

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

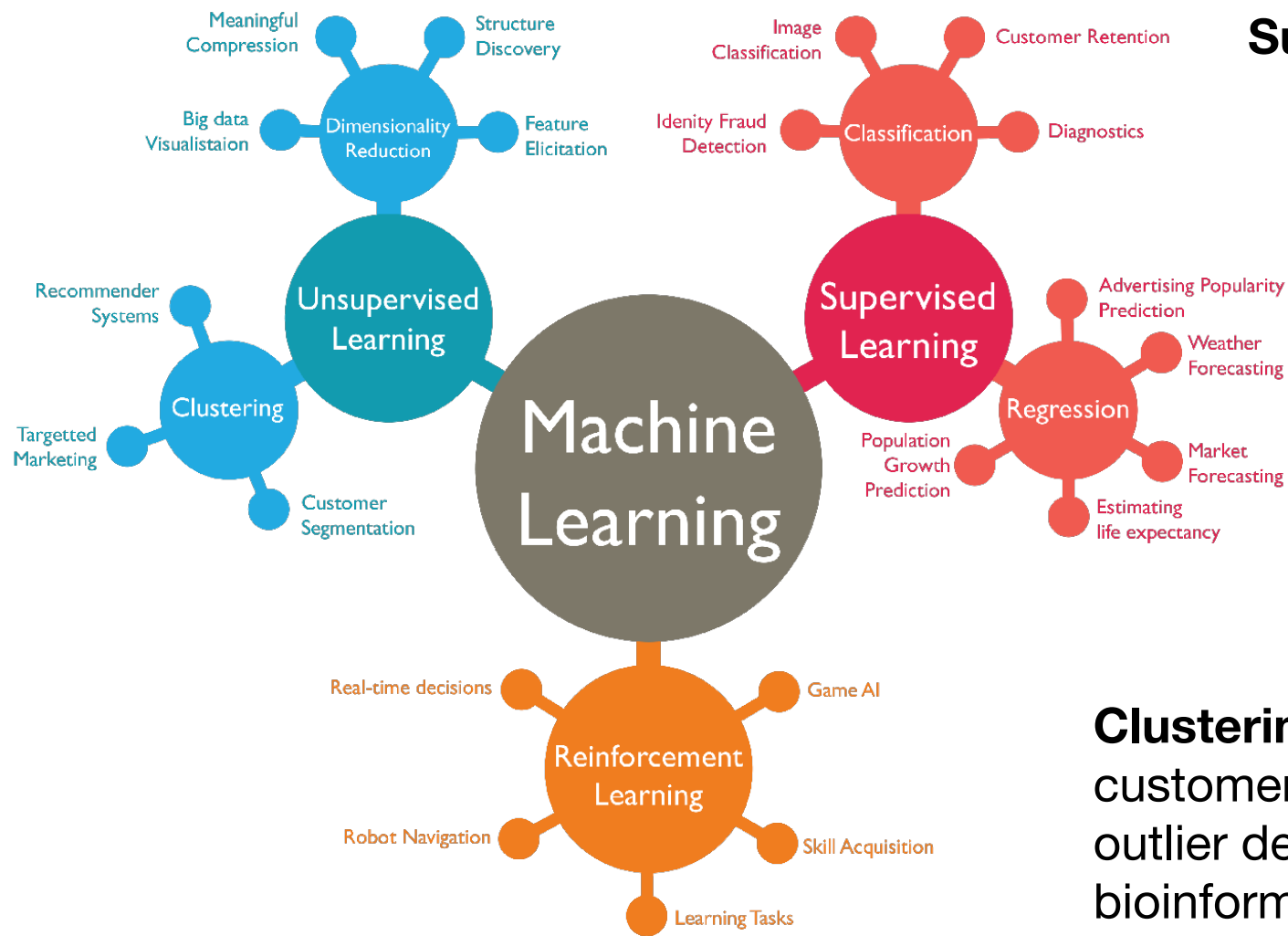
3.3 Factoring biological ingredient

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

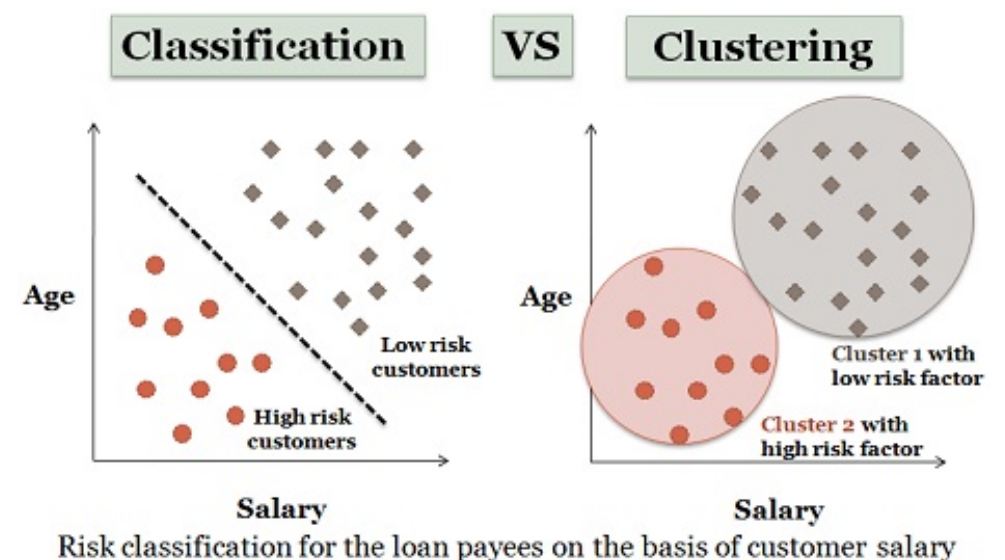
Unlabeled dataset

Find regularities from the input

Clustering:

customer segmentation, customer relationship management, outlier detection; Image compression

bioinformatics: DNA, RNA, amino acids, Motif, Proteins, sequence alignments

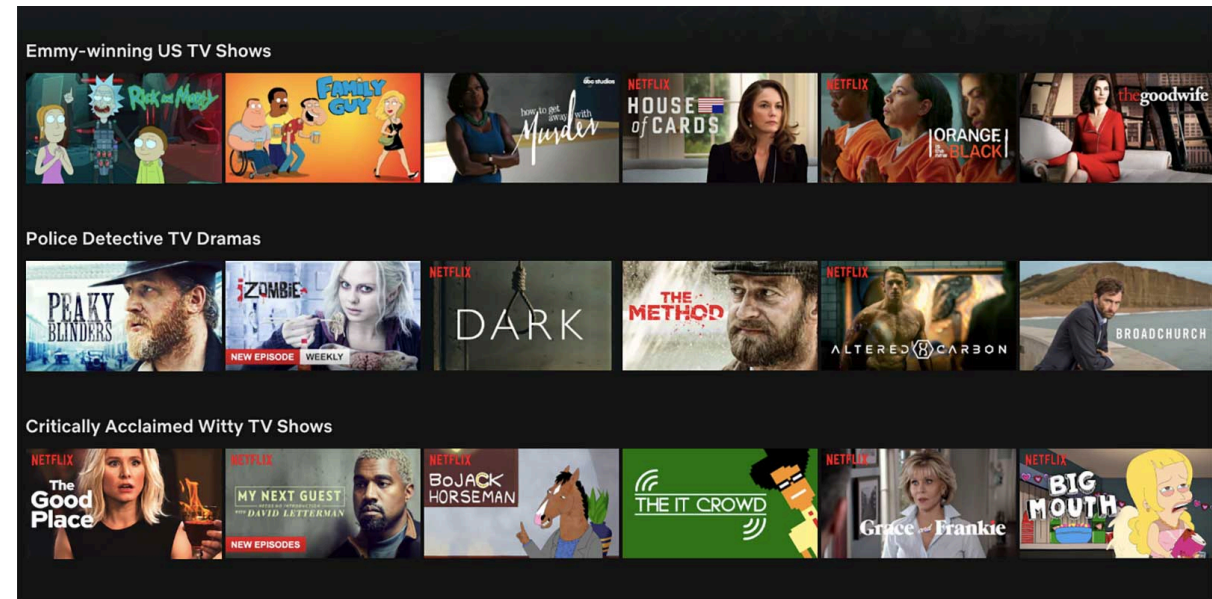


Clustering

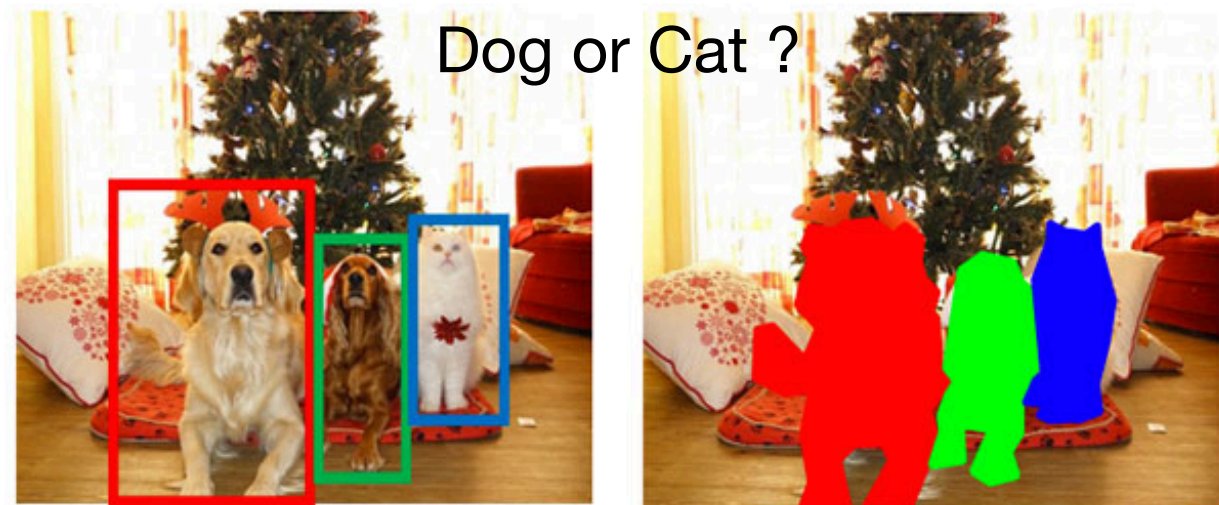
- 📌 Grouping of data points

“Clustering” literally means grouping similar things together

- 📌 Recommendation Engines



- 📌 Image Segmentation



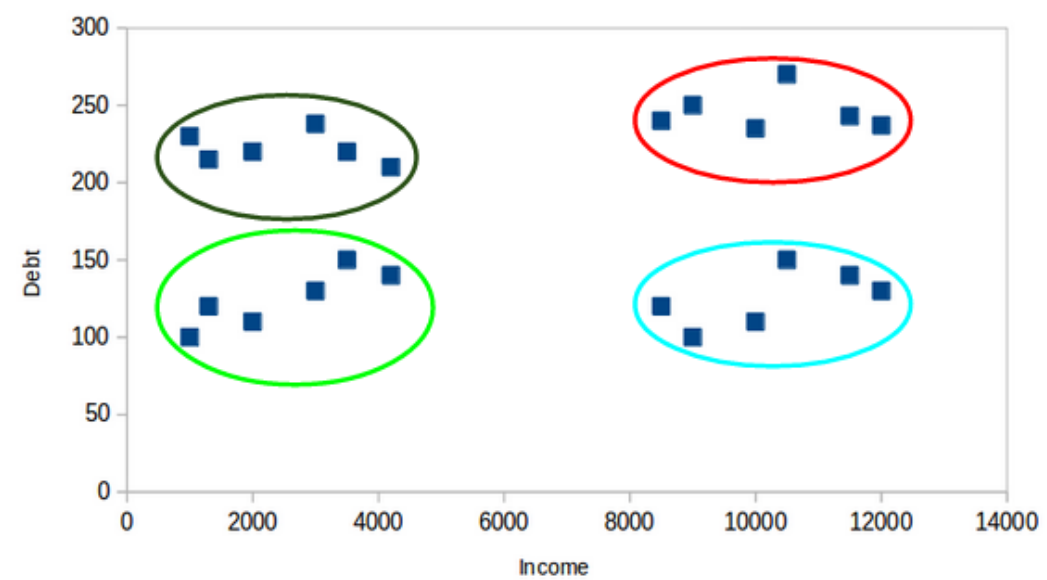
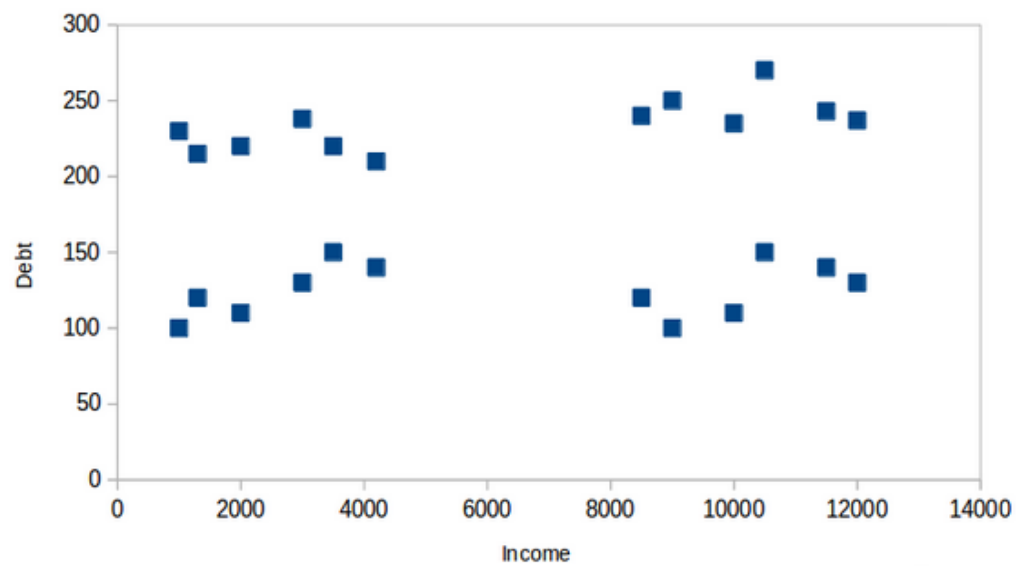
Good references:

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

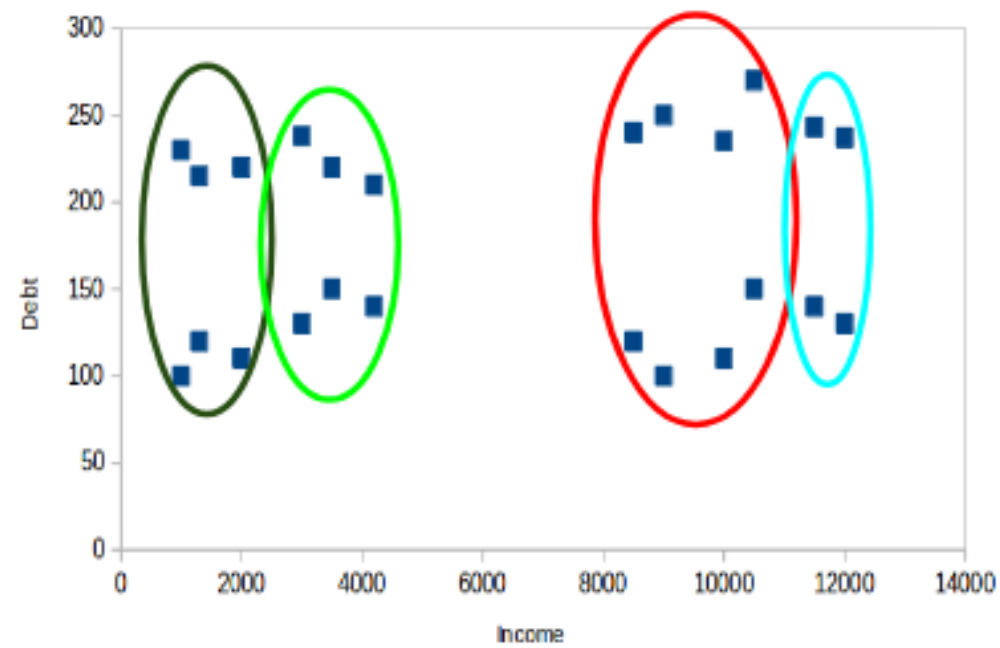
<https://towardsdatascience.com/k-means-clustering-from-a-to-z-f6242a314e9a>

Clustering

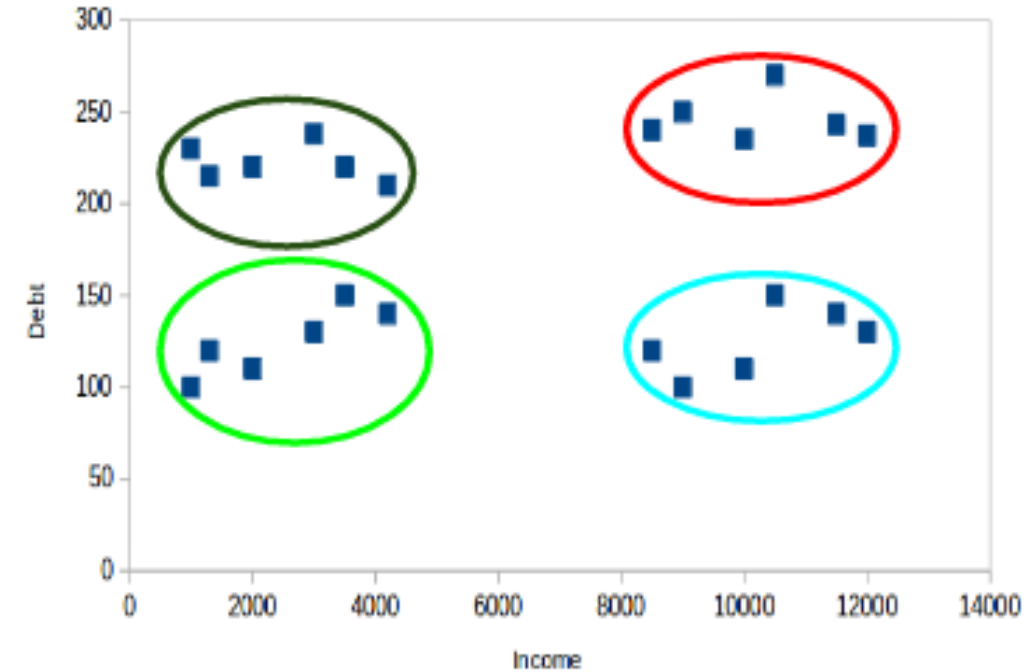
📌 All the data points in a cluster should be similar to one another



📌 The data points from different clusters should be as different as possible



Case - I

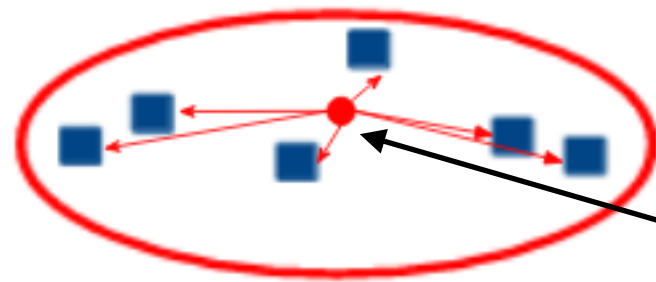


Case - II

Evaluation Metrics for Clustering

► Inertia: Sum of intraccluster distances

The lesser the inertia value, the better the cluster is



Intra cluster distance

Inertia: Sum of intraccluster distances

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

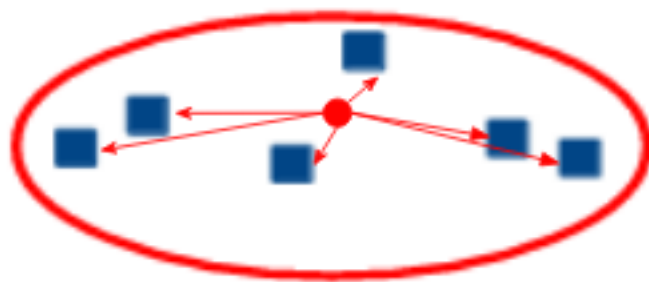
Centroid

► Dunn Index:

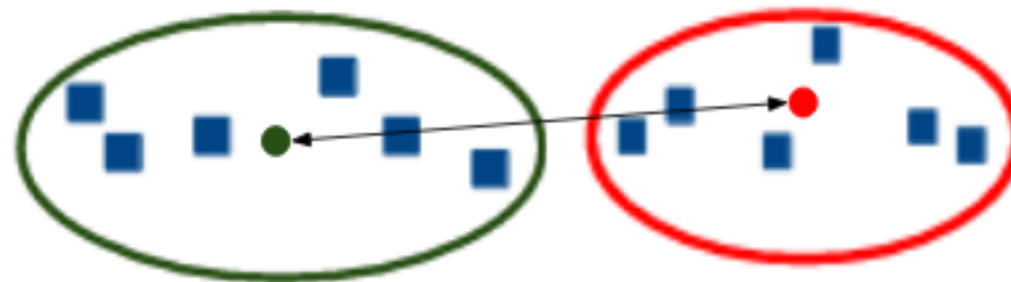
$$\text{Dunn Index} = \frac{\min(\text{Inter cluster distance})}{\max(\text{Intra cluster distance})}$$

Clusters are far apart

Clusters are compact



Intra cluster distance



Inter cluster distance

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

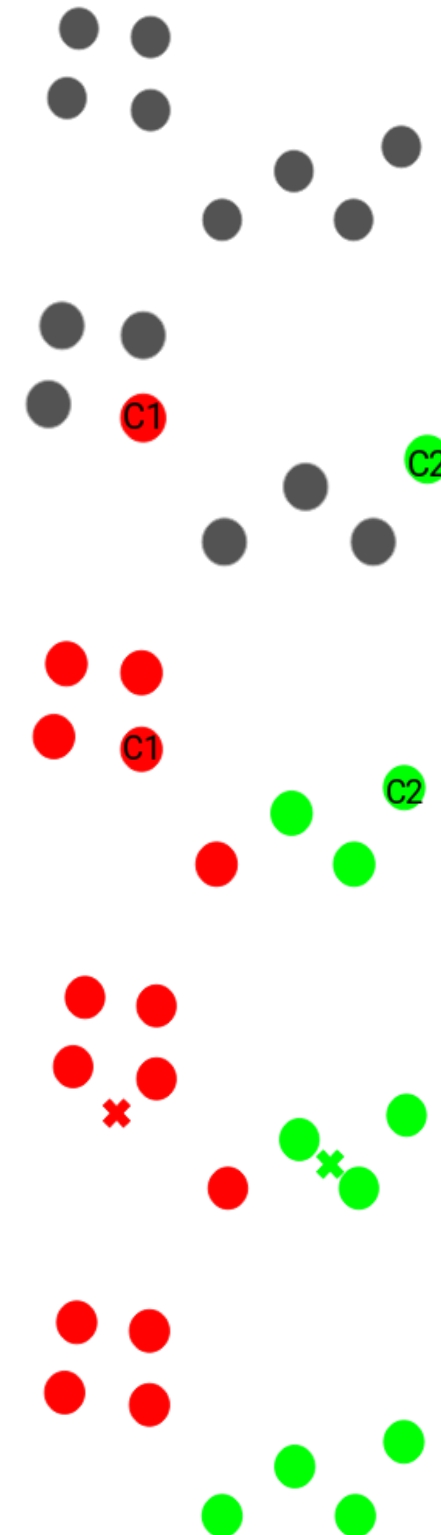
► Step 3: Assign all the points to the closest cluster centroid

► Step 4: Recompute the centroids of newly formed clusters

► Step 5: Repeat steps 3 and 4

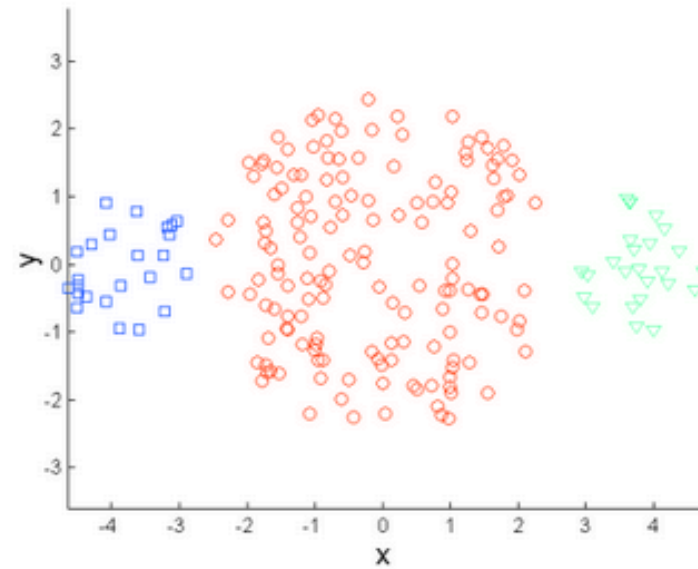
Stopping Criteria

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

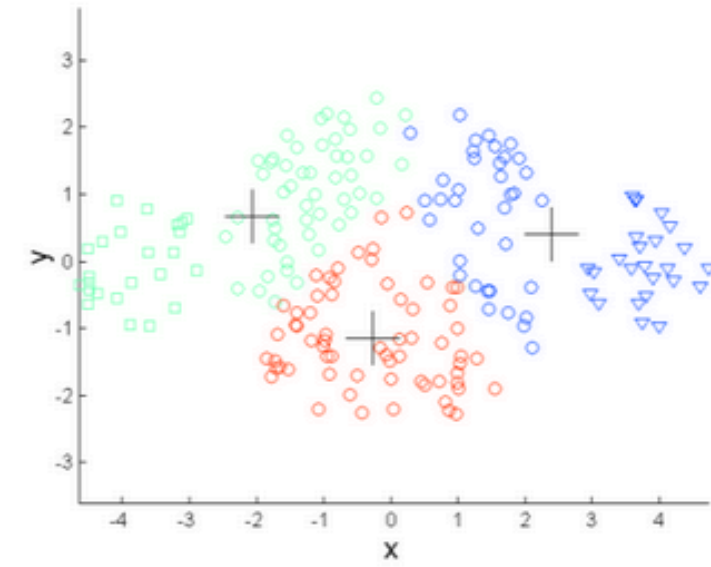


Challenges with the K-Means Clustering

The size of clusters is different

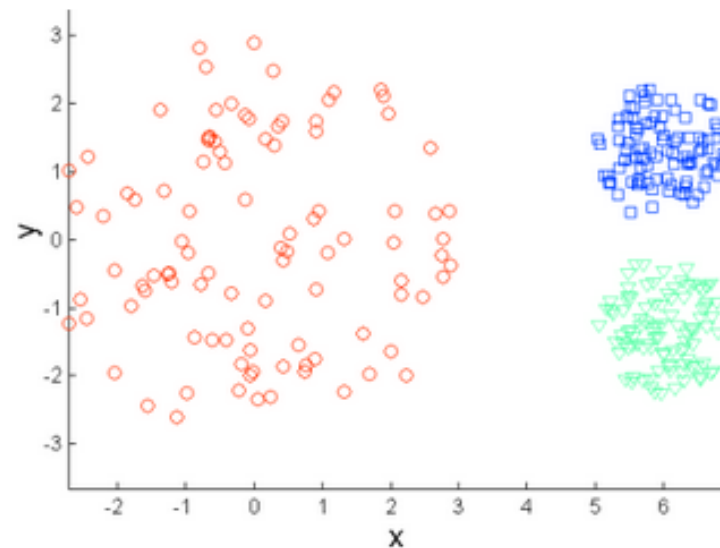


Original Points

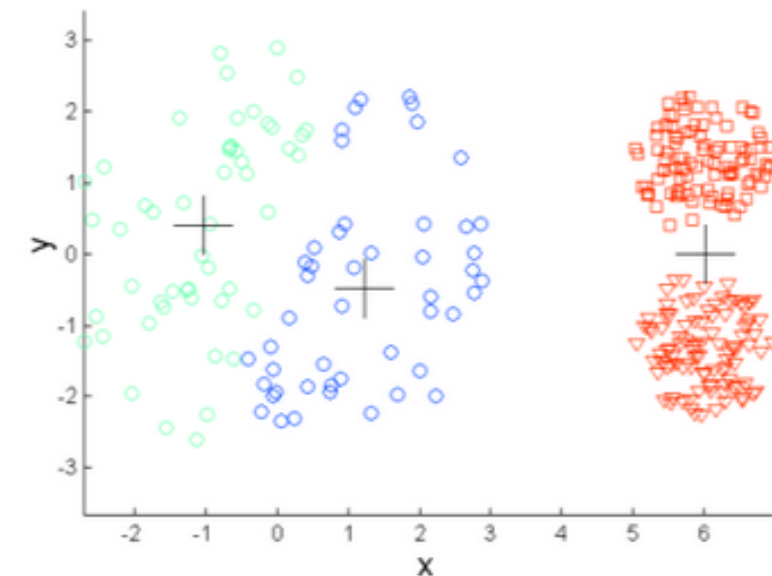


K-means ($k = 3$)

The densities of the original points are different



Original Points



K-means ($k = 3$)

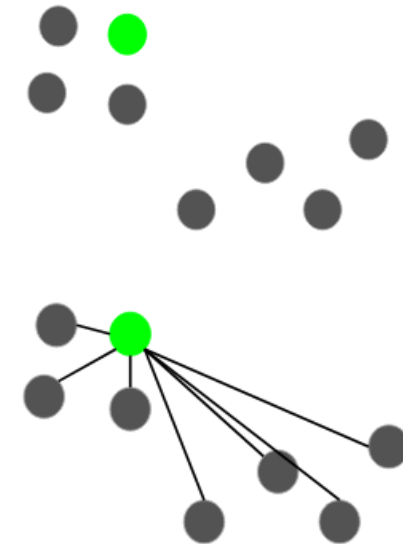
K-Means++ Clustering

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

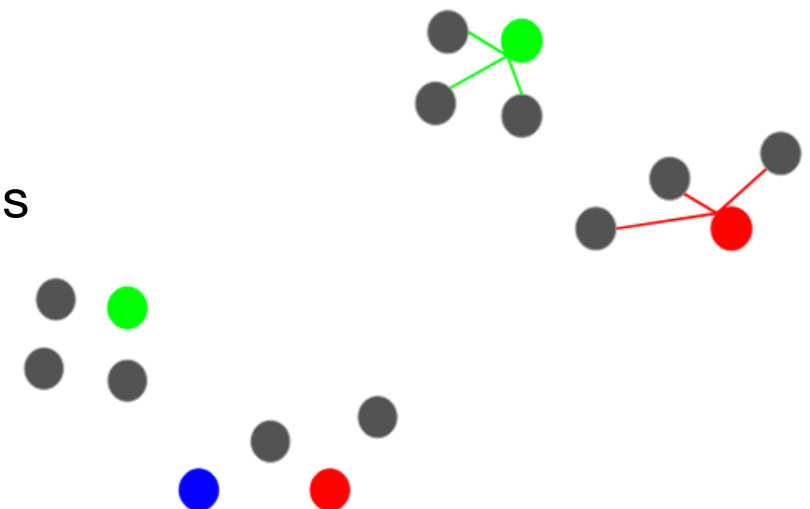


► Step 3: the next centroid is the one whose distance is the farthest from the current centroid

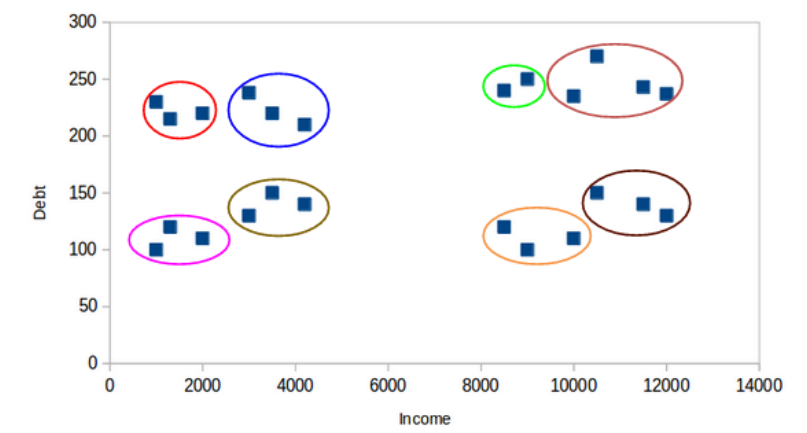
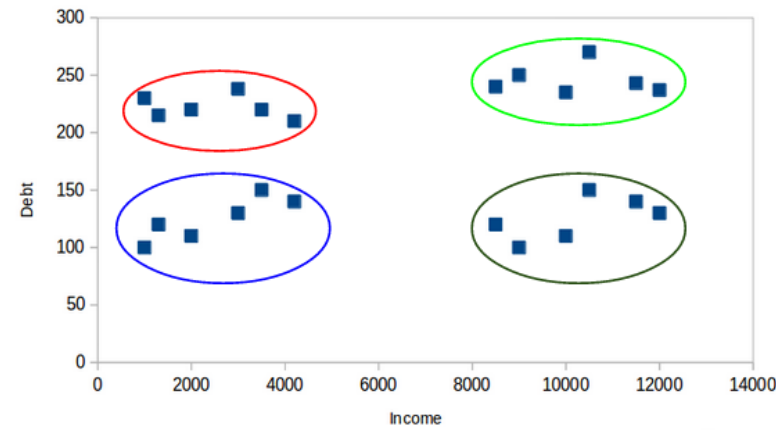
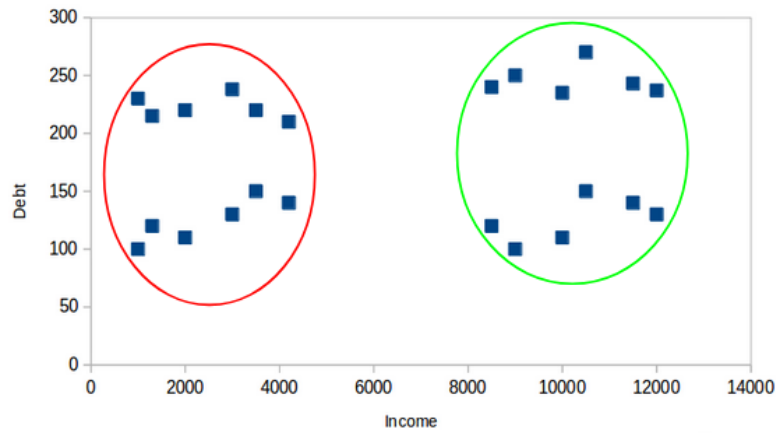
► Step 4: take the distance of each point from its closest centroid and the point having the largest distance will be selected as the next centroid



► 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

