K-Means:
an example of unsupervised learning

CMSC 422

SOHEIL FEIZI

sfeizi@cs.umd.edu

Slides adapted from SAMUEL DOOLEY and MARINE CARPUAT

Supervised Learning

Data comes in different formats:

$$\left\{(x^{(1)}, y^{(1)}), \ldots, (x^{(N)}, y^{(N)})\right\}$$

Trainin
g set

feature
s

target/labe
l variable

Goal: predict the label/target using features

Supervised Learning

Unsupervised Learning

Data comes in different formats:

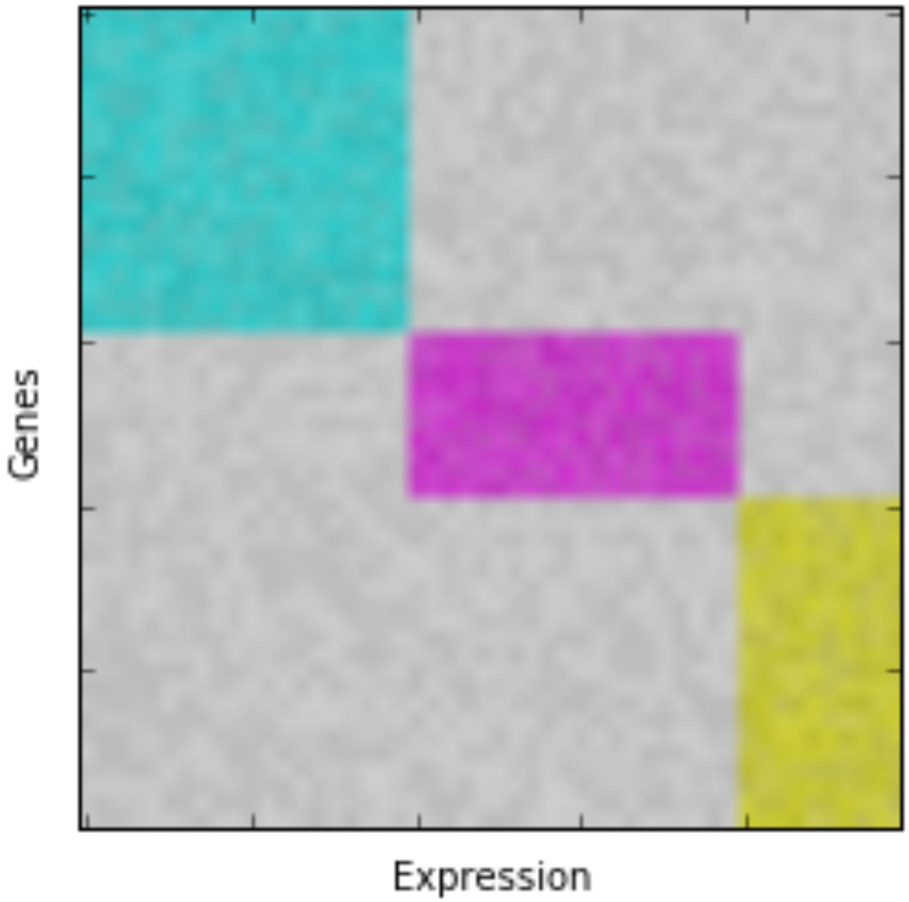
$$\left\{ x^{(1)}, x^{(1)}, \ldots, x^{(N)} \right\}$$ → Training set

features

Goal: find "interesting" patterns in data

→ Unsupervised Learning

Example



Clustering Problem

Today's Topics

- A new algorithm
  - K-Means Clustering
- Fundamental Machine Learning Concepts
  - Unsupervised vs. supervised learning

Supervised Machine Learning as Function Approximation

Problem setting

- Set of possible instances X
- Unknown target function $f: X \rightarrow Y$
- Set of function hypotheses $H = \{h \mid h: X \rightarrow Y\}$

Input

- Training examples $\{(x^{(1)}, y^{(1)}), \ldots (x^{(N)}, y^{(N)})\}$ of unknown target function f

Output

- Hypothesis $h \in H$ that best approximates target function f

Supervised vs. unsupervised learning

- Clustering is an example of unsupervised learning
- We are not given examples of classes y
- Instead we have to discover classes in data

Clustering

- Goal: automatically partition examples into groups of similar examples

- Why? It is useful for
  - Automatically organizing data
  - Understanding hidden structure in data
  - Preprocessing for further analysis

What can we cluster in practice?

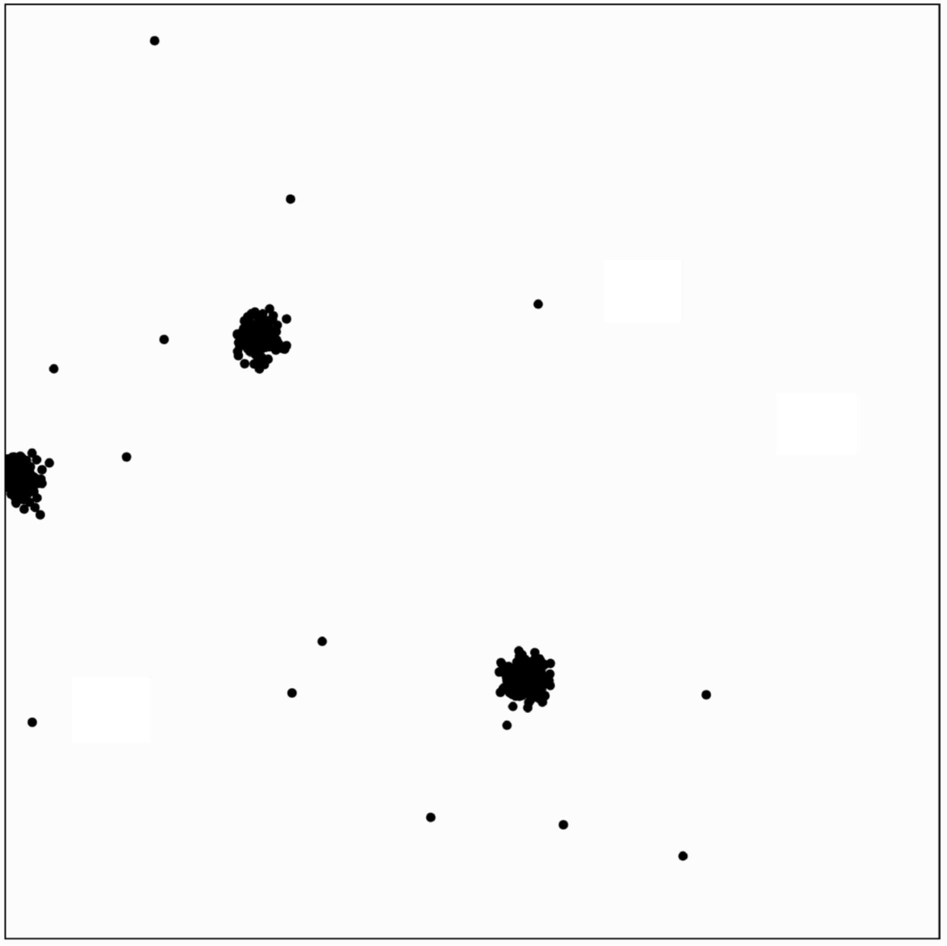
- news articles or web pages by topic
- protein sequences by function, or genes according to expression profile
- users of social networks by interest
- customers according to purchase history
- ...

Clustering

- Input
  - a set $S = \{x_1, x_2, \ldots, x_n\}$ of n points in feature space
  - a distance measure specifying distance $d(x_i, x_j)$ between pairs (x_i, x_j)
- Output
  - A partition $\{S_1, S_2, \ldots, S_k\}$ of S
  - Also represented as $\{z_1, \ldots, z_n\}$ where z_i is the index of the partition to which x_i belongs.

Illustration of Algorithm

Steps of Algorithm
- Gather data



Visualization from: http://stanford.edu/class/ee103/visualizations/kmeans/kmeans.html

Illustration of Algorithm

Steps of Algorithm
- Gather data
- Initialize means

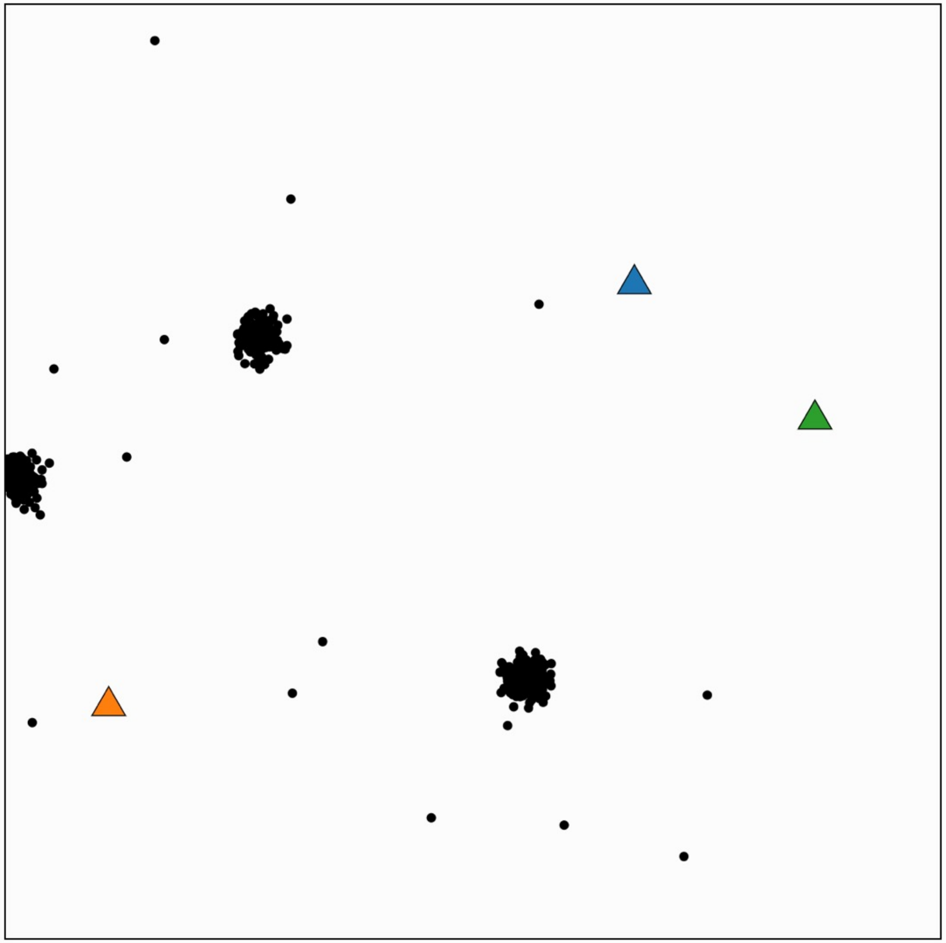


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Illustration of Algorithm

Steps of Algorithm
- Gather data
- Initialize means
- Repeat:
  - Assign classes

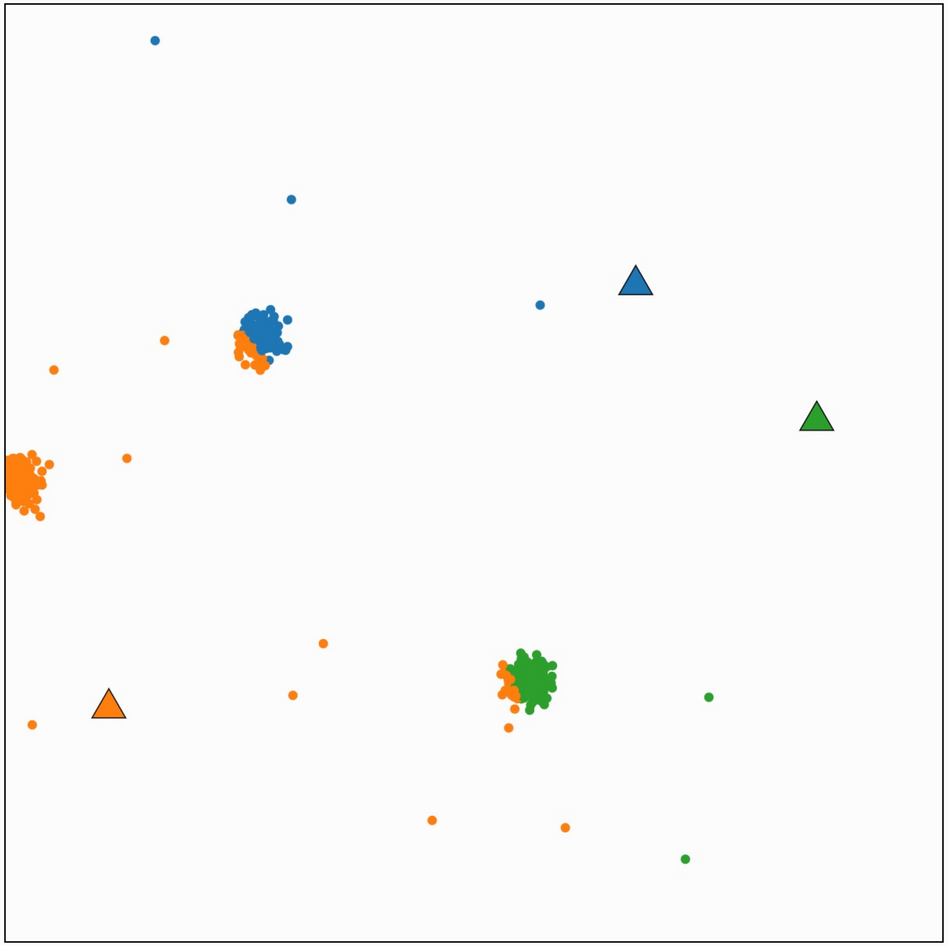

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Illustration of Algorithm

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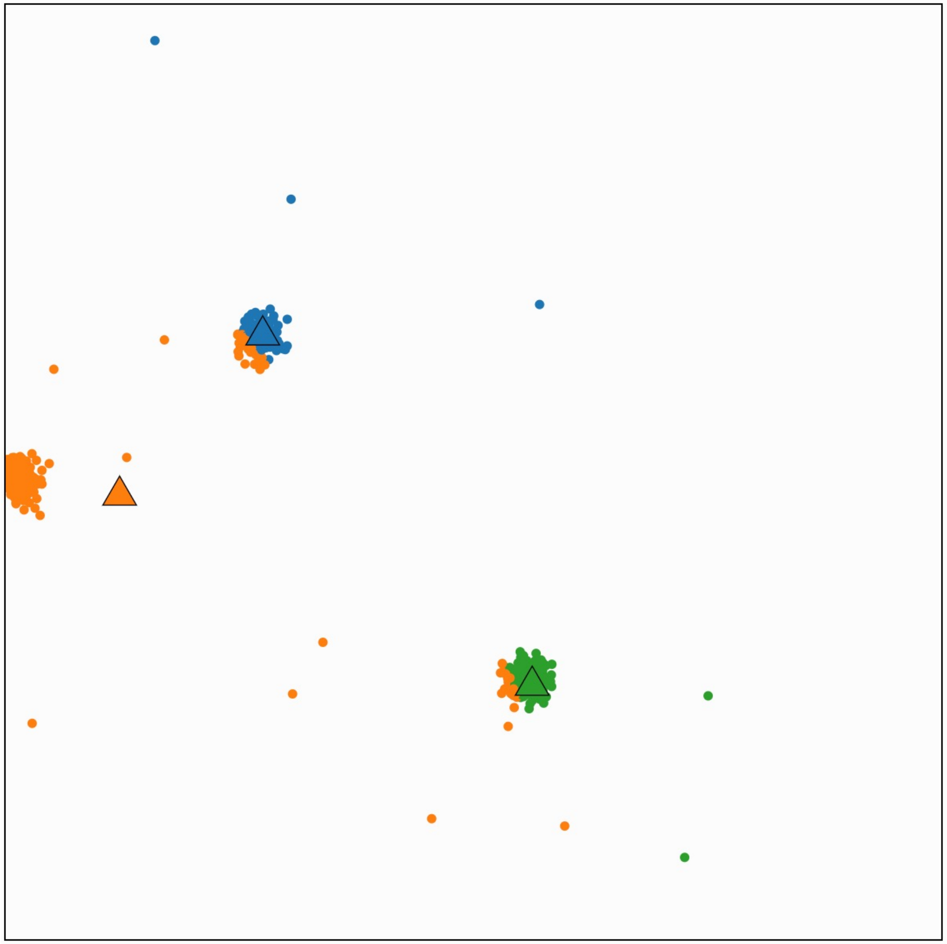
- Repeat:
  - Assign classes
  - Adjust means



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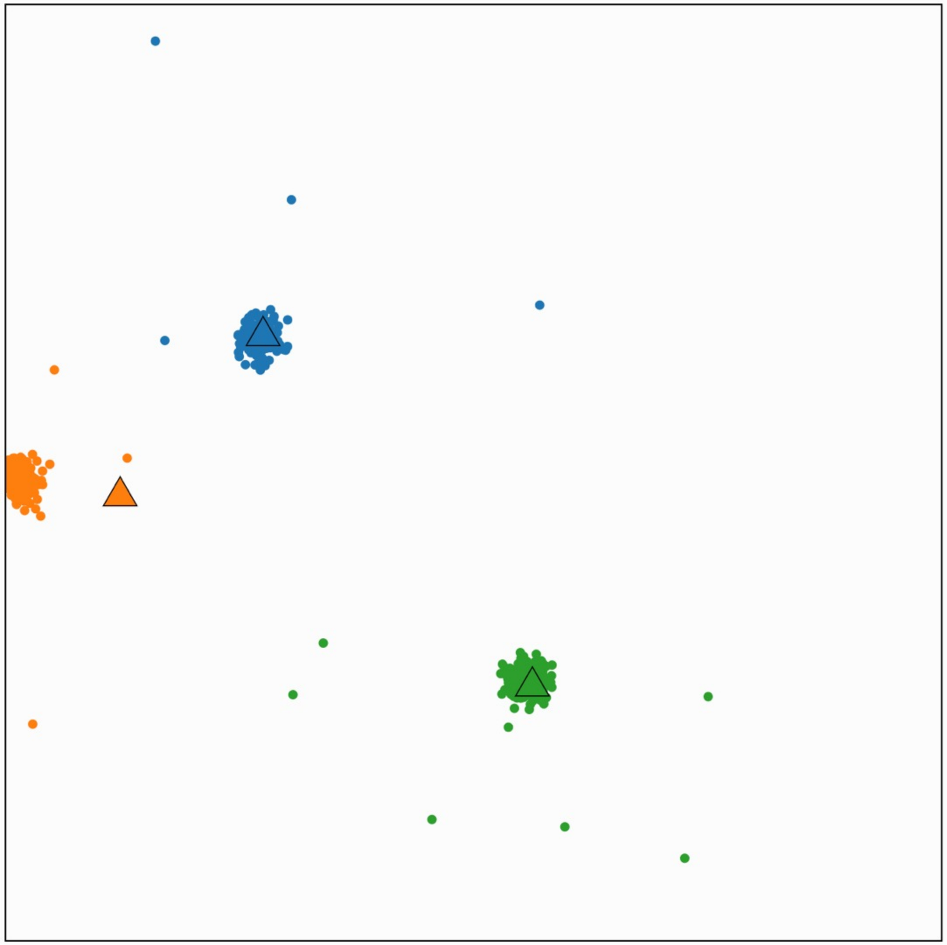

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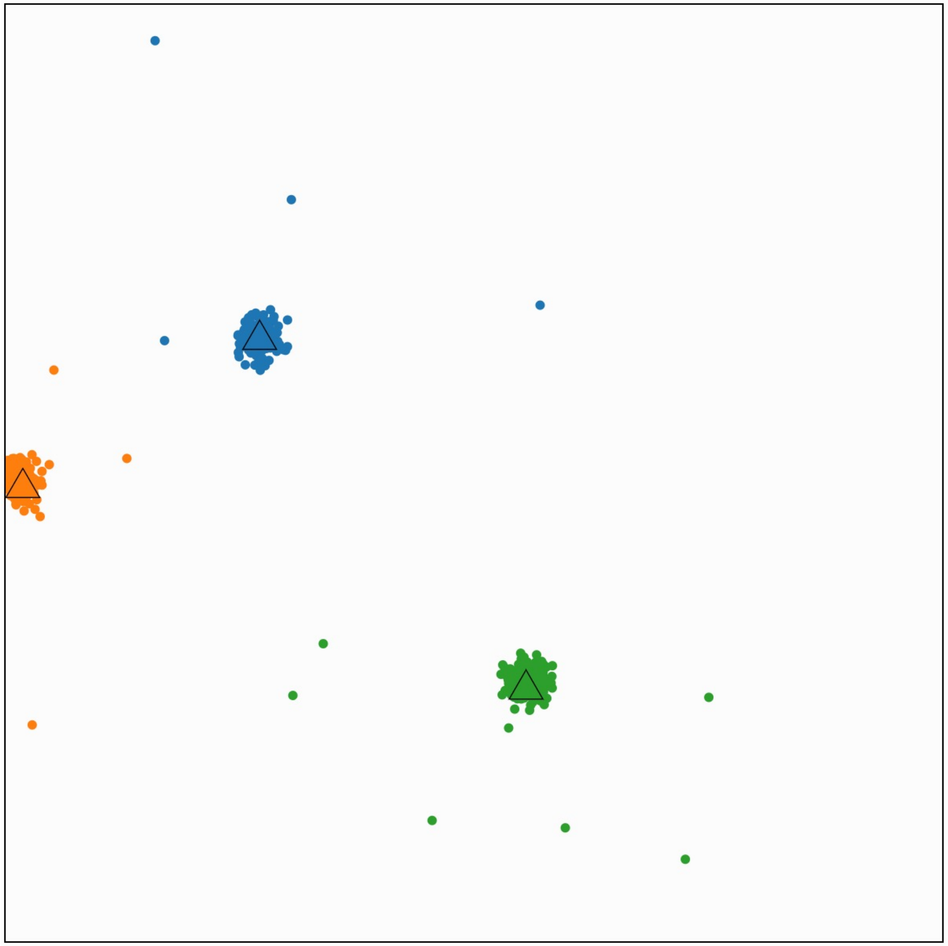

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The K-Means Algorithm

Training Data

K: number of clusters to discover

Algorithm 4 K-MEANS($\mathbf{D}$, K)

for $k = 1$ **to** K **do**
  $\boldsymbol{\mu}_k \leftarrow$ some random location // randomly initialize mean for kth cluster
end for
repeat
  for $n = 1$ **to** N **do**
    $z_n \leftarrow \text{argmin}_k \,||\boldsymbol{\mu}_k - \boldsymbol{x}_n||$ // assign example n to closest center
  end for
  for $k = 1$ **to** K **do**
    $\mathbf{X}_k \leftarrow \{\, \boldsymbol{x}_n : z_n = k \,\}$ // points assigned to cluster k
    $\boldsymbol{\mu}_k \leftarrow \text{MEAN}(\mathbf{X}_k)$ // re-estimate mean of cluster k
  end for
until $\boldsymbol{\mu}$s stop changing
return z // return cluster assignments

The K-Means Optimization

- Assignment objective: For each *i*,

$$\arg\min_{z_i} \|x_i - \mu_{z_i}\|^2$$

- Mean update objective:

$$\min_{\mu_j} \sum_{\{i|z_i=j\}} \|x_i - \mu_{z_i}\|^2$$

- Overall objective:

$$\arg\min_{S} \sum_{i=1}^{k} \sum_{x \in S_i} \|x - \mu_i\|^2 = \arg\min_{S} \sum_{i=1}^{k} |S_i| Var S_i$$

where μ_i is the mean of the points in S_i.

K-Means properties

- Time complexity: O(KNL) where
  - K is the number of clusters
  - N is number of examples
  - L is the number of iterations
- K is a hyperparameter
  - Needs to be set in advance (or learned on dev set)
- Different initializations yield different results!
  - Doesn’t necessarily converge to best partition
- “Global” view of data: revisits all examples at every iteration

Questions for you…

- For what types of data can we not use k-means?
- Are we sure it will find an optimal clustering?
- Does the initialization of the random means impact the result?
- Are there clusters that cannot be discovered using k-means?
- Do you know any other clustering algorithms?

What you should know

- New Algorithms
  - K-NN classification
  - K-means clustering
- Fundamental ML concepts
  - How to draw decision boundaries
  - What decision boundaries tells us about the underlying classifiers
  - The difference between supervised and unsupervised learning