

Content

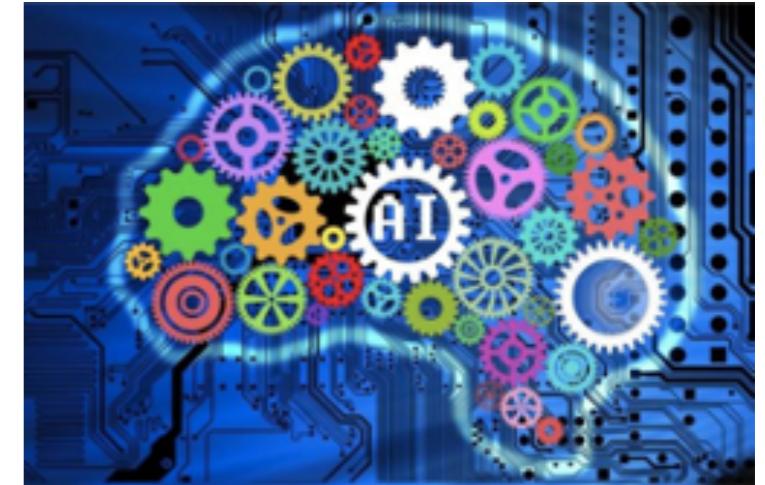
0. Introduction

1. Regression

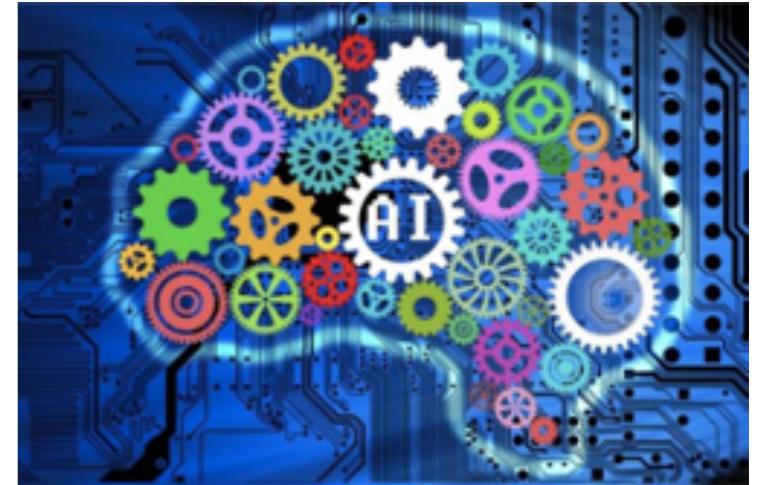
- 1.1 Multivariate Linear Regression (curve fitting)
- 1.2 Regularization (Lagrange multiplier)
- 1.3 Logistic Regression (Fermi-Dirac distribution)
- 1.4 Support Vector Machine (high-school geometry)

2. Dimensionality Reduction/feature extraction

- 2.1 Principal Component Analysis (order parameters)
- 2.2 Recommender Systems
- 2.3 Clustering (phase transition)



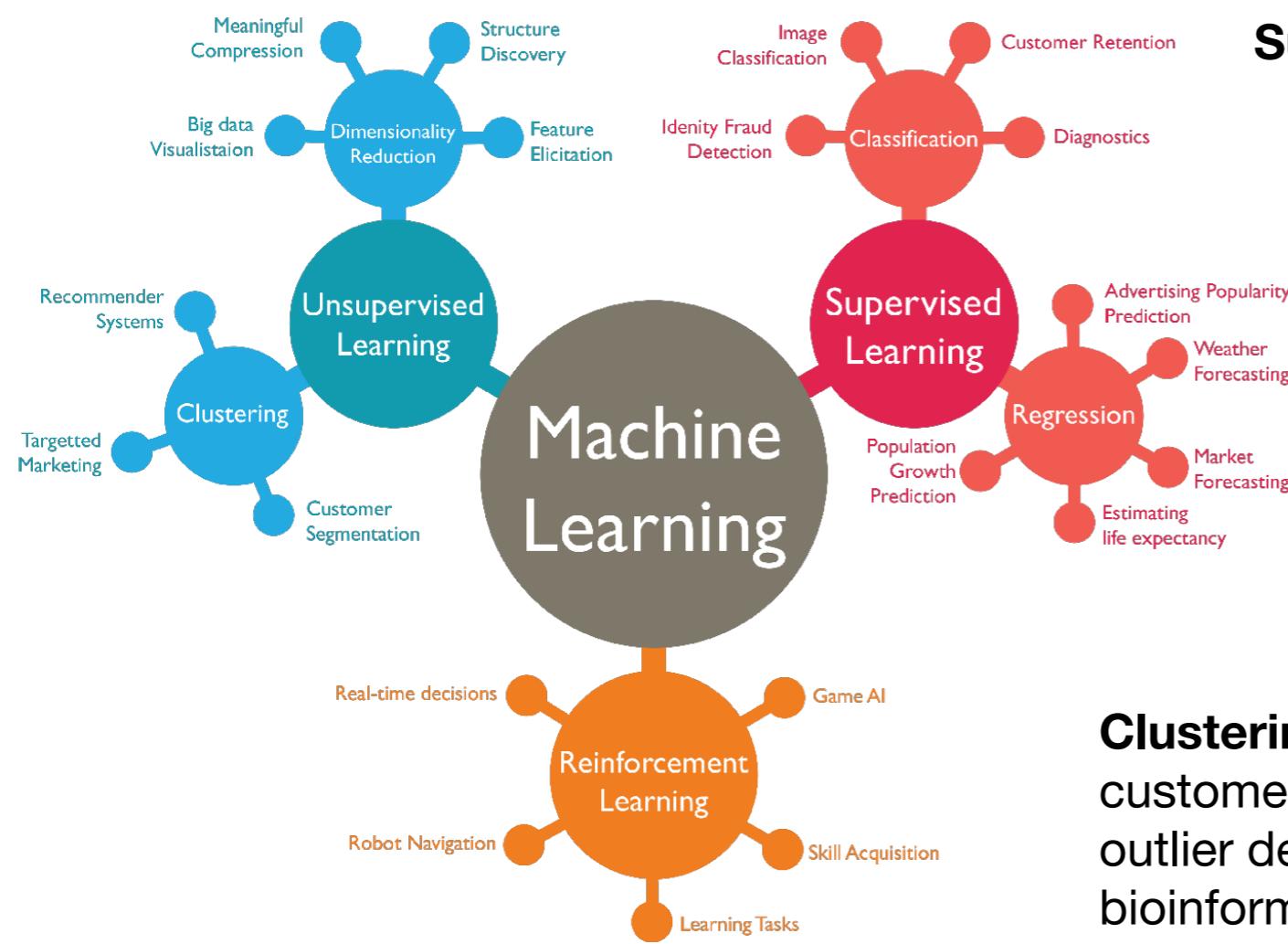
Content



3. Neural Networks

- 3.1 Biological neural networks**
- 3.2 Mathematical representation**
- 3.3 Factoring biological ingredient**
- 3.4 Feed-forward neural networks**
- 3.5 Learning algorithm**
- 3.6 Universal Approximation Theorem**

AI & Machine Learning Basics



Supervised Learning: Classification & Regression

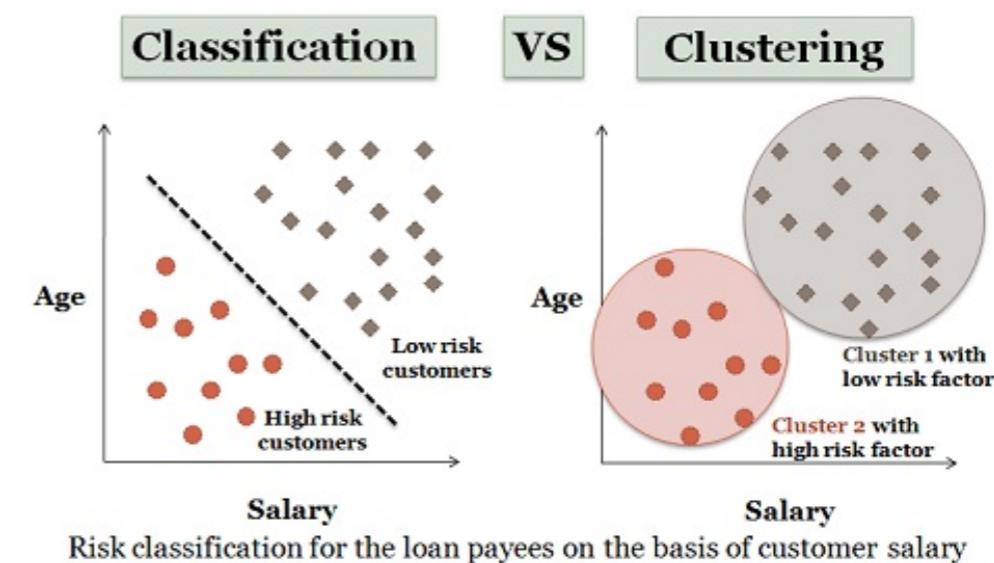
Labeled dataset
 Input → machine/model → Output
 Correct outputs are provided by the supervisor

Unsupervised Learning: only have input data

Unlabeled dataset
 Find regularities from the input

Clustering:

customer segmentation, customer relationship management, outlier detection; Image compression
 bioinformatics: DNA, RNA, amino acids, Motif, Proteins, sequence alignments

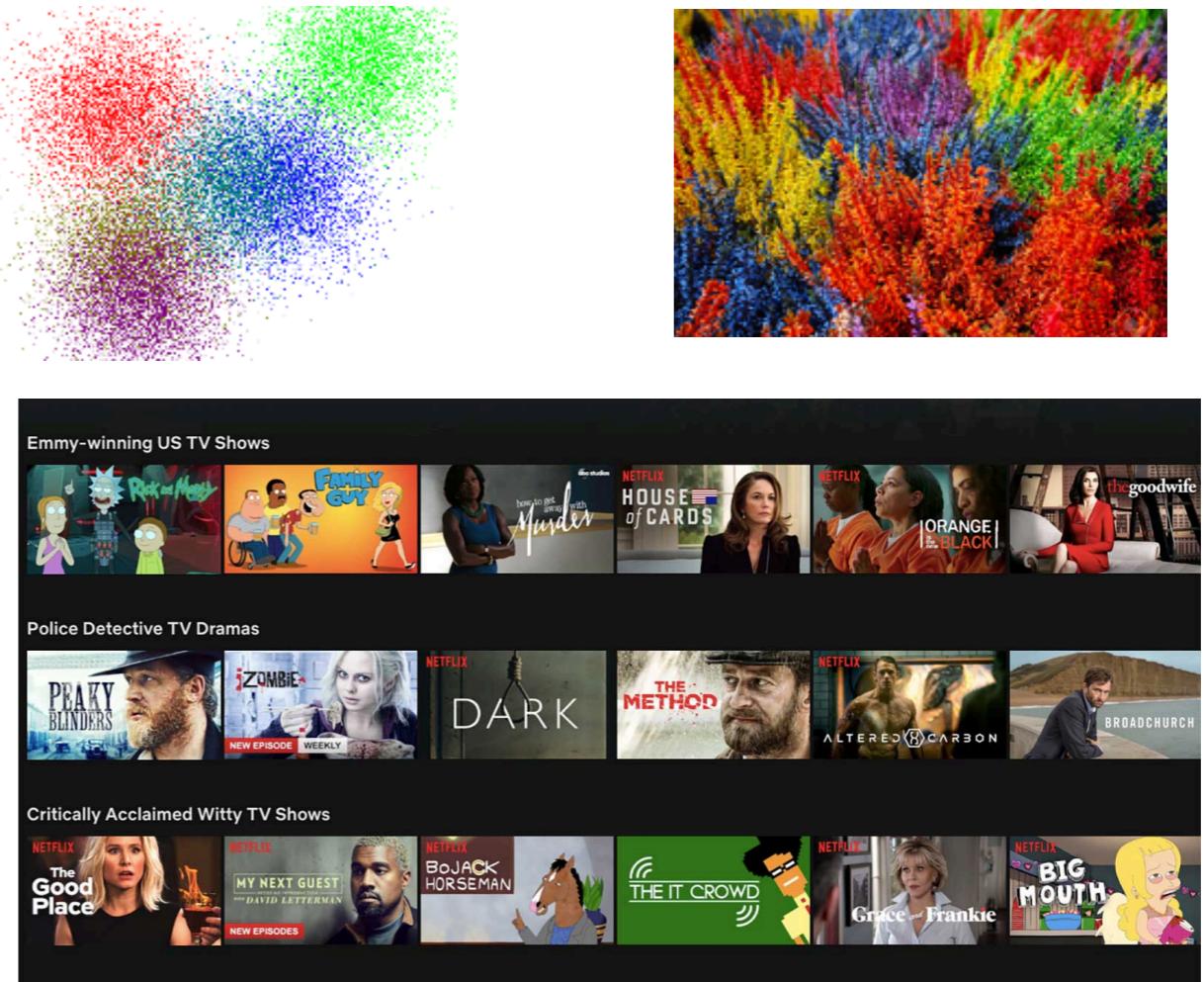


Clustering

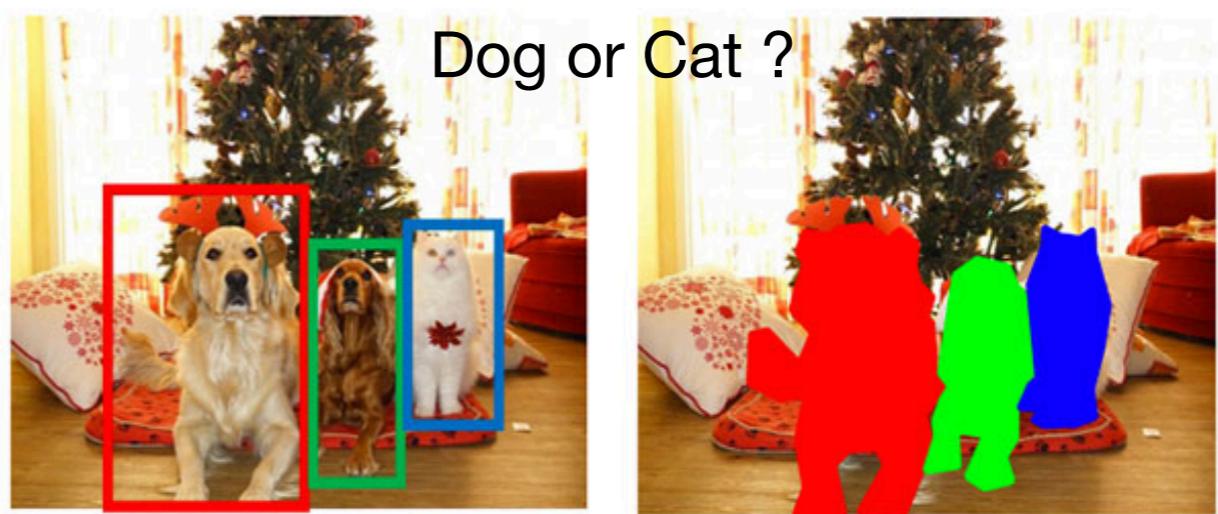
- Grouping of data points

“Clustering” literally means grouping similar things together

- Recommendation Engines



- Image Segmentation



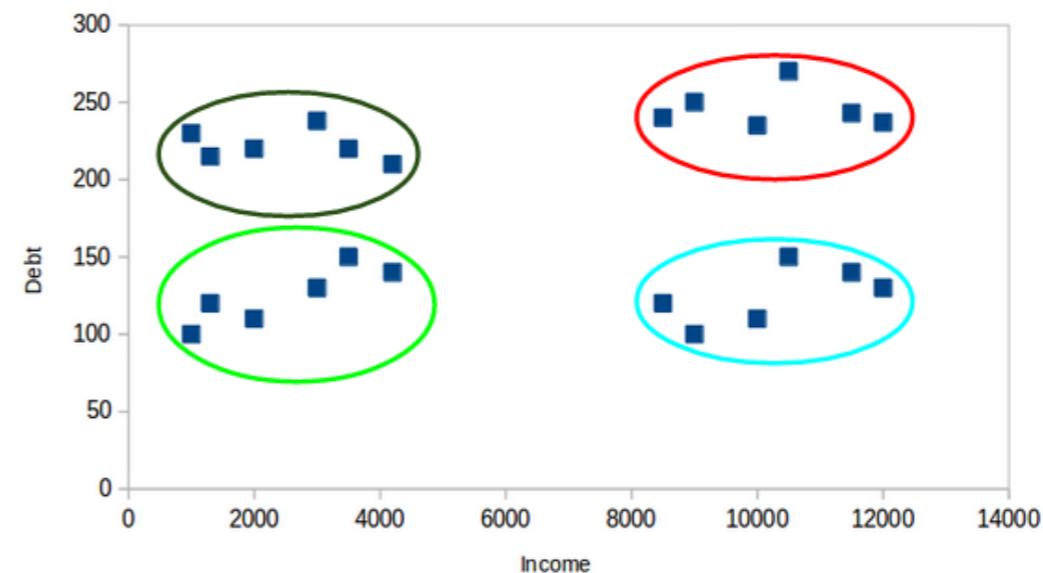
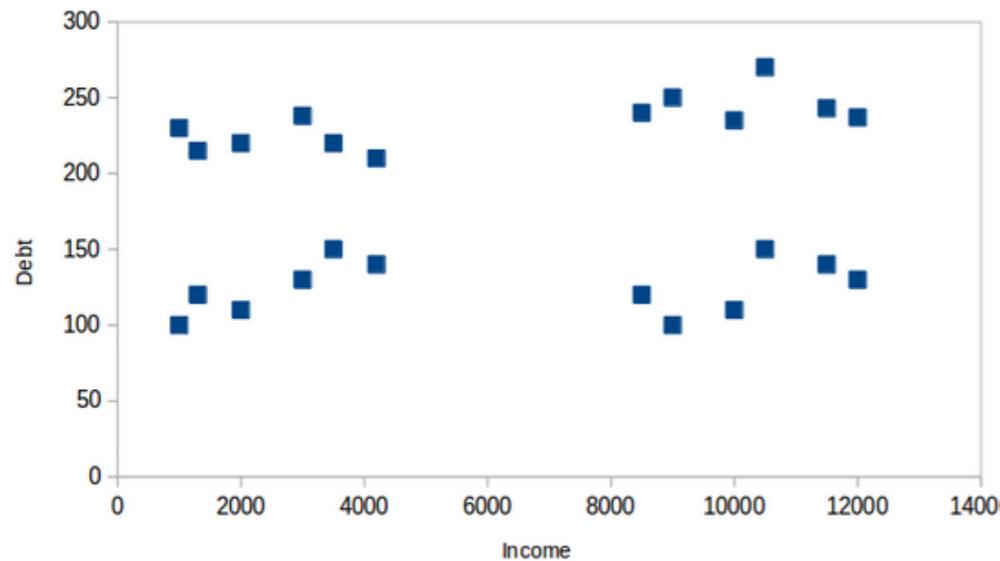
Good references:

<https://www.analyticsvidhya.com/blog/2019/08/comprehensive-guide-k-means-clustering/>

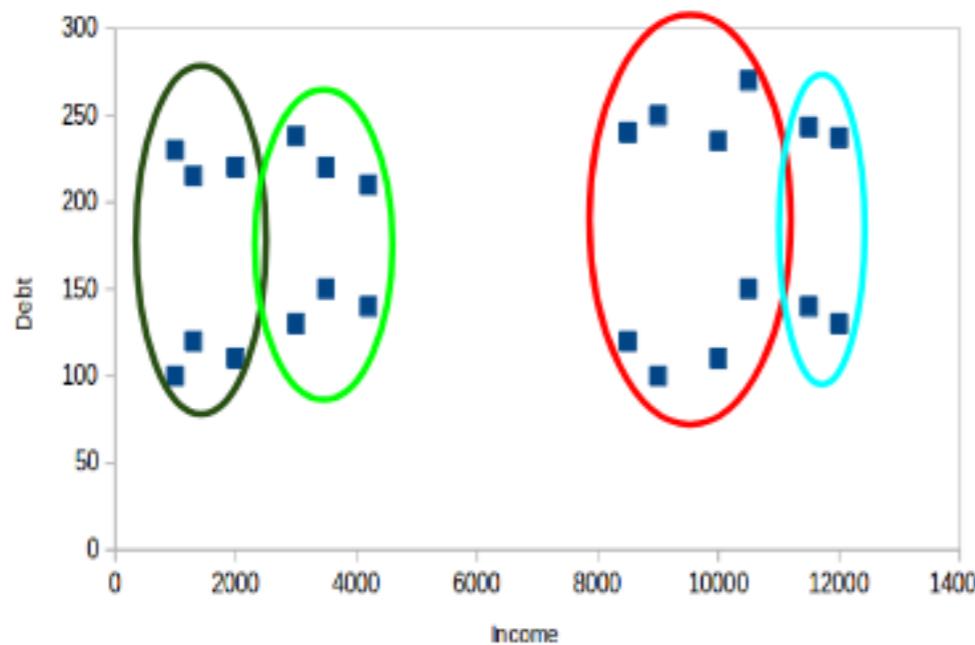
<https://towardsdatascience.com/k-means-clustering-from-a-to-z-f6242a314e9a>

Clustering

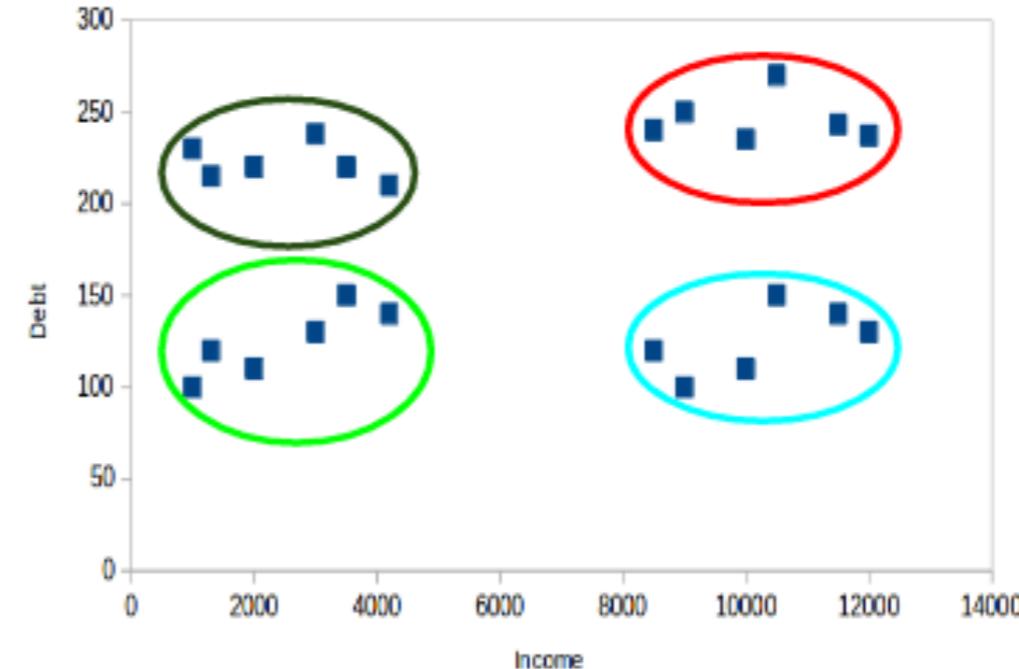
- 💡 All the data points in a cluster should be similar to one another



- 💡 The data points from different clusters should be as different as possible



Case - I

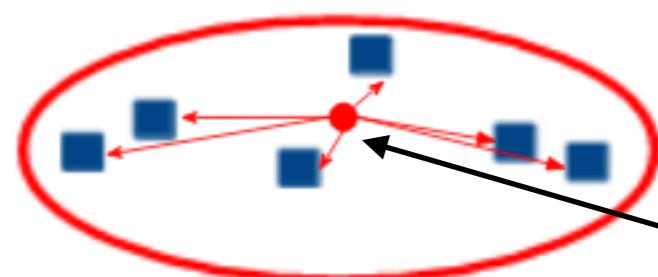


Case - II

Evaluation Metrics for Clustering

- Inertia: Sum of intracluster distances

The lesser the inertia value, the better the cluster is



Intra cluster distance

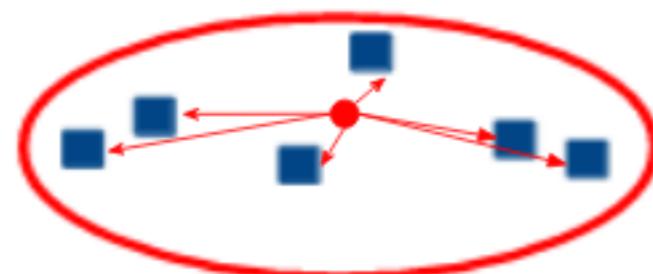
Inertia: Sum of intracluster distances

$$\sqrt{\sum_{i=1}^m |\vec{x}_i - \vec{c}_i|^2}$$

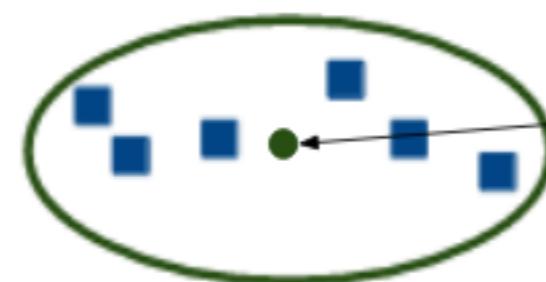
Centroid

- Dunn Index:

$$\text{Dunn Index} = \frac{\min(\text{Inter cluster distance})}{\max(\text{Intra cluster distance})}$$



Intra cluster distance



Inter cluster distance

Clusters are far apart

Clusters are compact

K-Means Clustering

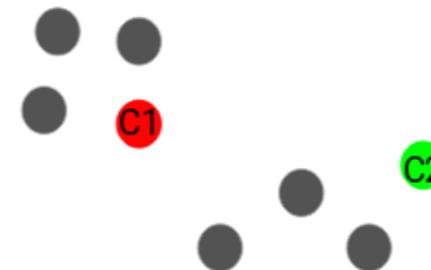
Centroid-based or distance-based algorithm, minimise the sum of distances

- ▶ Step 1: Choose the number of clusters k

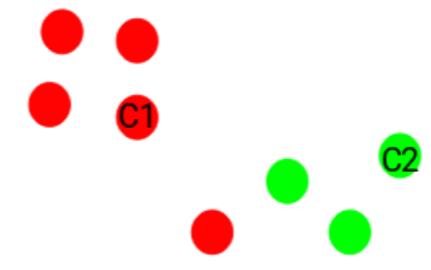
take k=2



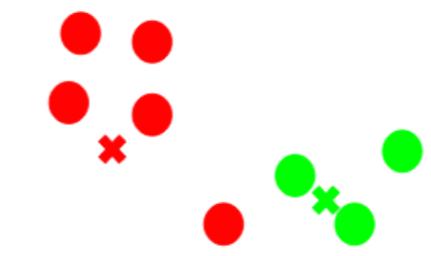
- ▶ Step 2: Select k random points from the data as centroids



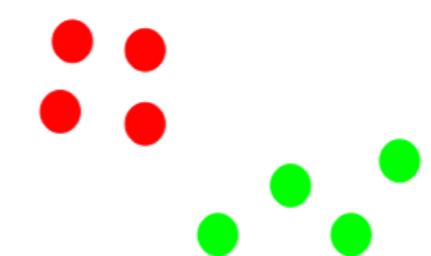
- ▶ Step 3: Assign all the points to the closest cluster centroid



- ▶ Step 4: Recompute the centroids of newly formed clusters



- ▶ Step 5: Repeat steps 3 and 4

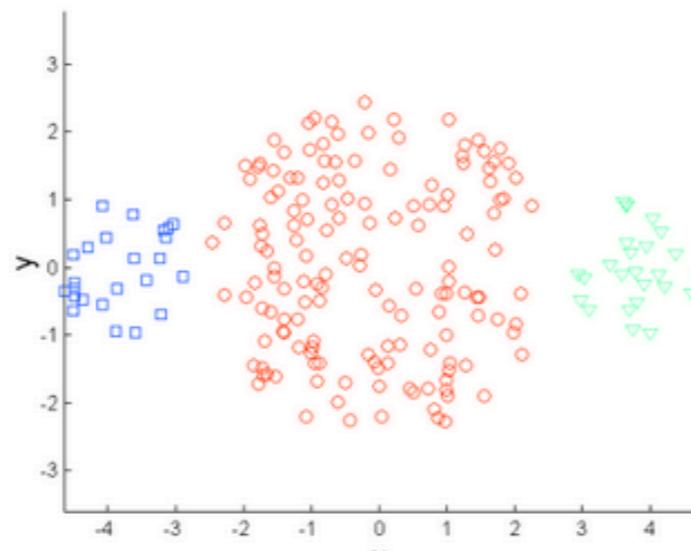


Stopping Criteria

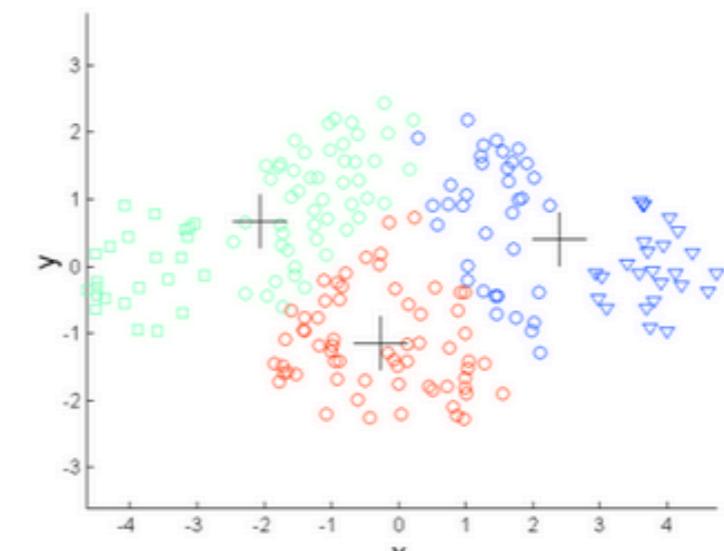
1. Centroids of newly formed clusters do not change
2. Points remain in the same cluster
3. Maximum number of iterations are reached

Challenges with the K-Means Clustering

The size of clusters is different

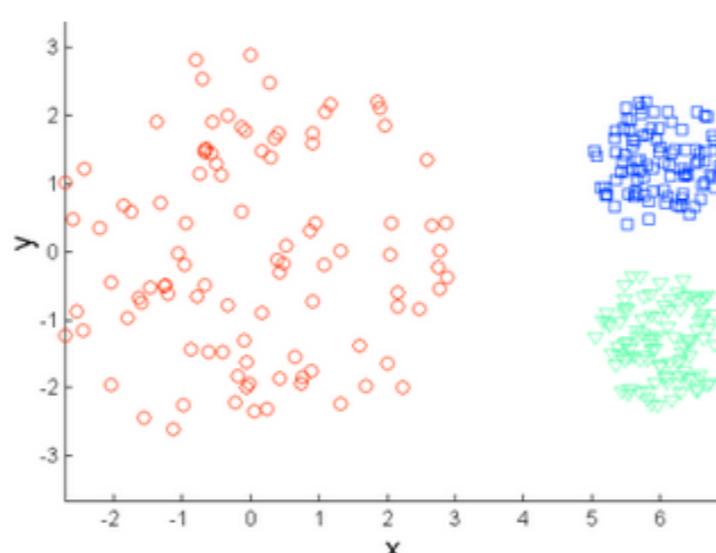


Original Points

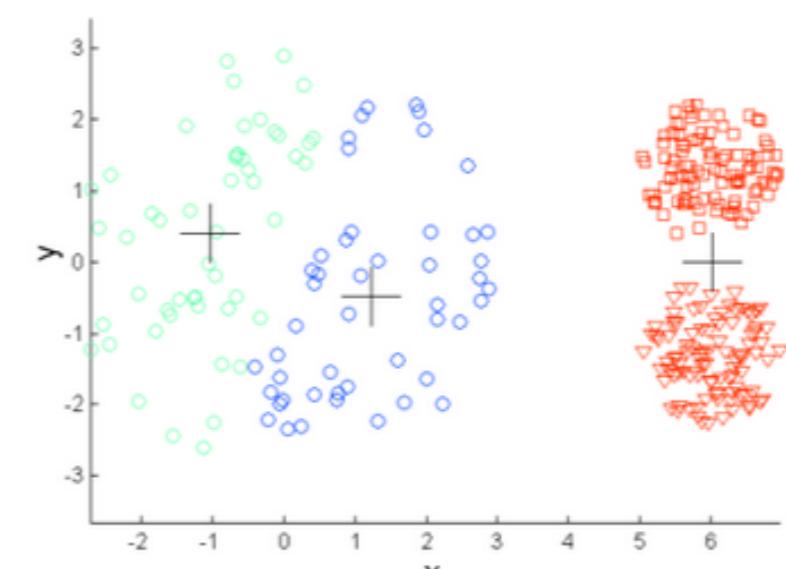


K-means ($k = 3$)

The densities of the original points are different



Original Points



K-means ($k = 3$)

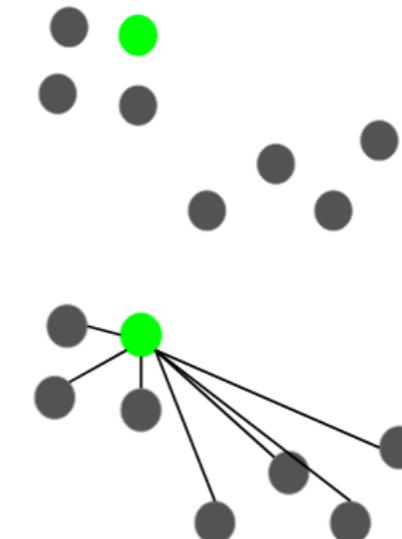
K-Means++ Clustering

Specifies a procedure to initialise the cluster centres before moving forward with k-means, take k=3

- ▶ Step 1: randomly pick **a** data point as **a** cluster centroid

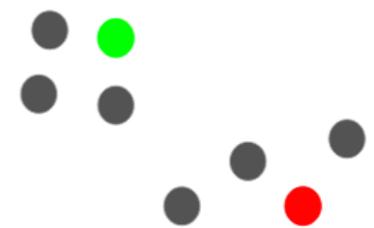
(not all the centroids but one)

- ▶ Step 2: calculate the distance of each data point with this centroid



- ▶ Step 3: the next centroid is the one whose distance is the farthest from the current centroid

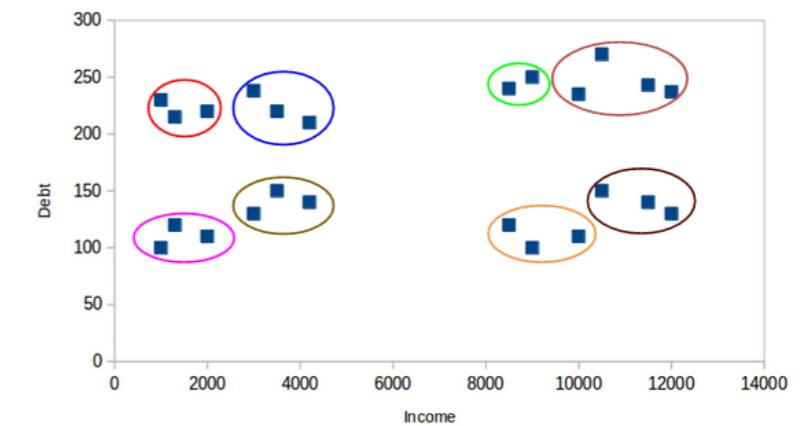
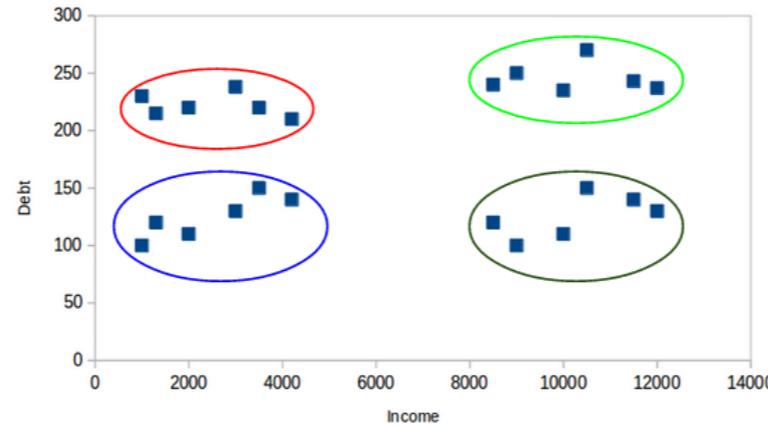
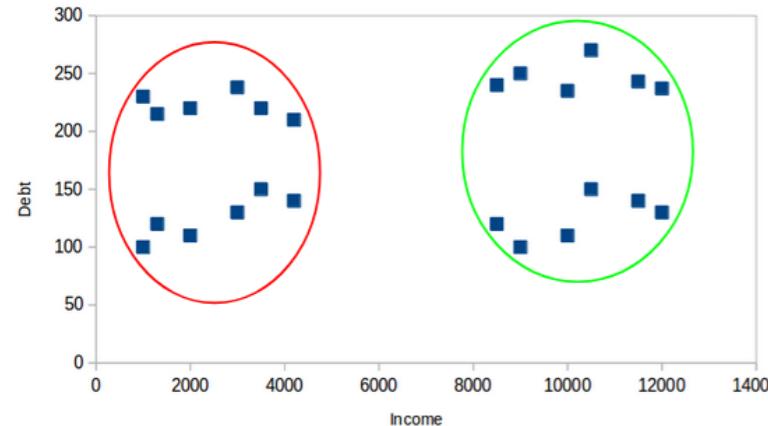
- ▶ Step 4: take the distance of each point from its closest centroid and the point having the largest distance will be selected as the next centroid



- ▶ Step 5: continue with the K-means after initialising the centroids



How to choose the right number of clusters



💡 Elbow curve, x-axis represent the number of clusters and y-axis the evaluation metric

