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# DATA SCIENCE 102: CLUSTERING

# AGENDA

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- Unsupervised Learning
- Clustering
  - Use Cases
  - Types of Clustering Algorithms
- K-Means Clustering
  - K-Means Algorithm
  - Optimal K
  - Coded Example

# UNSUPERVISED LEARNING

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- Unsupervised learning is used when there is **no outcome variable ( $y$ )** to predict or classify
- Attempts to learn patterns in the data other than predicting  $y$
- Unsupervised learning methods include:
  - Clustering Techniques
  - Association Rules
  - Dimension Reduction Methods

# CLUSTERING TECHNIQUES

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- Use Cases
- Types of Clustering Algorithm
- Distance Scoring



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- Segmentation of data into sets of homogenous clusters of records to generate insight
- Clustering can help improve the performance of supervised methods by modelling each cluster rather than the entire heterogeneous dataset
- Cluster analysis helps to form groups (clusters) of similar observations based on several measurements made on those observations





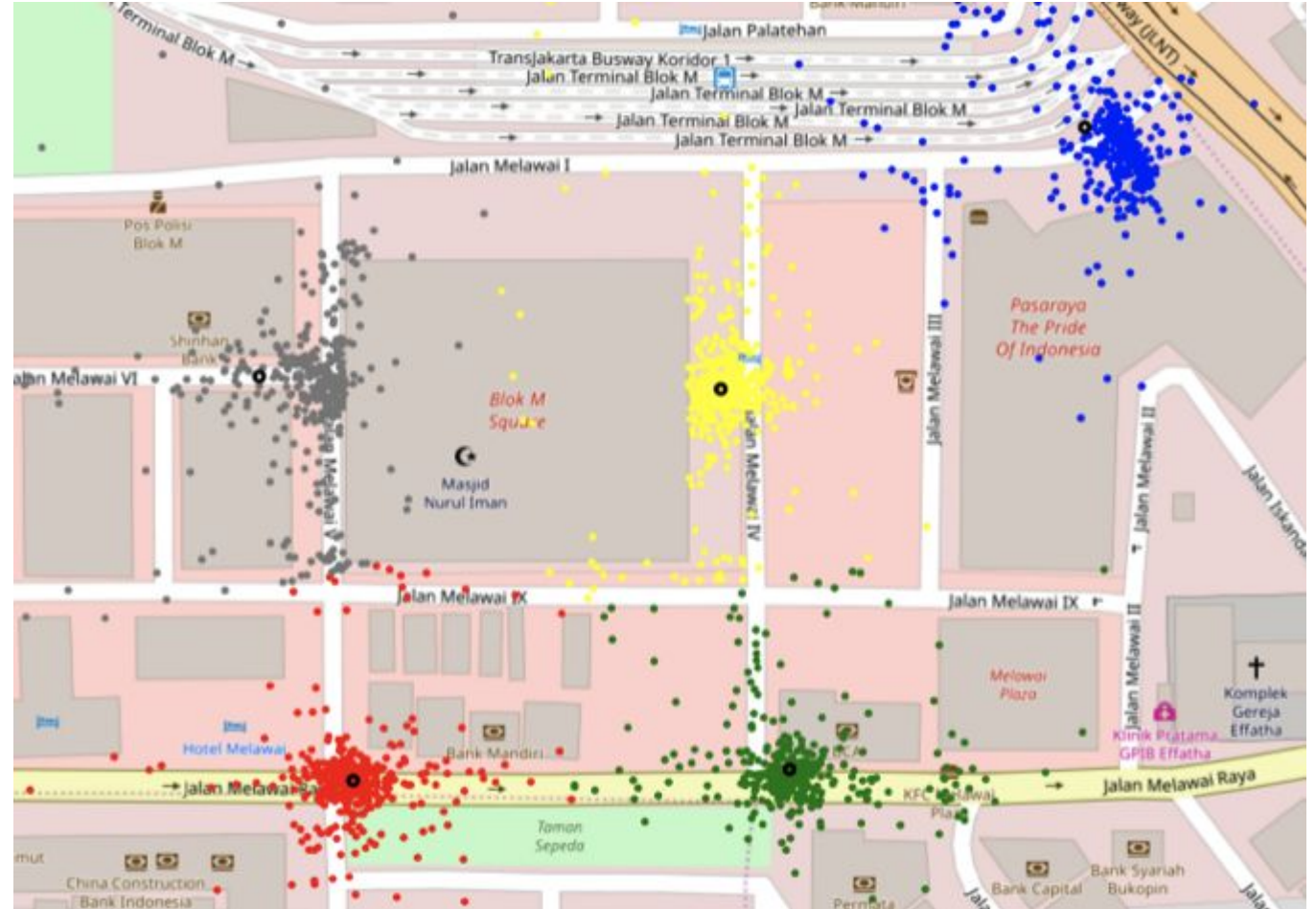
- Marketing
  - **Market segmentation** of customers based on demographic and transaction history and tailored marketing strategy
  - **Market structure analysis** identifying groups of similar products according to competitive measures of similarity
- Finance
  - **Balanced portfolios** by choosing stocks from different clusters
  - **Industry Analysis** finding similar firms through “market measures”
- Accounting
  - **Group transactions** by type
  - **Anomaly detection**

*Data Mining for Business Analytics: Concepts, Techniques, and Applications in R* by  
GalitShmueli, Peter C. Bruce, InbalYahav, Nitin R. Patel, Kenneth C. Lichtendahl Jr. (2018)

# USE CASE - GO-JEK FANTASTIC DRIVERS



- Go-Jek used K-Means algorithm to identify their better drivers
- It also helped them “pin” pick up points at popular locations



Find out more here: <https://blog.gojekengineering.com/fantastic-drivers-and-how-to-find-them-a88239ef3b29>



# TYPES OF CLUSTERING ALGORITHMS

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- There are two general types of clustering algorithms:
  - a. Hierarchical
    - Agglomerative - begins with  $n$  clusters and sequentially merge similar clusters until a single cluster is obtained
    - Divisive - starts with a single cluster including all records and does the opposite
  - b. Non-hierarchical (*Focused for this class; k-means clustering*)
    - Using predetermined number of clusters to assign observations to each cluster
    - Less computationally intensive and preferred for larger datasets

*Data Mining for Business Analytics: Concepts, Techniques, and Applications in R* by Galit Shmueli, Peter C. Bruce, Inbal Yahav, Nitin R. Patel, Kenneth C. Lichtendahl Jr. (2018)

# K-MEANS CLUSTERING

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- K-Means Algorithm
- Distance Scoring
- Optimal K
- Limitations of K-Means



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# K-MEANS ALGORITHM

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- Start with  $k$  initial clusters ( $k$  needs to be pre-defined)
- At every step, each record is reassigned to the cluster with the “closest” centroid
- Recompute the centroids of clusters that lost or gained a record, and repeat Step 2
- Stop when moving any more records between clusters **increases cluster dispersion**

# DISTANCE SCORING - BETWEEN TWO OBSERVATIONS



- Suppose two different observations are  $i$  and  $j$ , the distance metric for them is  $d_{ij}$
- The formula to calculate the distance between two observed points is the **Euclidean Distance**:

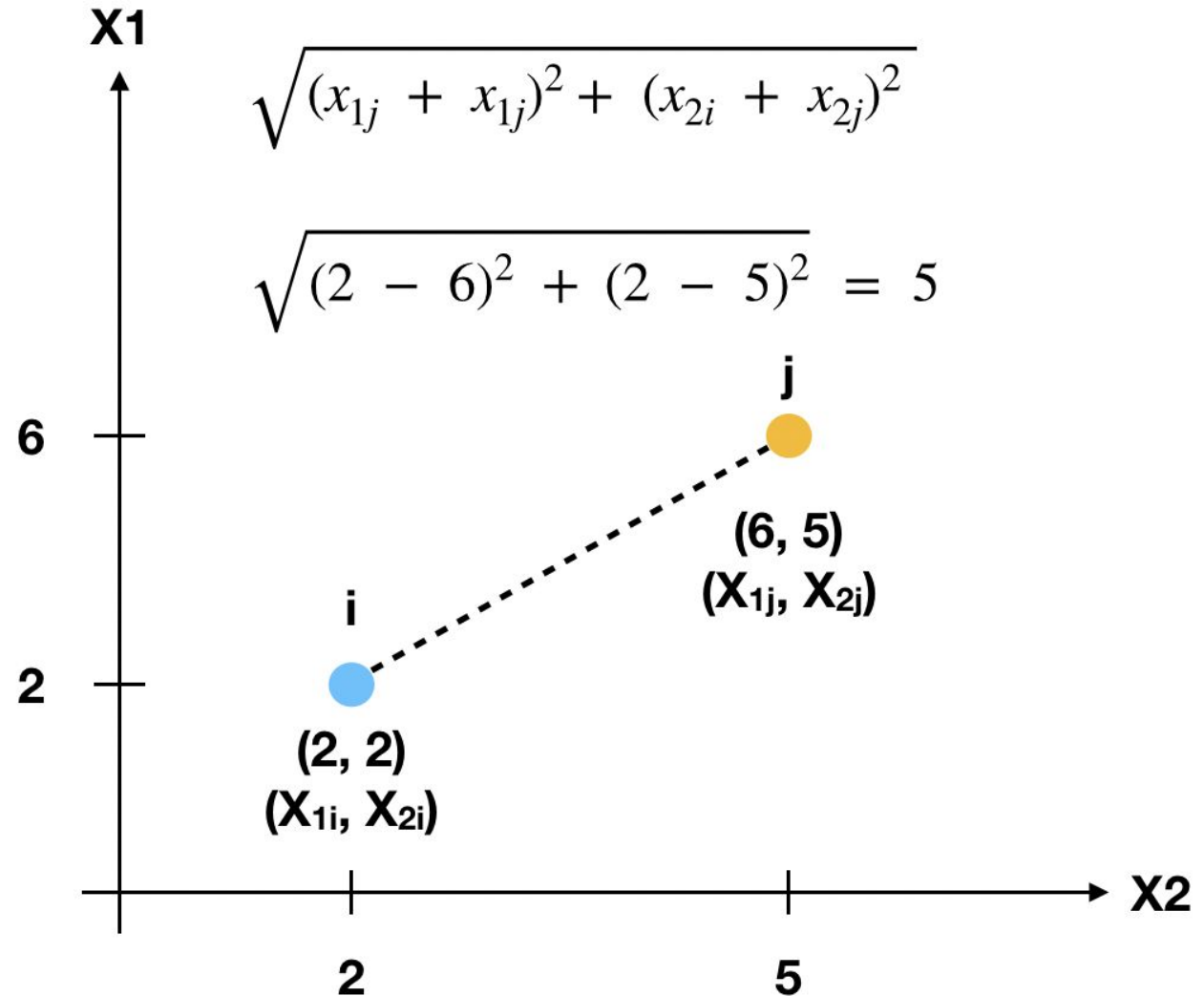
$$d_{ij} = \sqrt{(x_{i1} - x_{j1})^2 + (x_{i2} - x_{j2})^2 + \dots + (x_{ip} - x_{jp})^2}$$

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# DISTANCE SCORING - BETWEEN TWO OBSERVATIONS

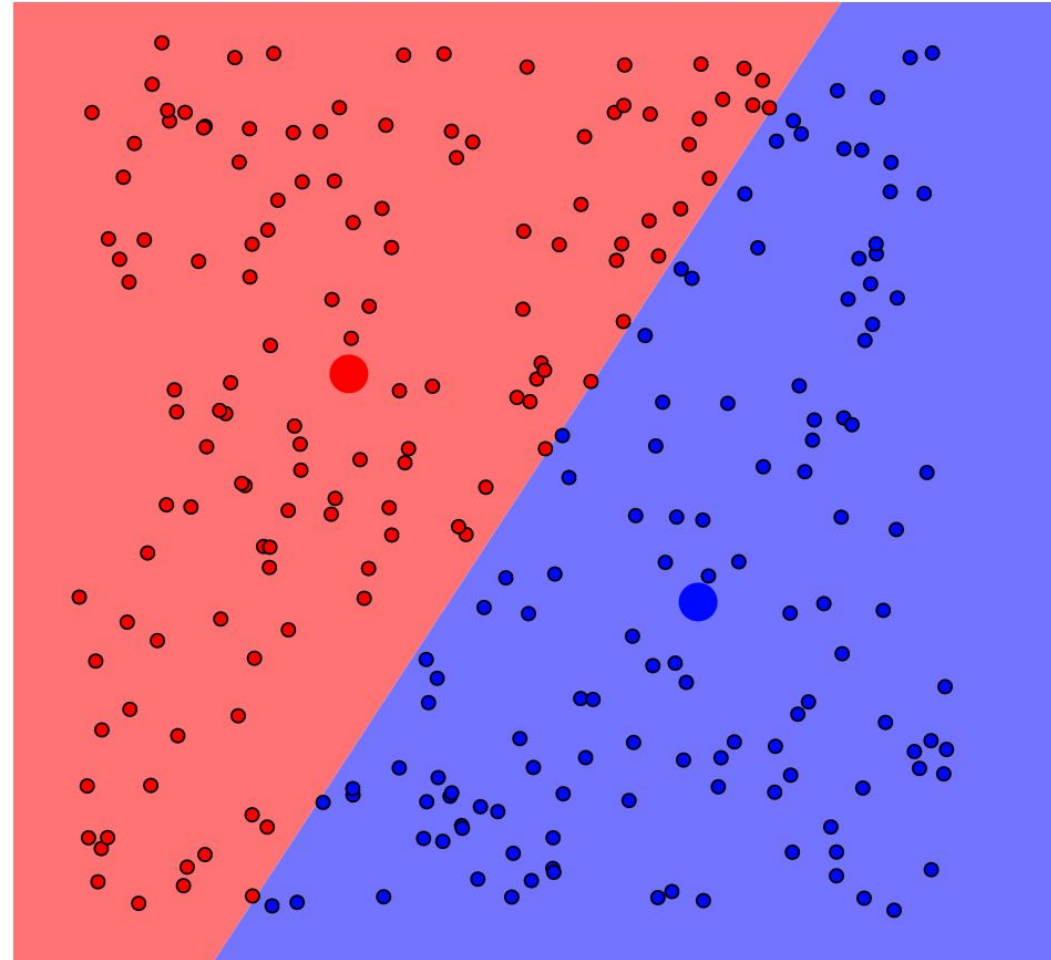


ID	X1	X2
i	2	5
j	2	6





# K-MEANS ALGORITHM - VISUALIZED



Click here for an interactive k-means algorithm animation: <https://www.naftaliharris.com/blog/visualizing-k-means-clustering/>



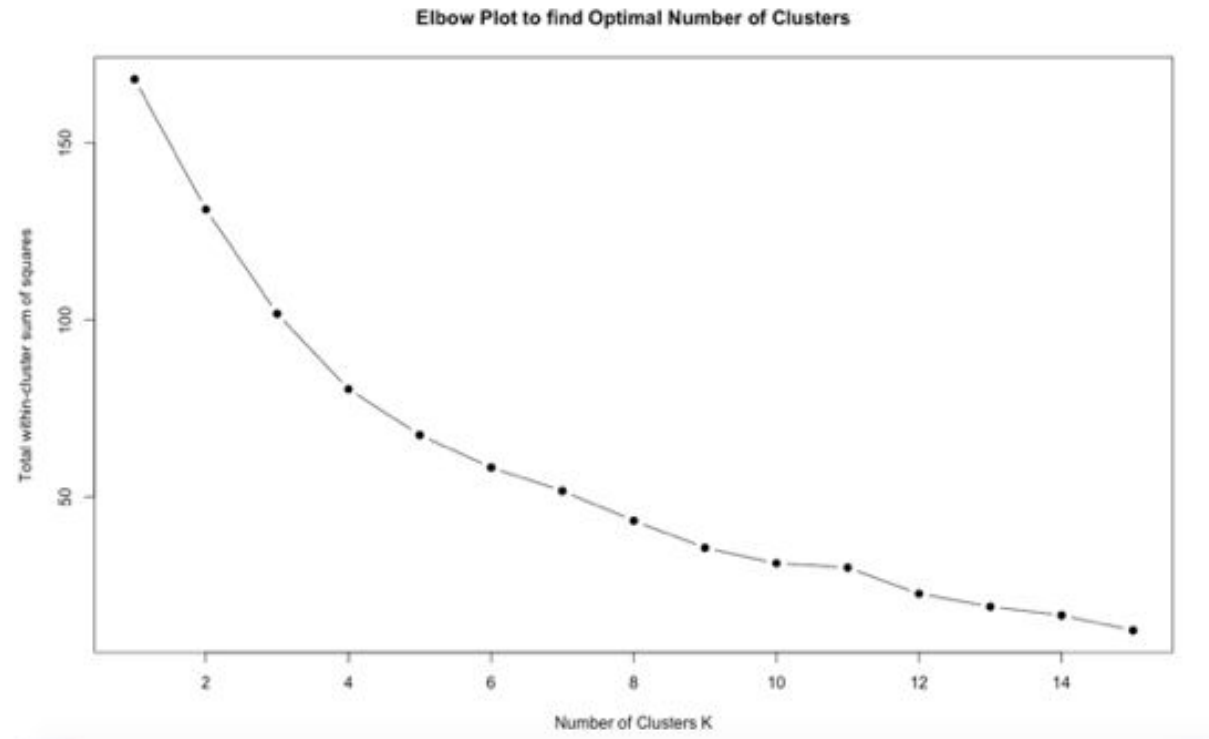
- In many cases, there is a lack of information to be used for the initial number of  $k$ .
- K-means algorithm, like other clustering algorithms, work towards compressing the  $k$  number of data-points by summarising them by their “means” (hence, k-means)
- There is no right number of  $k$ 's. However, information on within-cluster dispersion can assist in determining the optimal number of  $k$
- With an “elbow chart”, we can graphically evaluate whether there is a decline in cluster heterogeneity when more clusters are added (i.e  $k$  is increased)

# OPTIMAL K - ELBOW PLOT



- Select a K where the next increase in K has **little to no improvement** in the total within cluster sum of squares (WSS)
- Higher the K, the more computation required

choose the k with the sharpest drop



# SPOTIFY DATASET - SELECTING K\*



```
4 X = df_spotify_cluster # <<< Numerical DataFrame here
5 distortions = []
6 for k in range(2, 20):
7     kmeans = KMeans(n_clusters=k)
8     kmeans.fit(X)
9     distortions.append(kmeans.inertia_)
10
11 fig = plt.figure(figsize=(15, 5))
12 plt.plot(range(2, 20), distortions)
13 plt.grid(True)
14 plt.title('Elbow curve')
```

Loops for clusters from 2 to 19

Initialises based on K clusters

Calculates within cluster sum of squared

Plots elbow plot

# SPOTIFY DATASET - K-MEANS ALGORITHM\*



```
1 k = 5
2 model = KMeans(n_clusters=k, # < Initialise Number Of Clusters here
3               random_state=0)
4
5 spotify_kmeans = model.fit(df_spotify_cluster) # < DataFrame of All Variables
6 print(spotify_kmeans)
```

Initialises the KMeans  
model based on K clusters

```
KMeans(algorithm='auto', copy_x=True, init='k-means++', max_iter=300,
       n_clusters=5, n_init=10, n_jobs=1, precompute_distances='auto',
       random_state=0, tol=0.0001, verbose=0)
```

Trains the model by fitting in  
all variables into the model  
and **returns a kmeans  
result set**



# IN-CLASS PRACTICE - CLUSTERING\*

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- Try out the in-class practice with the credit card spending behaviour
- Do a summary statistics on the different clusters of credit card spending behaviours