Implementation K-medoids (PAM) algorithm for clustering objects

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Outline

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Clustering

Cluster analysis or clustering is the task of grouping a set of objects in such a way that objects in the same group (called a cluster) are more similar (in some sense) to each other than to those in other groups (clusters).

- It is a main task of exploratory data mining
- Common technique for statistical data analysis, used in many fields, including:
  - Pattern recognition
  - Image analysis
  - Information retrieval
  - Machine learning

Medoid

- Medoids are representative objects of a data set or a cluster with a data set whose average dissimilarity to all the objects in the cluster is minimal
- Medoids are similar in concept to means or centroids
- Medoids are always restricted to be members of the data set.
- Most commonly used on data when a mean or centroid cannot be defined, such as graphs

k-medoids vs k-means similarities

- The k-medoids problem is a clustering problem similar to k-means
- Both the k-means and k-medoids algorithms break the dataset into clusters and attempt to minimise the distance between points labelled to be in a cluster and a point designated as the centre of that cluster

k-medoids vs k-means differences

- In contrast to the k-means algorithm, k-medoids chooses data points as centres, and thereby allows for greater interpretability of the cluster centres than in k-means where the centre of a cluster is not necessarily one of the input data points (it is the average between the points in the cluster)
- K-medoids can be used with arbitrary dissimilarity measures, whereas k-means generally requires Euclidean distance for efficient solutions
- More robust to noise and outliers than k-means

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Algorithms

- In general, the k-medoids problem is NP-hard to solve exactly. Many heuristic solutions exist
- Voronoi iteration
- approximate algorithms
  - CLARA
  - CLARANS
- Partitioning Around Medoids (PAM). Uses a greedy search which may not find the optimum solution, but it is faster than exhaustive search

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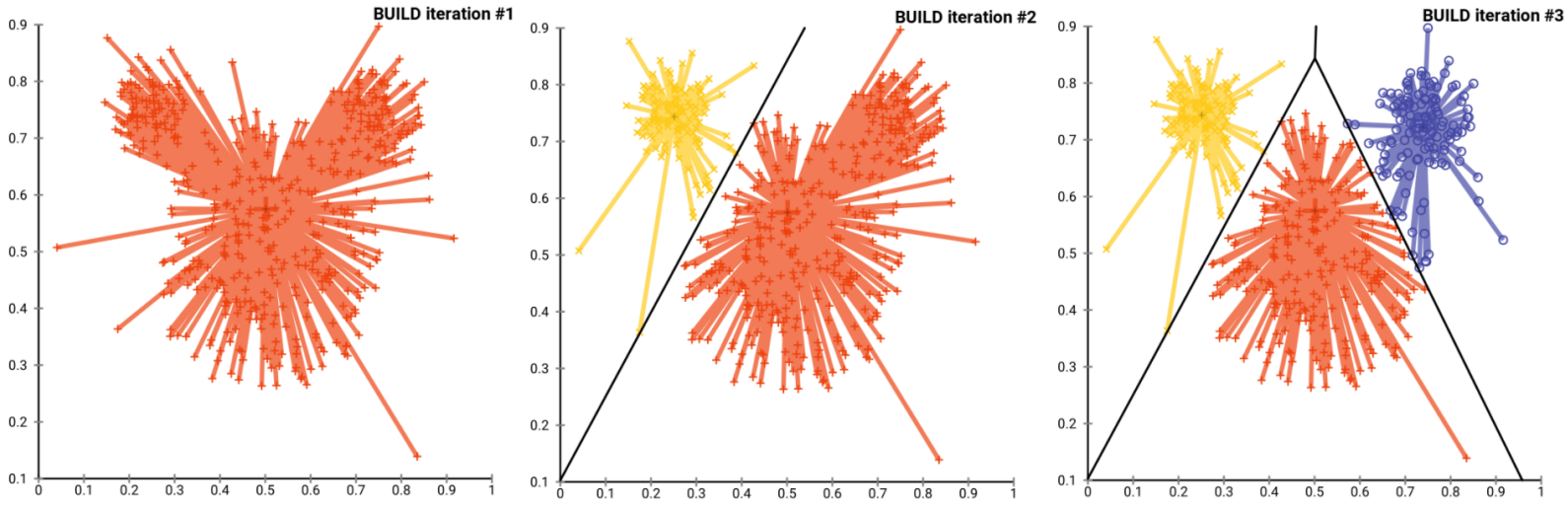
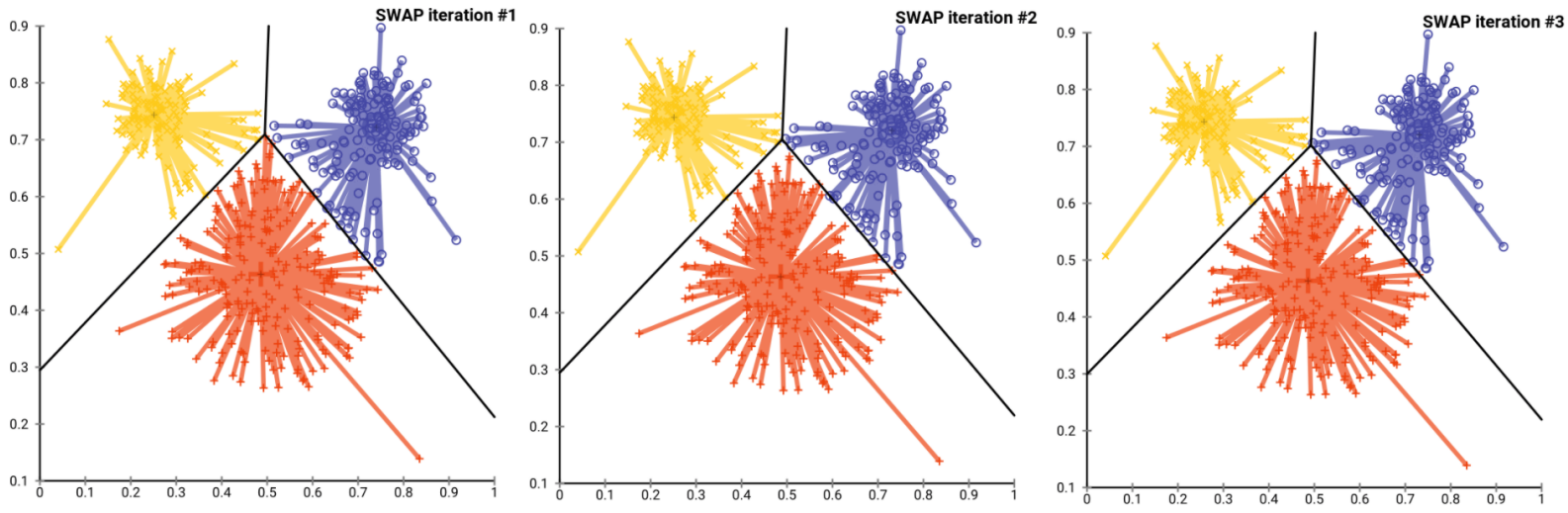
Partitioning Around Medoids (PAM)

1. (BUILD) Initialize: greedily select k of the n data points as the medoids to minimize the cost
2. Associate each data point to the closest medoid
3. (SWAP) While the cost of the configuration decreases:
    1. For each medoid m, and for each non-medoid data point o:
        1. Consider the swap of m and o, and compute the cost change
        2. If the cost change is the current best, remember this m and o combination
    2. Perform the best swap if it decreases the cost function. Otherwise, terminate

Build



SWAP



Thank you for your attention

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