THE UNIVERSITY OF MELBOURNE

Workshop 9

COMP20008

Elements of Data Processing

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Agenda

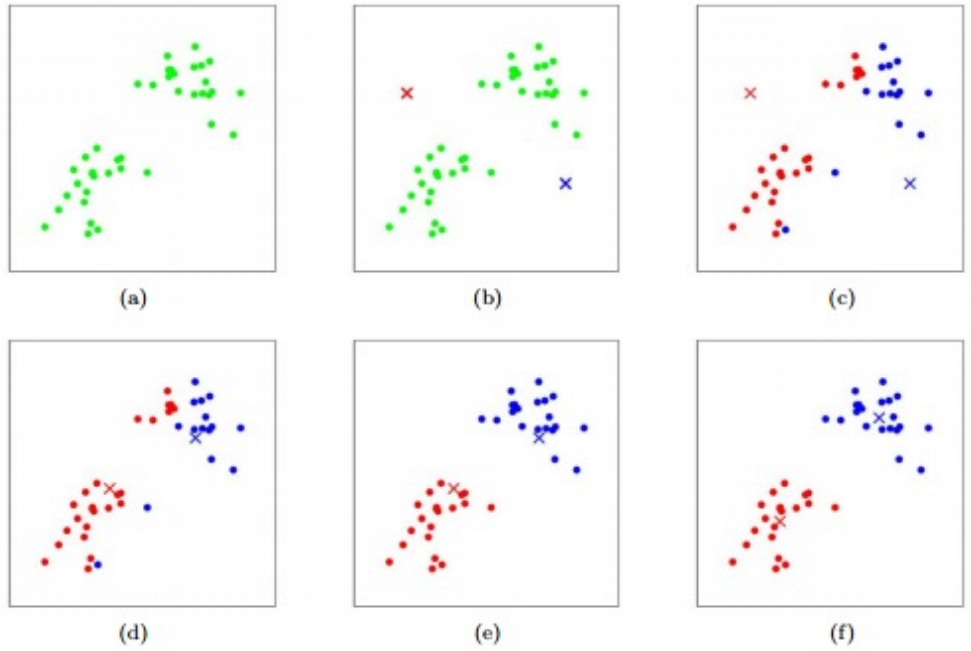
- Unsupervised machine learning
  - Clustering
- Clustering algorithms
  - *k*-means clustering
  - Agglomerative hierarchical clustering
- Principal Component Analysis (PCA)

Unsupervised learning

- In supervised learning
  - Labelled data
  - Learns a function that predicts the correct output for unseen input
  - e.g. Classification, regression
- In unsupervised learning
  - Unlabelled data
  - Learns to discover patterns, structures, or relationships within the data without any specific guidance on what to look for
  - e.g. Clustering

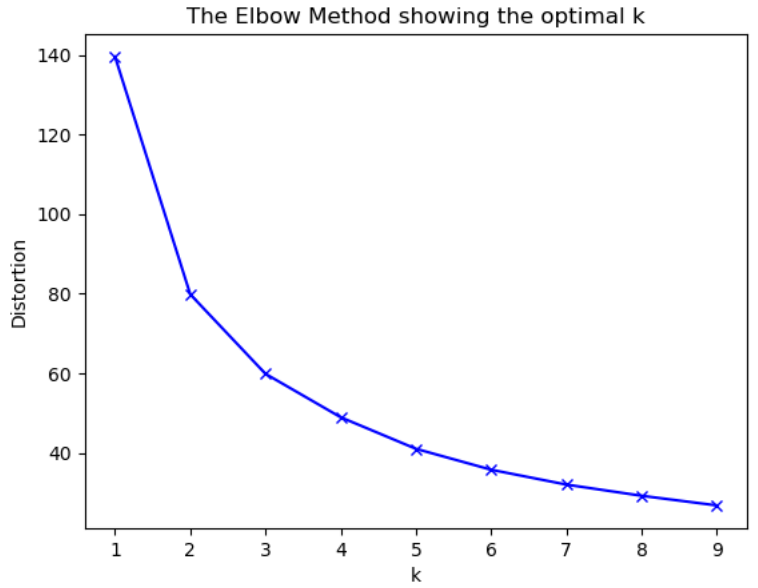
k-Means Clustering

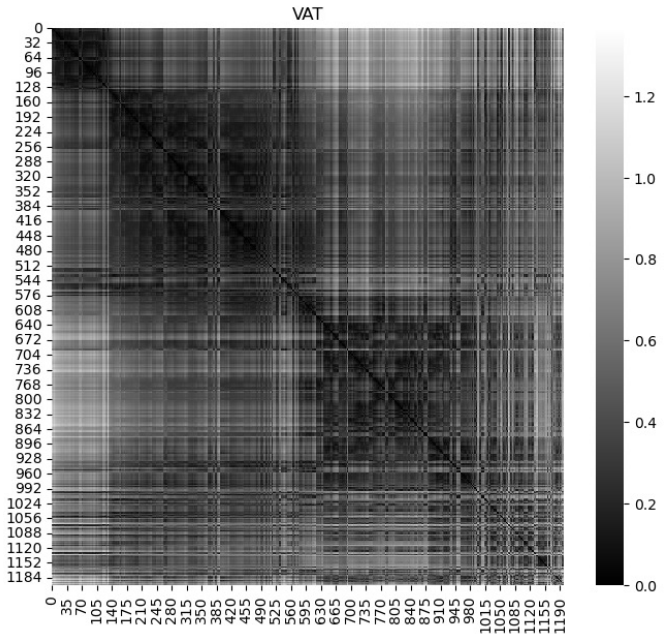
- Assumption: Similar data points belong to same cluster
- Idea: Alternate between
  - Assigning data points to centroids
  - Adjusting centroids based on current assignment
- Data points are categorised by their closet centroid



k-Means Clustering

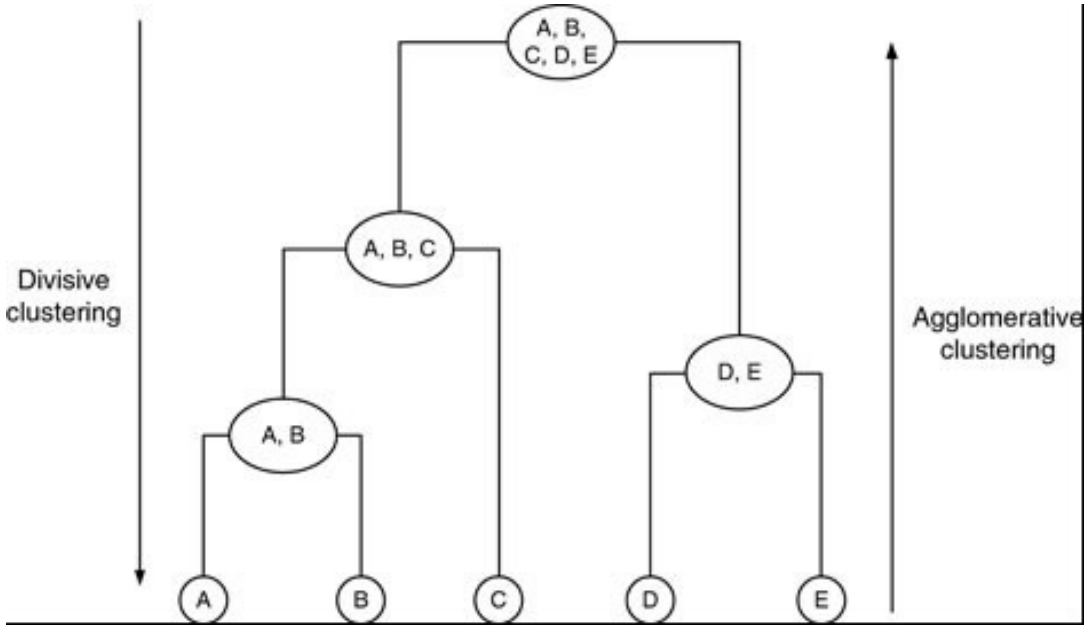
- Need to decide on:
  - Number of clusters *k*
  - Distance metric (may need normalisation)
- Some methods to help on deciding *k*
  - Elbow method: Sum of Squared Errors (SSE) for different *k*
  - VAT: Heatmap on a reordered dissimilarity matrix





Agglomerative hierarchical clustering

- Assumption: There is a hierarchical structure within the data
- Divisive: Top-down
- Agglomerative: Bottom-up
- Idea of agglomerative HC:
  - Merge two closest cluster
  - Update dissimilarity matrix
- Data are put into a dendrogram

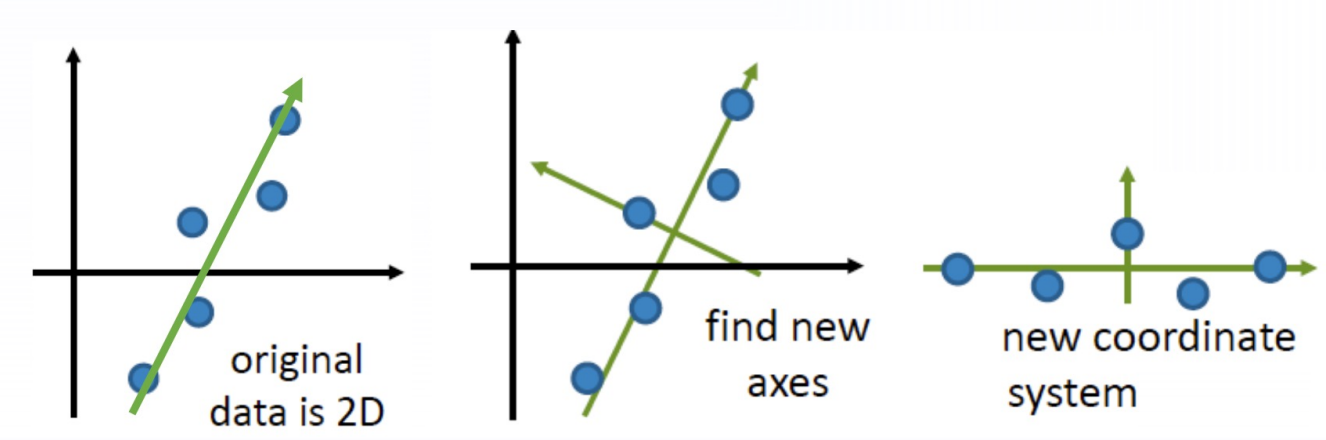


Agglomerative hierarchical clustering

- Need to decide on
  - Distance metric between clusters
  - Examples:
    - Single linkage: two most similar parts
    - Complete linkage: two least similar parts
    - Average linkage: centre of clusters

Principal Component Analysis (PCA)

- Too many features can cause problems (curse of dimensionality)
- PCA provides one way to perform dimensionality reduction
- Idea: transforms the original variables into principal components (PC)
  - PCs are linear weighted combinations of the original variables
  - Each PC captures as much variance in data as possible
  - Each PC are linearly uncorrelated with each other



Principal Component Analysis (PCA)

- Once we performed PCA:
  - The first few PC capture most of the variance in the dataset
  - We can discard some higher order PC as they don't tell us much about the data, thereby reducing the dimension of the data
- E.g. Reducing 10-D data into 2D/3D allows for visualisation

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Thank you

More Resources: Canvas