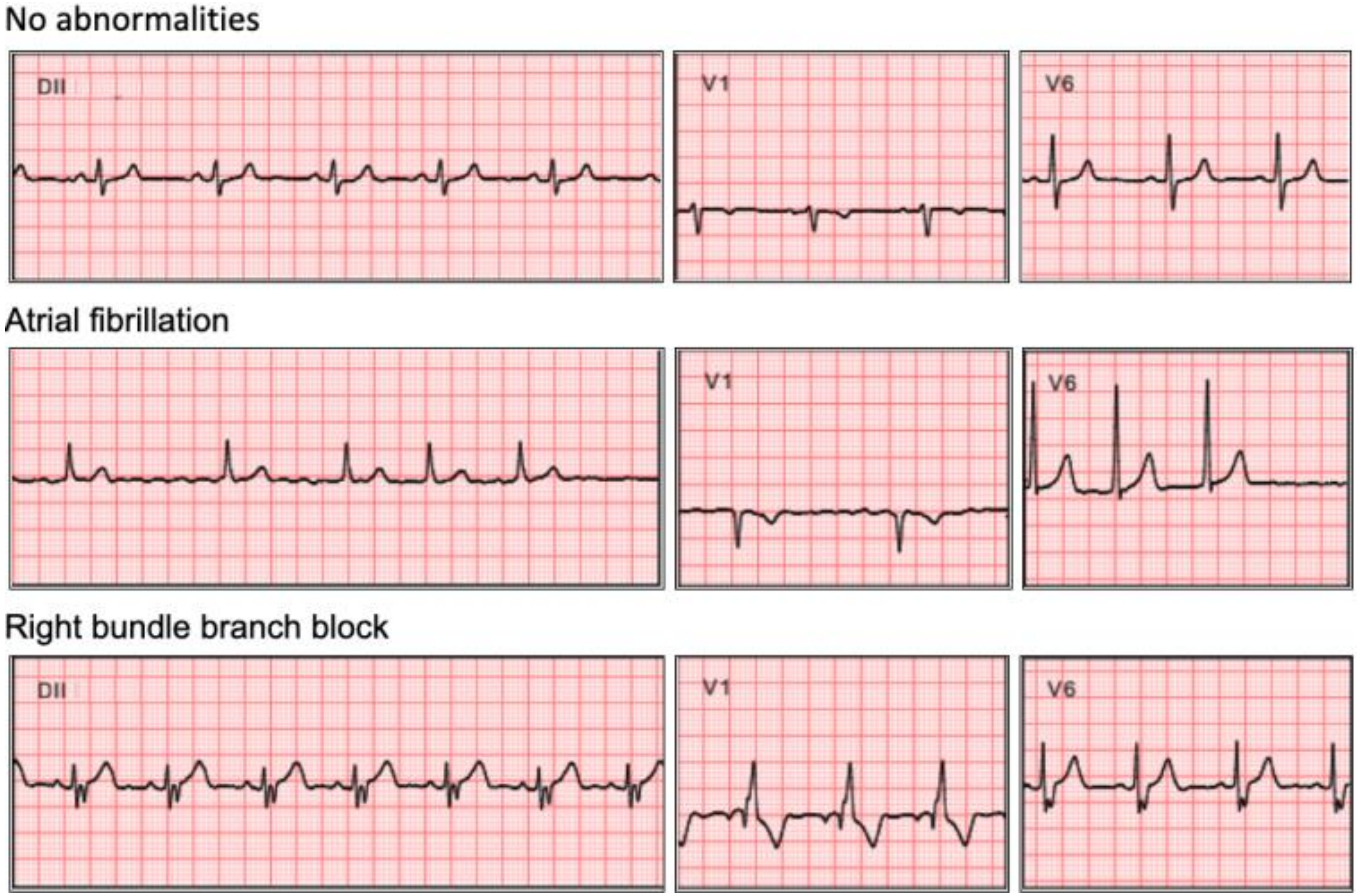

- Which model to make use of?
  - ✓ Guided by the machine learning engineer's insights generated when looking at the available data and the practitioner's general understanding of the problem

# 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 be extremely challenging!

- **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 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

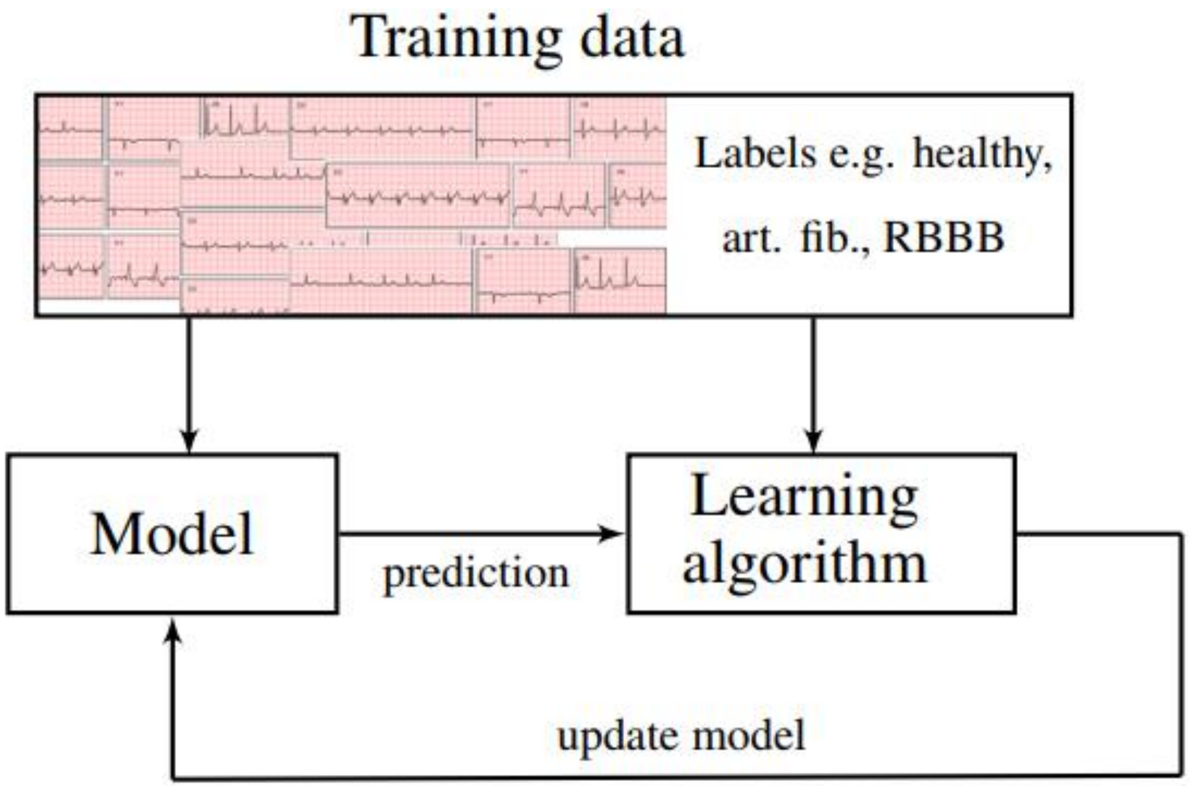
6. The ultimate goal of the trained ML model is to obtain accurate predictions in future. We say that the predictions made by the model must *generalise beyond the training data*

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

# Examples of machine learning : Example 1

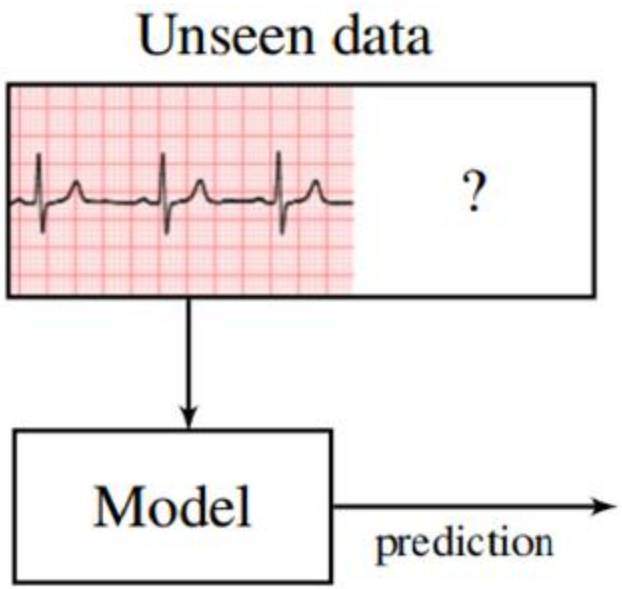
**Automatically diagnosing heart abnormality**

**Training phase**




Values for the unknown parameters of the model are set 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

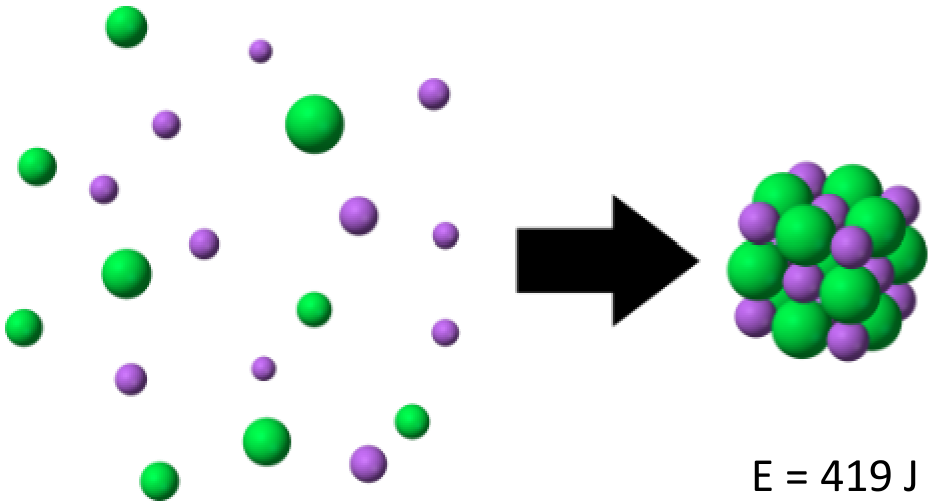
Normal or Abnormal?

# 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

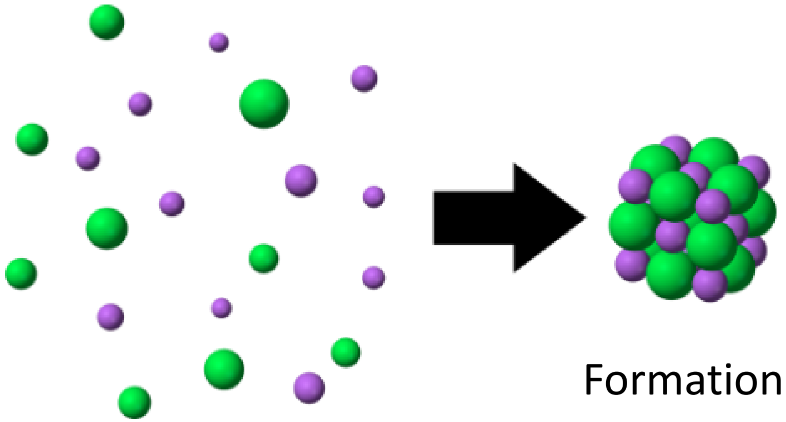
- **Machine learning approach:** Train an ML model that mimics the DFT but is computationally fast
  - Input → Description of the positions and atoms in the candidate crystal
  - Output → Formation energy of the candidate crystal computed using DFT
  - Faber et. al. (2016) used kernel ridge regression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

# 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 unlabelled data

## Reinforcement

Teacher provides rewards

- Decision process
- Rewards
- Learn series of actions

- Gaming
- Control