Introduction to Machine Learning

Lecture 1: Preliminaries and K-Means Clustering

Ali Bereyhi

ali.bereyhi@utoronto.ca

Department of Electrical and Computer Engineering

University of Toronto

Winter 2026

What is Machine Learning?

It's a hard question to answer accurately

Mitchel defines ML as *". . . the study of computer algorithms that improve automatically through experience. . ."*

and

Goodfellow et al. *informally* define ML as *". . . a form of applied statistics with increased emphasis on the use of computers to statistically estimate complicated functions. . ."*

and . . .

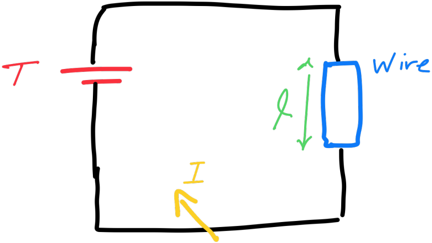
What is Machine Learning?

But not too hard to answer practically

We define ML as *the set of data-driven approaches that help us understand the environment and its behavior, and generalize it!*

Data-driven approaches have long been with us in science and engineering!

Early Example from 1827: *Ohm's Law*



What Did Ohm Do?

Georg Ohm did three major steps

- He saw a pattern and hypothesized some mathematical model
  - ↳ *Electric current increases with voltage*
  - ↳ *The constant changes with the length and material*
  - ↳ . . .
- He collected data
  - ↳ *Electric currents and voltages*
- He used mathematical tools to extract the modeled pattern
  - ↳ *Some curve-fitting technique*

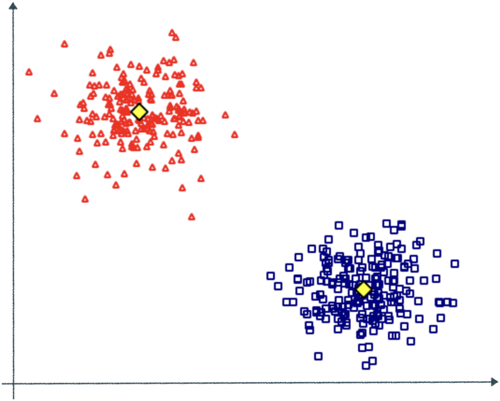
Learning Task

Any learning task has three components

- Model *that captures the Pattern*
- Data
- Learning Algorithm

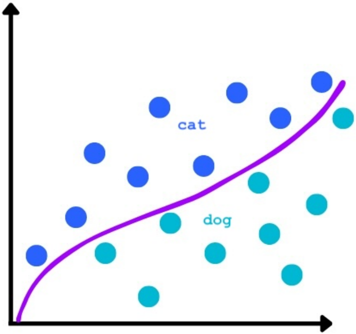
Example: *Clustering*

Monthly amount of transactions versus *# of transactions per month*



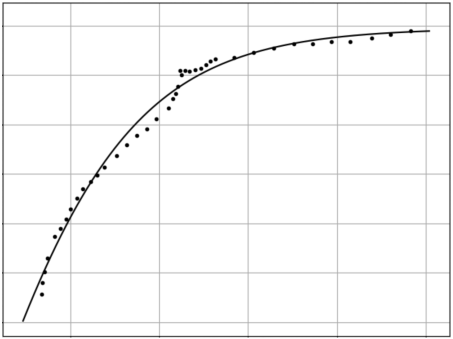
Example: *Classification*

Sleep time versus *# of times the pet makes noise*

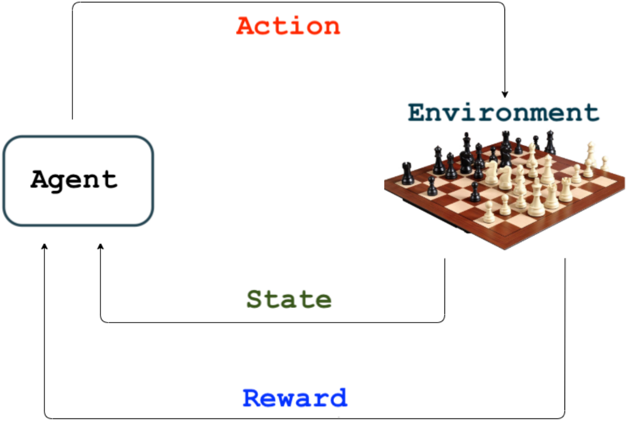


Example: *Regression*

Salary versus *years of experience*



Example: *Playing Chess*



Dataset

A set of data samples

$$\mathbb{D} = \{\boldsymbol{x}_n : n = 1, \dots, N\}$$

with $\boldsymbol{x}_n \in \mathbb{R}^d$

Let's think about data in our examples

- Clustering
- Classification
- Regression
- Playing Chess

Model

A pre-assumed function

$$f : \boldsymbol{x} \mapsto y$$

for a data sample $\boldsymbol{x}$ and output y that *fits the learning task*

Let's formulate model in our examples

- Clustering
- Classification
- Regression
- Playing Chess

Learning Algorithm

Algorithm that gets dataset and returns the exact model

$$\mathcal{A} : \mathbb{D} \mapsto f^\star$$

$f^\star$ does the mapping such that we get to the desired output

Let's formulate learning algorithm in our examples

- Clustering
- Classification
- Regression
- Playing Chess

? *How can we define a "good" learning algorithm?*

Unsupervised Learning

Data samples are not labeled

$$\mathbb{D} = \{\boldsymbol{x}_n : n = 1, \ldots, N\}$$

Here, we are looking for a pattern in the data

Other components of an unsupervised task

- Model *captures the pattern hidden in data*
- Learning Algorithm

Examples of unsupervised learning

- ✔ Clustering
- Dimensionality Reduction
- Distribution Learning

Supervised Learning

Data samples are labeled

$$\mathbb{D} = \{(\boldsymbol{x}_n, v_n) : n = 1, \ldots, N\}$$

Here, we are looking for a model that describes the relation

Other components of a supervised task

- Model *describes the relation between data samples and their labels*
- Learning Algorithm

Examples of supervised learning

- Classification
- Regression

Reinforcement Learning

Data samples are series of *actions*, *states* and *rewards*

$$\mathbb{D} = \left\{ \left\{ \left(a_n^t, s_n^t, r_n^t \right) : t = 1, \ldots \right\} : n = 1, \ldots, N \right\}$$

Here, we are looking for optimal policy, i.e., policy that maximizes future returns

$$G_t = r^t + r^{t+1} + \ldots$$

Other components of a reinforcement task

- Model *describes a policy*
- Learning Algorithm

Examples of reinforcement learning

- Playing Game, Control Robots, . . .

Reinforcement learning is not discussed in this course, but you may consider taking Reinforcement Learning in next Fall

Further Read

- Bishop
  - ↳ Chapter 1: *Sections 1.1 and 1.3* — ***Introductory***
- ESL
  - ↳ Chapter 1 — ***Introductory***
  - ↳ Chapter 2: *Sections 2.1 and 2.2* — ***Supervised***
  - ↳ Chapter 14: *Sections 14.1 and 14.2* — ***Unsupervised***
- Mitchell
  - ↳ Chapter 13: *Sections 13.1 and 13.2* — ***Reinforcement***
- Goodfellow, et al.
  - ↳ Chapter 5: *Sections 5.1 and 5.2* — ***Introductory***

Unsupervised Learning

Why do we start with *unsupervised learning*?

- Many basic problems are unsupervised
  - ↳ *We naturally cluster everything around us*
  - ↳ *We get sense about quantities by understanding its statistical behavior*
- It helps us to recap some basics we need later
  - ↳ *Linear Algebra*
  - ↳ *Probability Theory*

Problem of Clustering

This is a basic sign of intelligence

- *We cluster everything around us*
  - ↳ *Trees, flowers, animals, . . .*
- *We often start with simple clustering and extend hierarchically*
  - ↳ *Plants and animals*
  - ↳ *Plants could be trees, flowers, . . .*
  - ↳ *Animals could be mammals, birds, . . .*
- *The further we go, the more intelligent we get!*

Basic Clustering Task: *Data*

Data samples are points in d-dimensional space

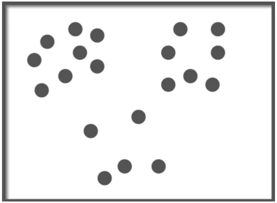
$$\mathbb{D} = \{\boldsymbol{x}_n : n = 1, \dots, N\}$$

with $\boldsymbol{x}_n \in \mathbb{R}^d$

In Examples

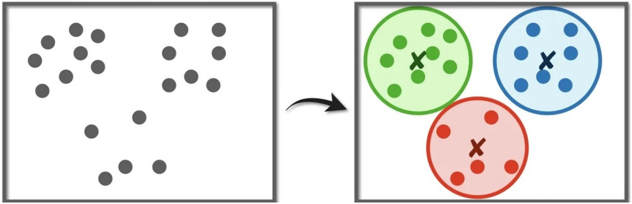
In examples, we always think of two dimensions for sake of simplicity

Recall our bank record example



Basic Clustering Task: *Pattern*

We assume that the samples can be grouped into clusters



Recall our bank record example

Basic Clustering Task: *Model*

We use a model to capture the clustering pattern

$$f\left(\boldsymbol{x}\right) \to k \in \{1, \ldots, K\}$$

for some integer number of clusters K

Some definitions and assumptions

- *Cluster subspace* k

$$\mathbb{C}_k = \{\boldsymbol{x} : f\left(\boldsymbol{x}\right) = k\}$$

- *Cluster subspaces partition the data space*

$$\mathbb{C}_1 \cup \ldots \cup \mathbb{C}_K = \mathbb{X} \rightsquigarrow \textit{all possible samples}$$
$$\mathbb{C}_j \cap \mathbb{C}_k = \varnothing \rightsquigarrow \forall j \neq k$$

Basic Clustering Task: *Learning Algorithm*

The learning algorithm gets a dataset and finds a good f

$$\mathcal{A} : \mathbb{D} \mapsto f^{\star}$$

? *What is a "good" model?*

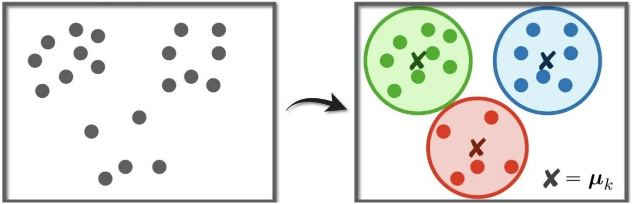
! *We'll answer it!*

An Intuitive Model: *K Centroids*

Let's use a simple and intuitive model

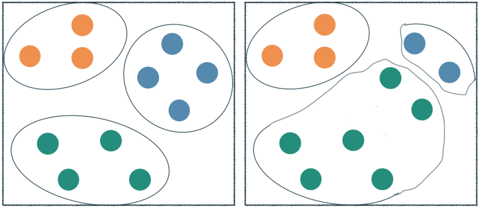
$$f(\boldsymbol{x}) = \underset{k \in \{1,\dots,K\}}{\operatorname{argmin}} \|\boldsymbol{x} - \boldsymbol{\mu}_k\|$$

for K centroids $\boldsymbol{\mu}_1, \dots, \boldsymbol{\mu}_K \in \mathbb{R}^d$



K Centroids: *Learning Algorithm*

This model is valid for any set of centroids!



The learning algorithm is to start from $\mathbb{D}$ and learn good centroids

$$\mathcal{A} : \mathbb{D} \mapsto \boldsymbol{\mu}_1^\star, \ldots \boldsymbol{\mu}_K^\star$$

? *What is a "good" set of centroids?*

! *We'll answer it!*

K-Means Clustering Algorithm: *Intuitive Derivation*

Given the centroids, we can easily assign each $\boldsymbol{x}_n \in \mathbb{D}$ *to a cluster-set*

`Cluster_Assignment`$(\boldsymbol{\mu}_1, \ldots, \boldsymbol{\mu}_K)$:

`# we want to find` $\mathcal{C}_1 \cup \ldots \cup \mathcal{C}_K = \mathbb{D}$

1: **for** $n = 1 : N$ **do**

2: Find the index of the closest centroid

$$k^\star \leftarrow \operatorname*{argmin}_{k \in \{1,\ldots,K\}} \|\boldsymbol{x}_n - \boldsymbol{\mu}_k\|$$

3: Assign $\boldsymbol{x}_n$ to cluster-set $\mathcal{C}_{k^\star}$

4: **end for**

5: Return $\mathcal{C}_1, \ldots, \mathcal{C}_K$

K-Means Clustering Algorithm: *Intuitive Derivation*

Given the cluster sets, we can move centroids to the center of cluster-sets

`Centroid_Update`$(\mathcal{C}_1, \ldots, \mathcal{C}_K)$:

`# we want to find` $\boldsymbol{\mu}_1, \ldots, \boldsymbol{\mu}_K$

1: **for** $k = 1 : K$ **do**
2:     **if** $\mathcal{C}_k \neq \emptyset$ **then**
3:         Move $\boldsymbol{\mu}_k$ to the center of cluster $\mathcal{C}_k$, i.e.,

$$\boldsymbol{\mu}_k \leftarrow \frac{1}{|\mathcal{C}_k|} \sum_{\boldsymbol{x}_n \in \mathcal{C}_k} \boldsymbol{x}_n$$

4:     **else**
5:         Leave $\boldsymbol{\mu}_k$ unchanged
6:     **end if**
7: **end for**
8: Return $\boldsymbol{\mu}_1, \ldots, \boldsymbol{\mu}_K$

K-Means Clustering Algorithm

We could iterate till we converge

K`-Means()`:

1: Initiate $\boldsymbol{\mu}_1, \ldots, \boldsymbol{\mu}_K$
2: **while** $\boldsymbol{\mu}_1, \ldots, \boldsymbol{\mu}_K$ changing **do**
3: Set $\mathcal{C}_1, \ldots, \mathcal{C}_K \leftarrow$ `Cluster_Assignment`$(\boldsymbol{\mu}_1, \ldots, \boldsymbol{\mu}_K)$
4: Update $\boldsymbol{\mu}_1, \ldots, \boldsymbol{\mu}_K \leftarrow$ `Centroid_Update`$(\mathcal{C}_1, \ldots, \mathcal{C}_K)$
5: **end while**
6: Return $\boldsymbol{\mu}_1, \ldots, \boldsymbol{\mu}_K$

Example: *2-Means Clustering*[1]

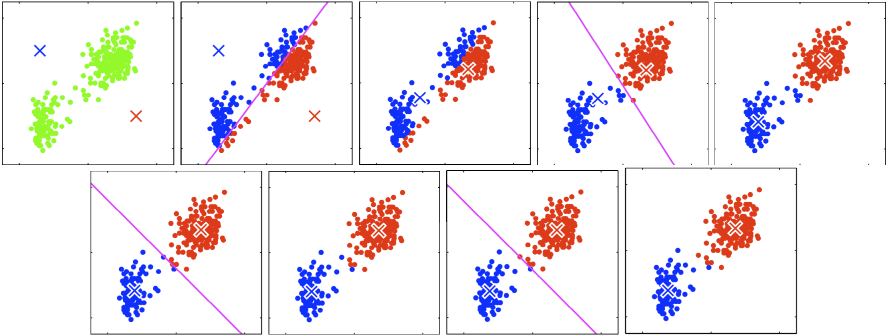
Initial centroids

Iteration 1

Iteration 2

Iteration 3

Iteration 4 – Converged



[1] *This example is taken from Bishop's book, Chapter 9*

Further Read

- MacKay
  - ↳ Chapter 20 — K***-means***
- Bishop
  - ↳ Chapter 9: *Section 9.1* — K***-means***
- ESL
  - ↳ Chapter 14: *Section 14.3* — ***Clustering***