CEE 616: Probabilistic Machine Learning

M5 Unsupervised Learning: L5c: Clustering

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Outline

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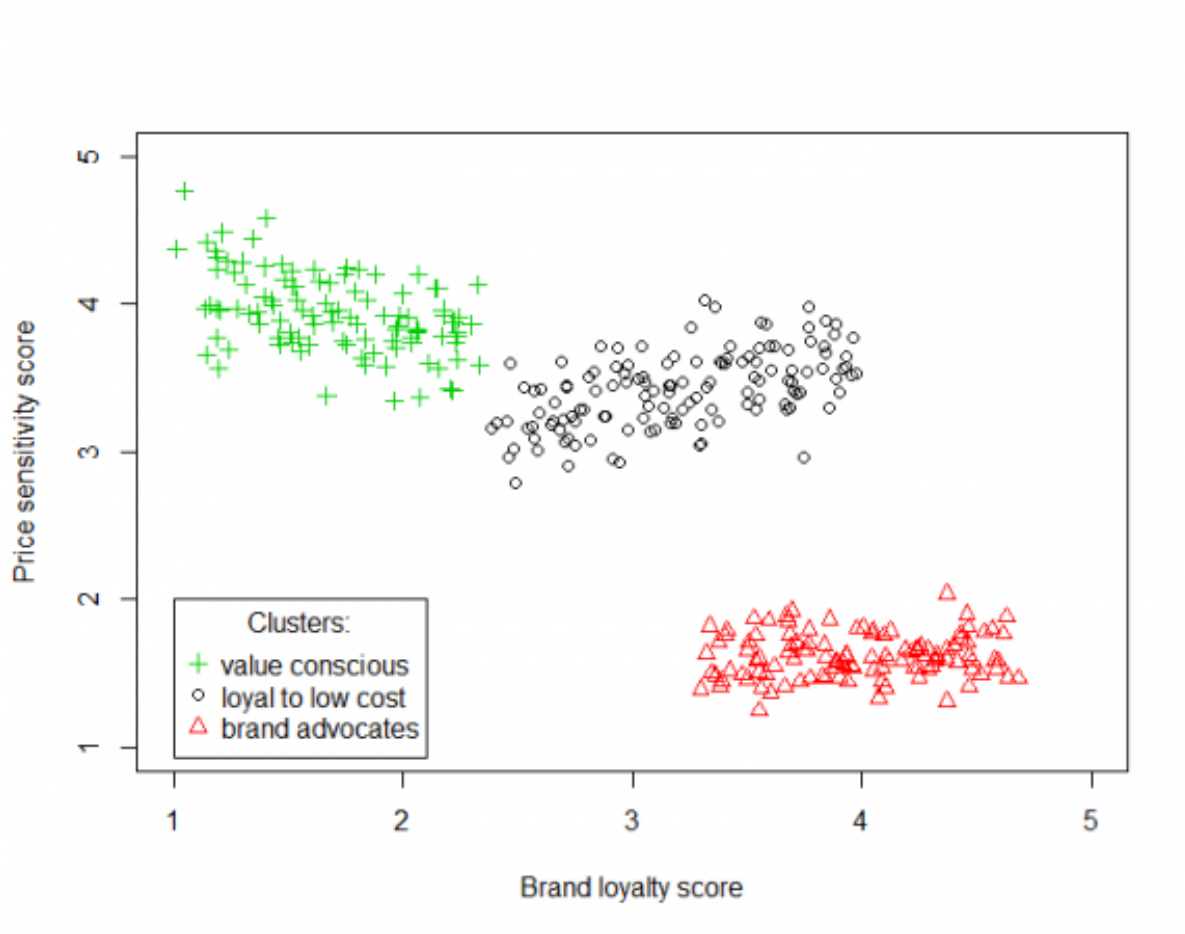

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Similarity Measures

- How similar are two observations?
  - Geographical distance
  - Vehicle color
  - Vehicle type
  - Vehicle brand
  - Engine type
  - Engine power
  - ...

Figure: Vehicles as items for cluster analysis

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$$d(\mathbf{x}_i, \mathbf{x}_k) = \left[\sum_{j=1}^{p} |x_{ij} - x_{kj}|^m \right]^{1/m} \tag{3}$$

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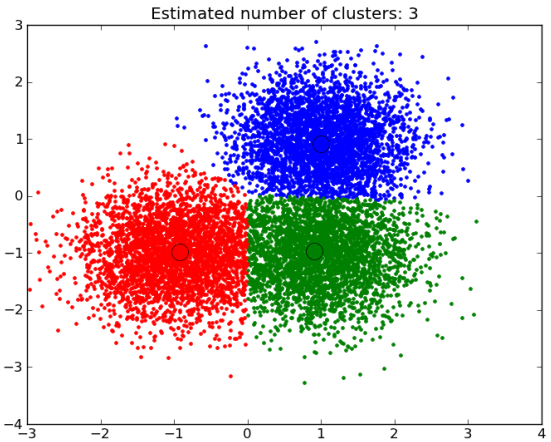

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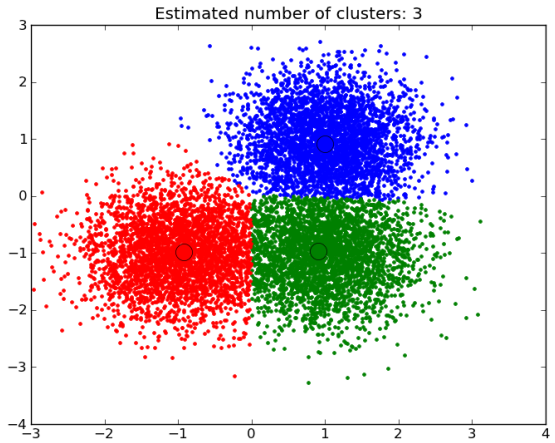

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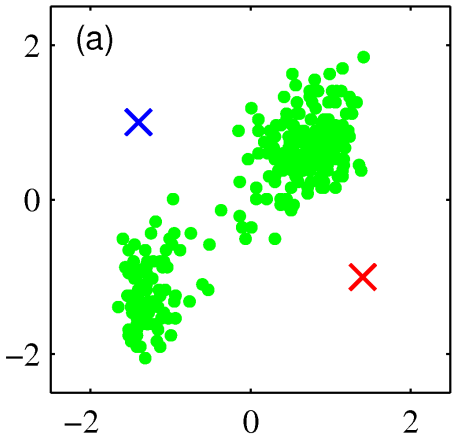

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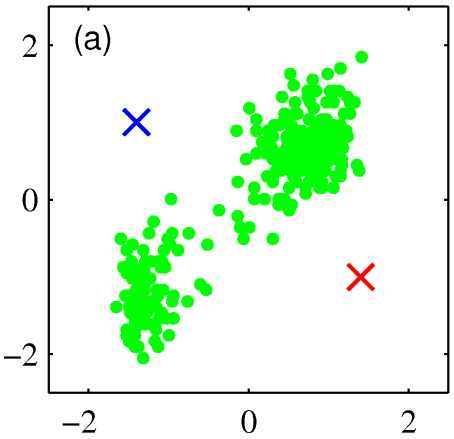

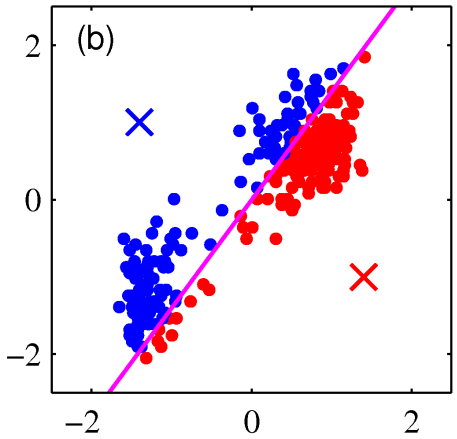

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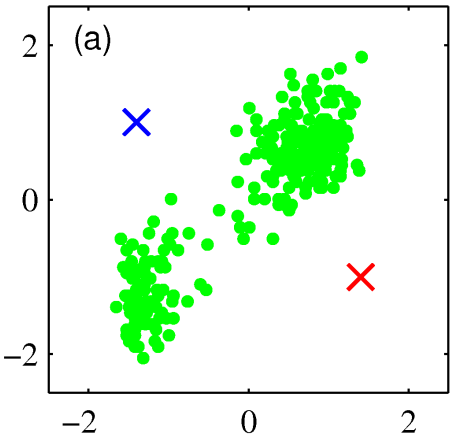

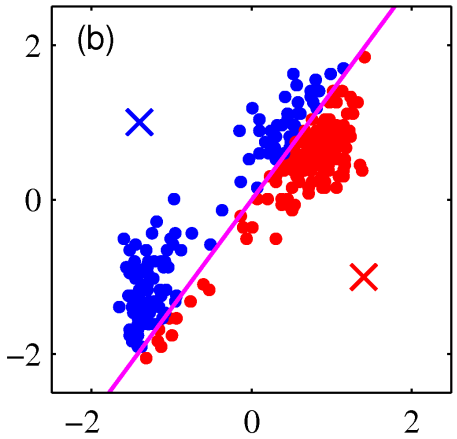

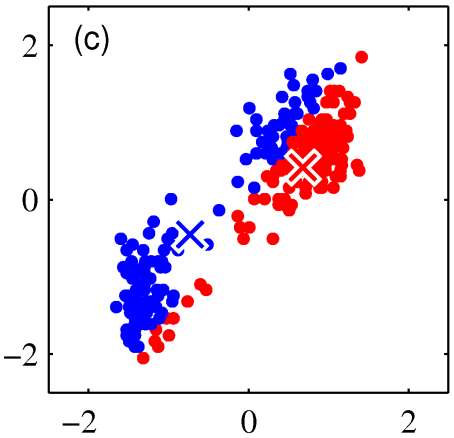

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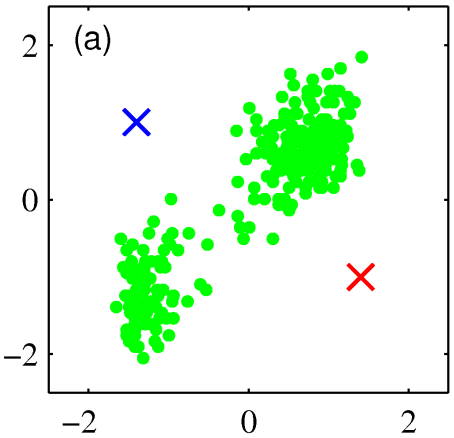

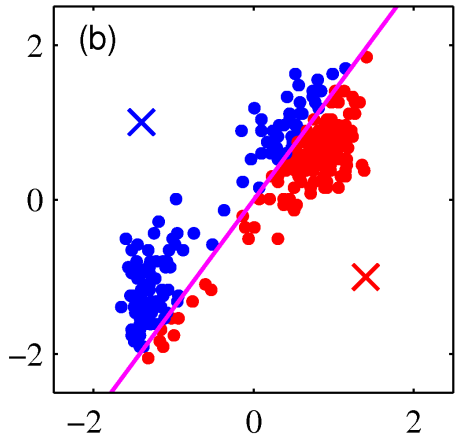

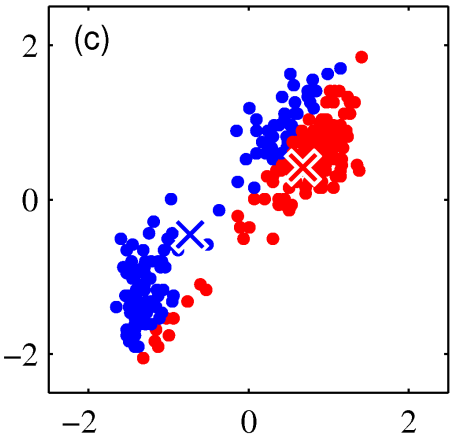

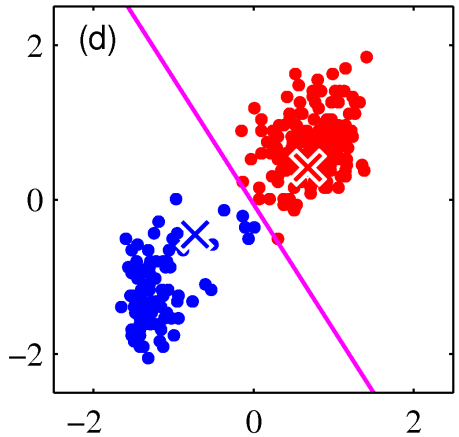

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K-means Clustering: Illustration (e) - (h)

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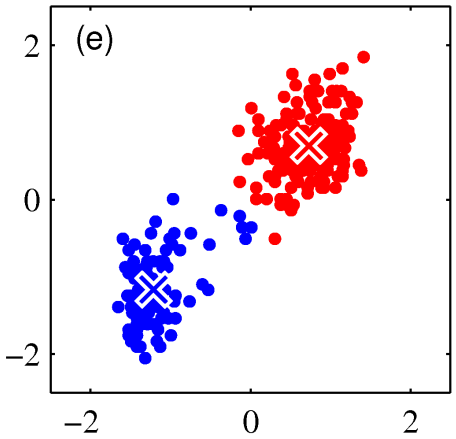

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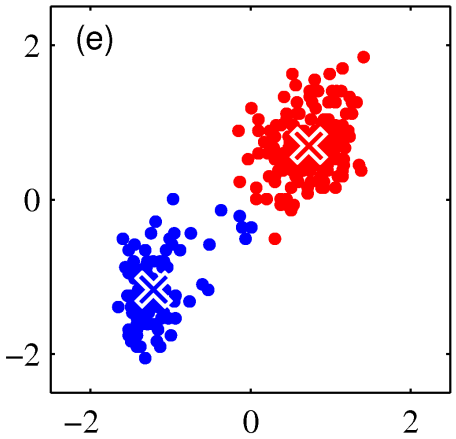

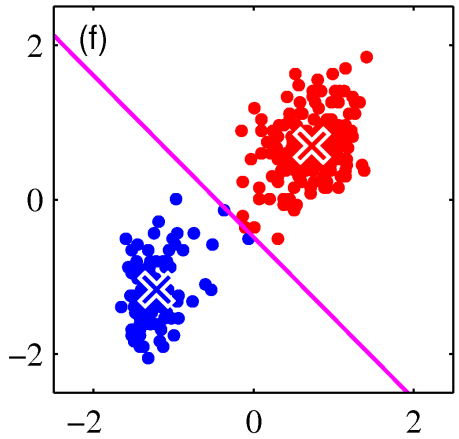

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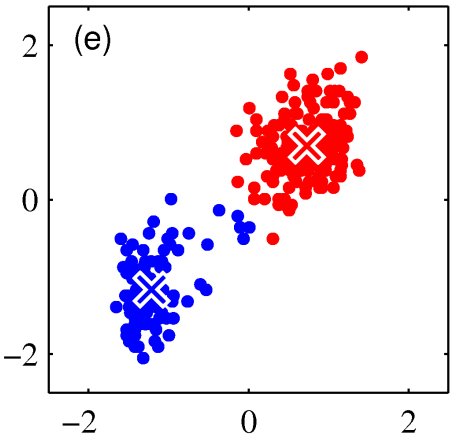

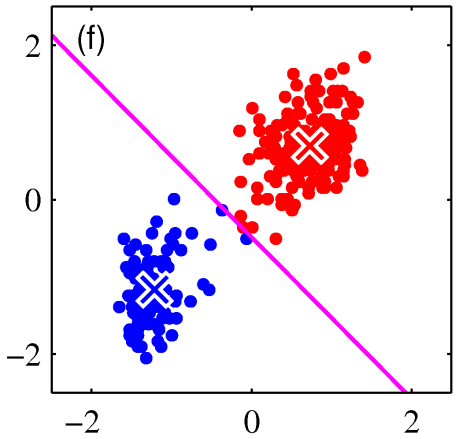

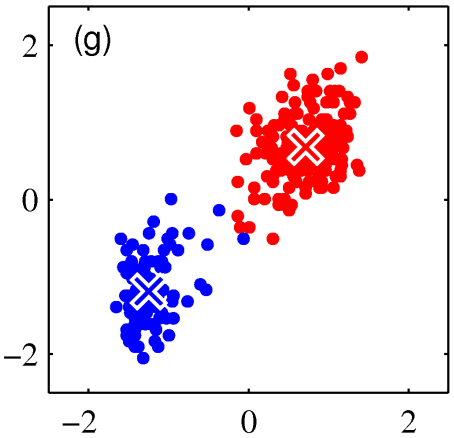

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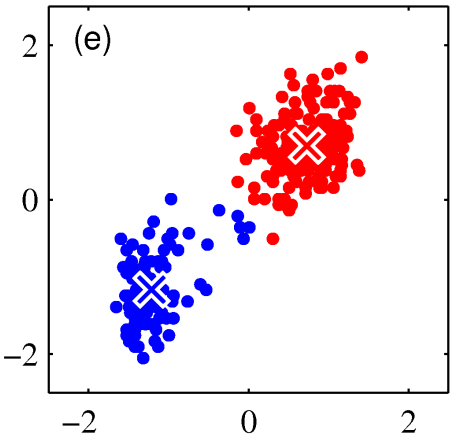

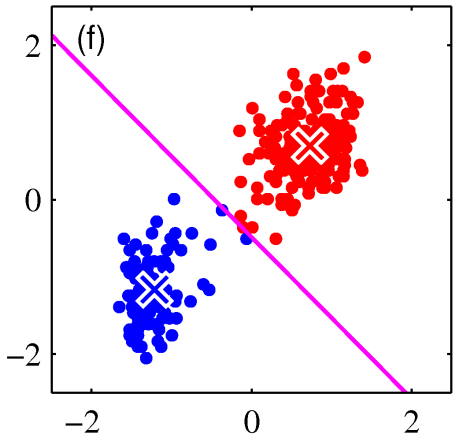

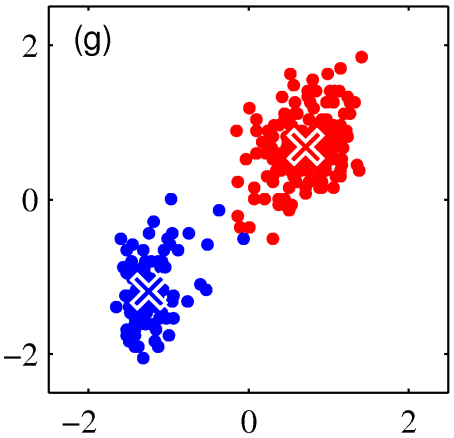

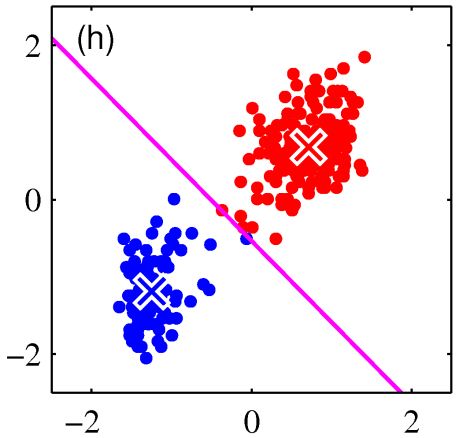

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K-means Clustering: Algorithm

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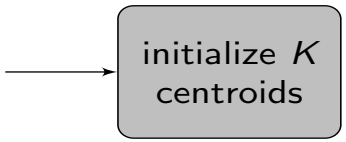
initialize K centroids

K-means Clustering: Algorithm



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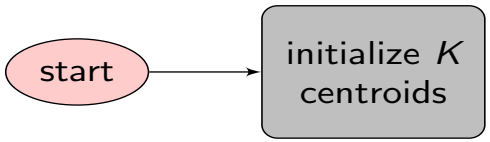

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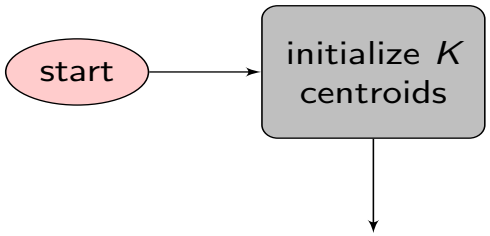

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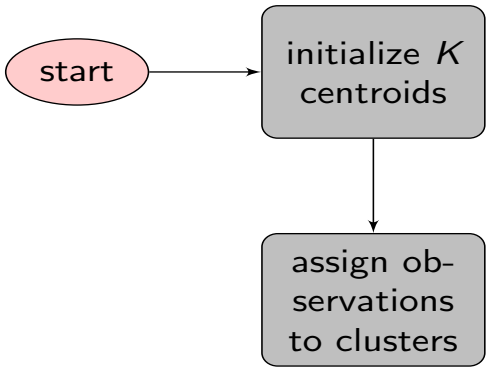

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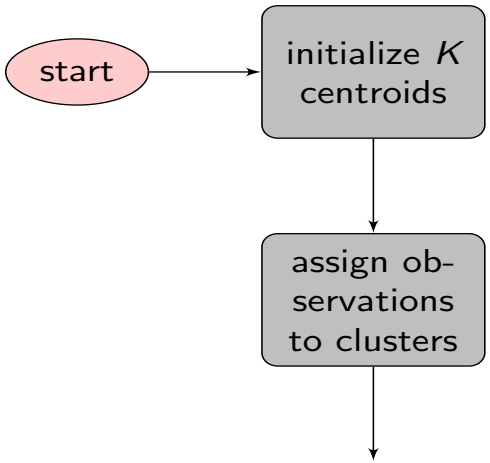

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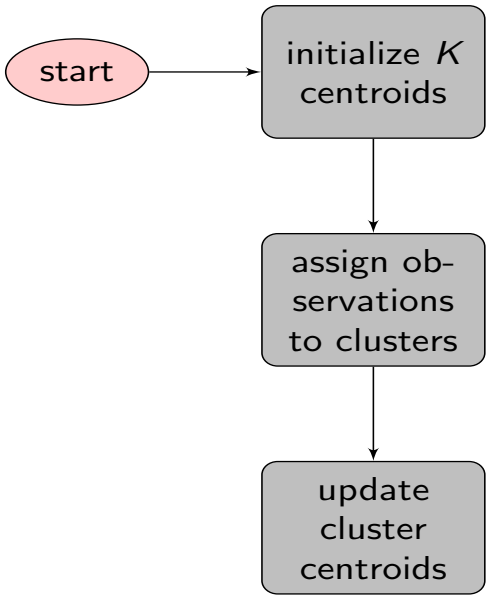

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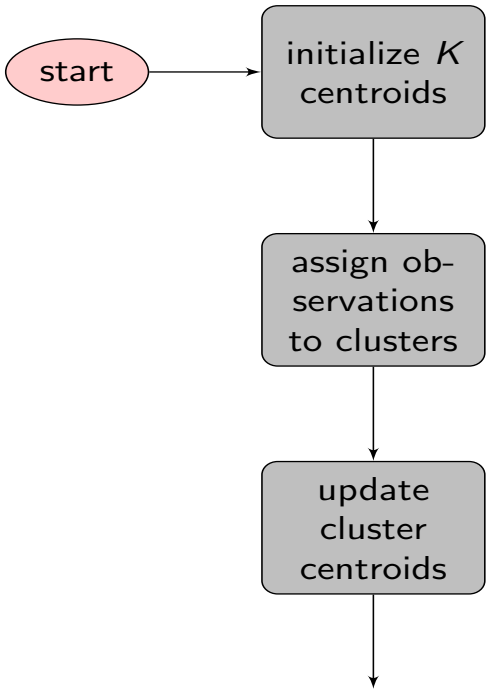

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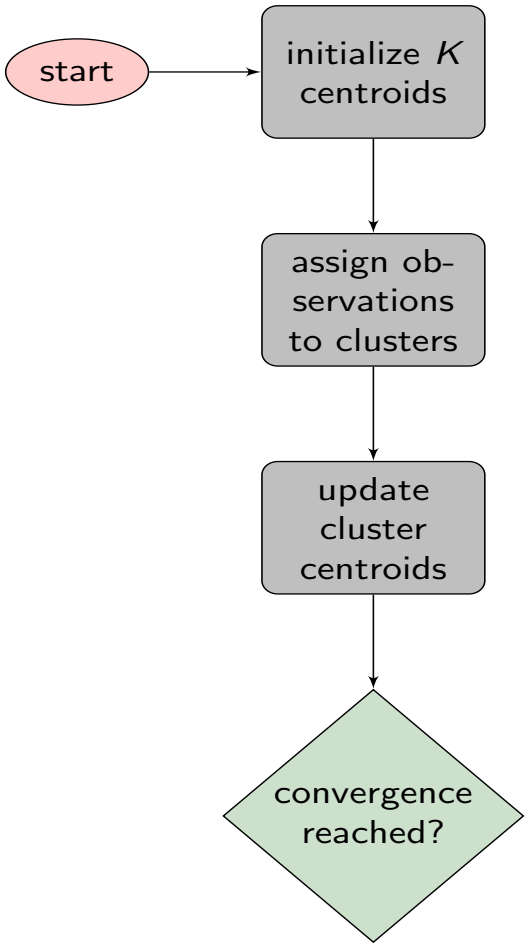

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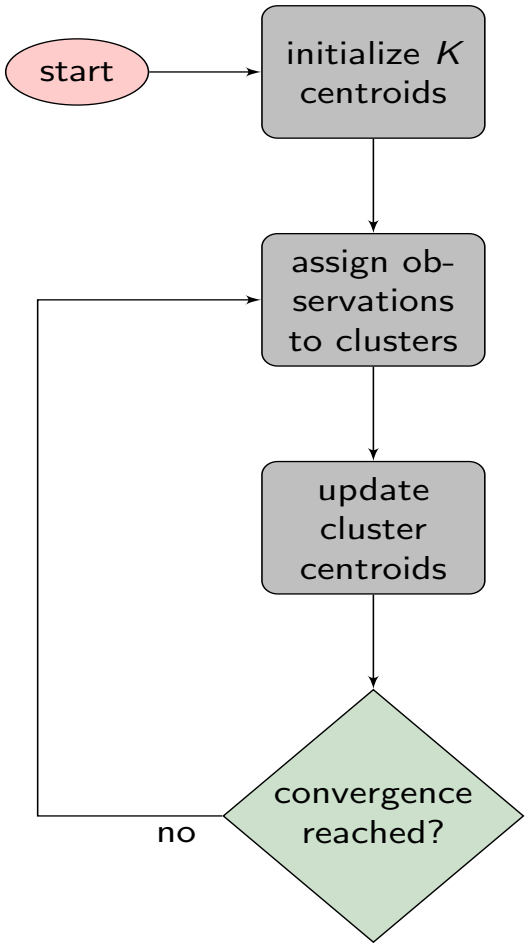

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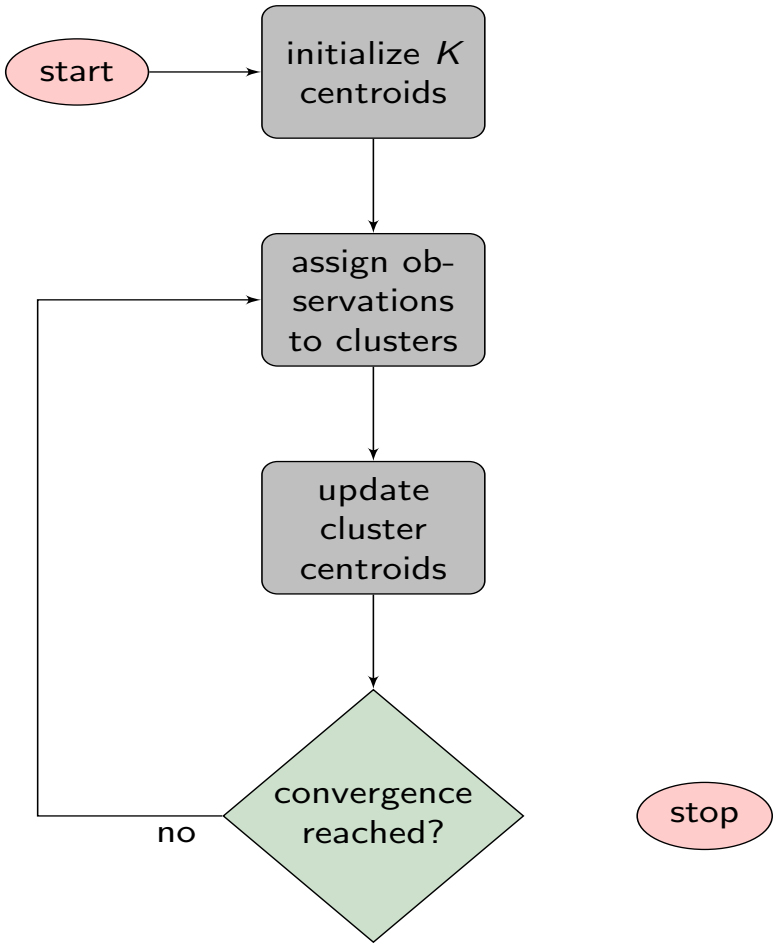

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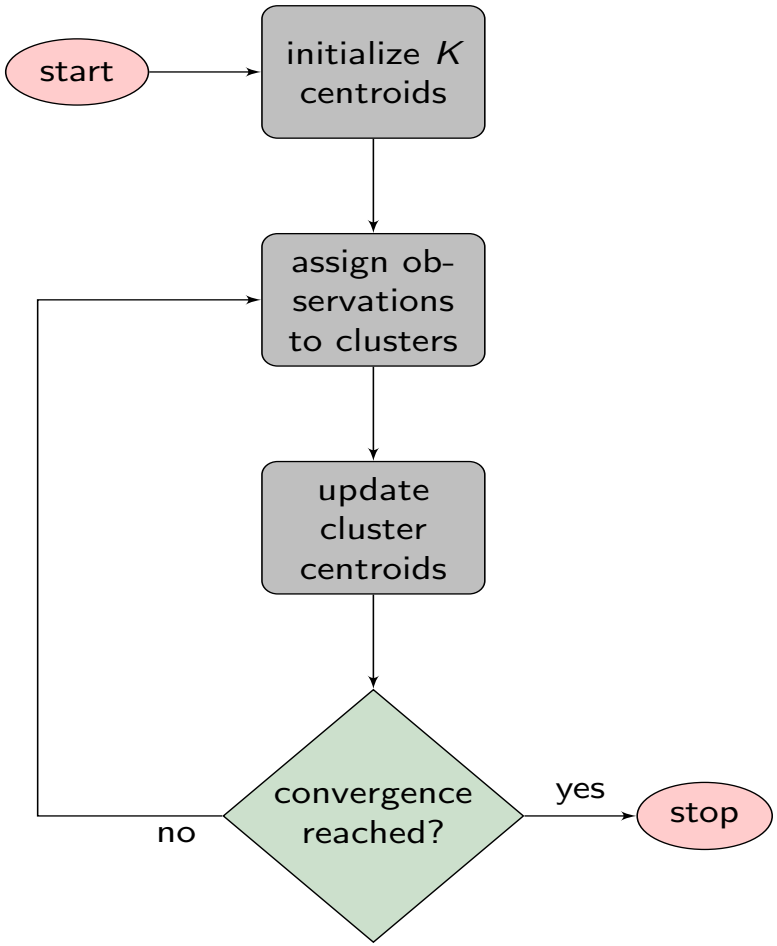

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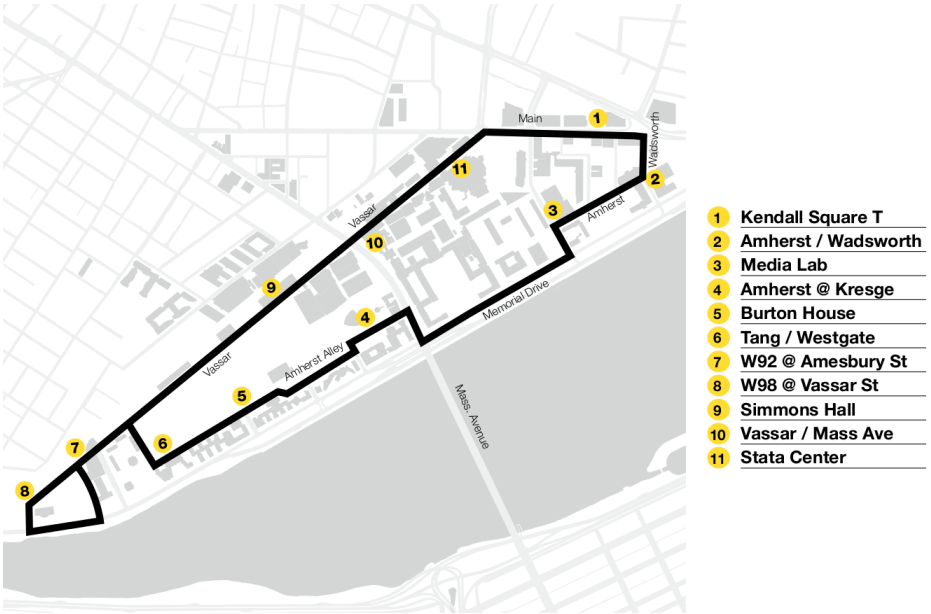
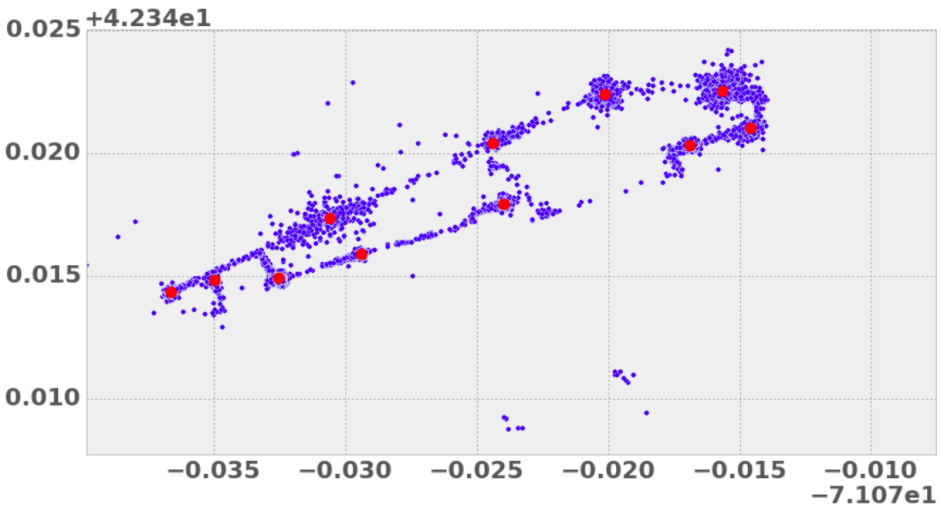
KMeans example: MIT tech shuttle

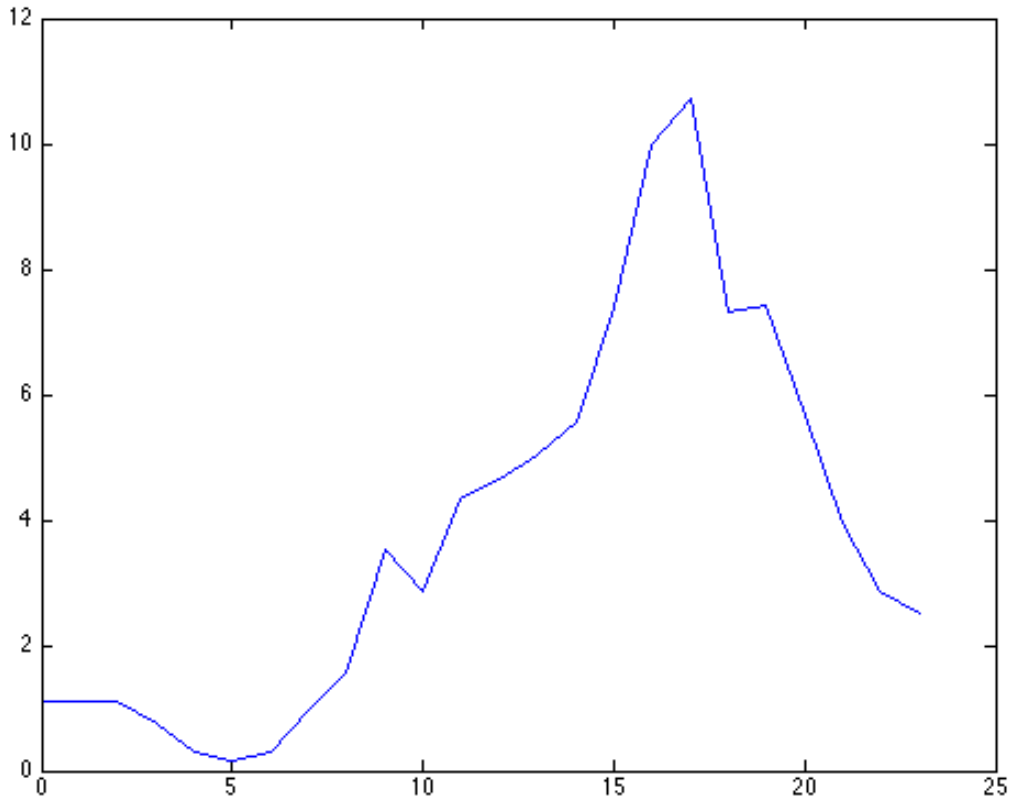




Purple dots: GPS points from buses; Red dots: centroids

Clustering Hubway rentals

- Comparing patterns
- Challenge: group stations according to similar demand patterns



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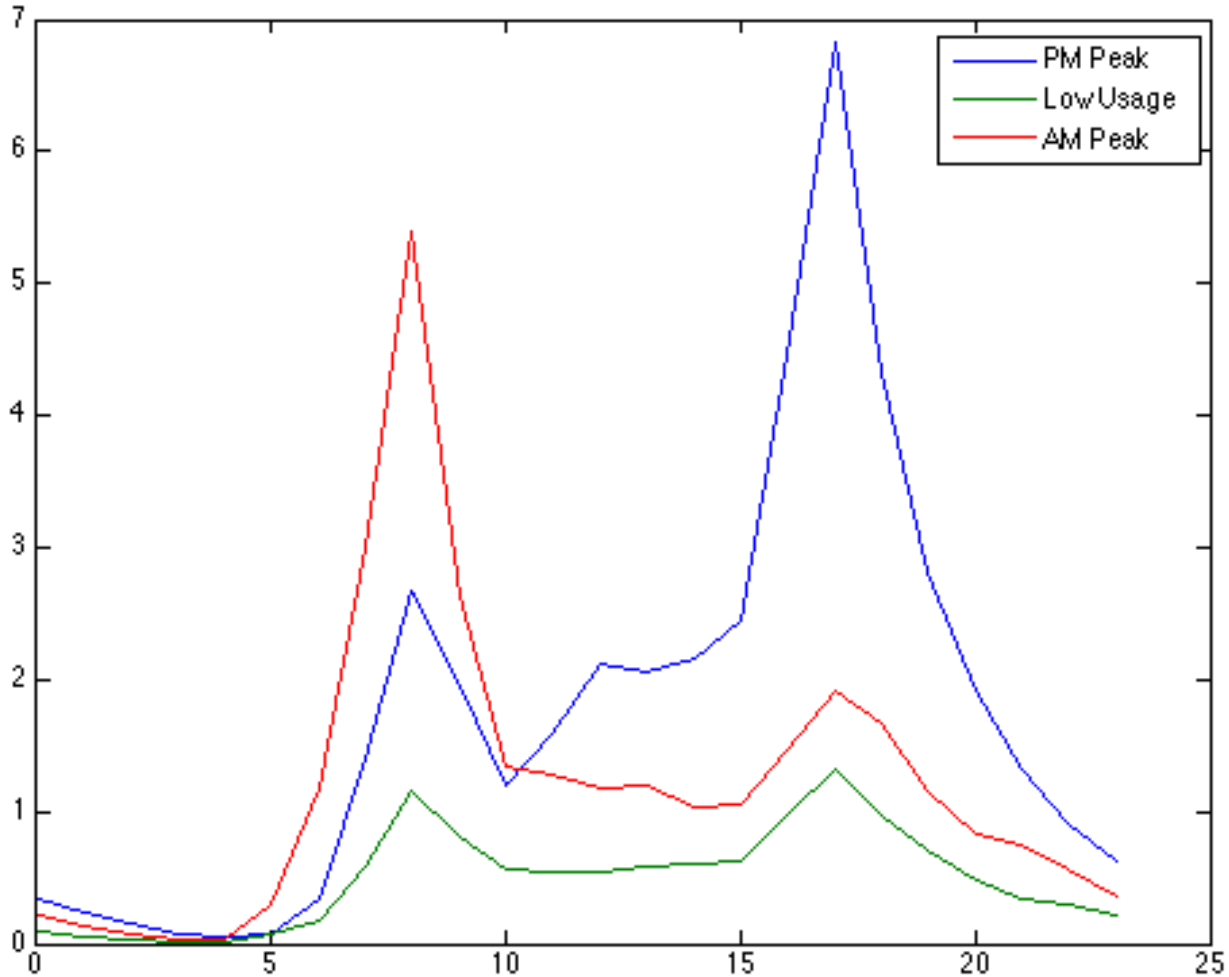

Clustering Hubway rentals (cont.)

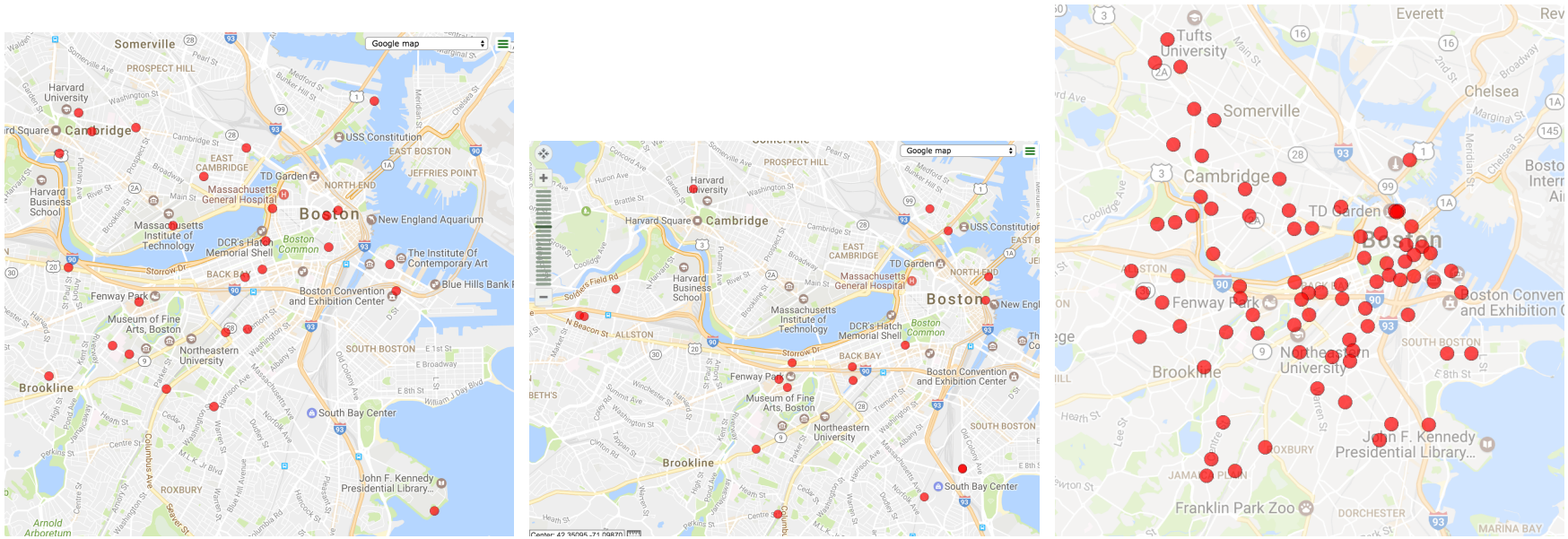

Figure: AM Peak, PM Peak, Low Usage docks

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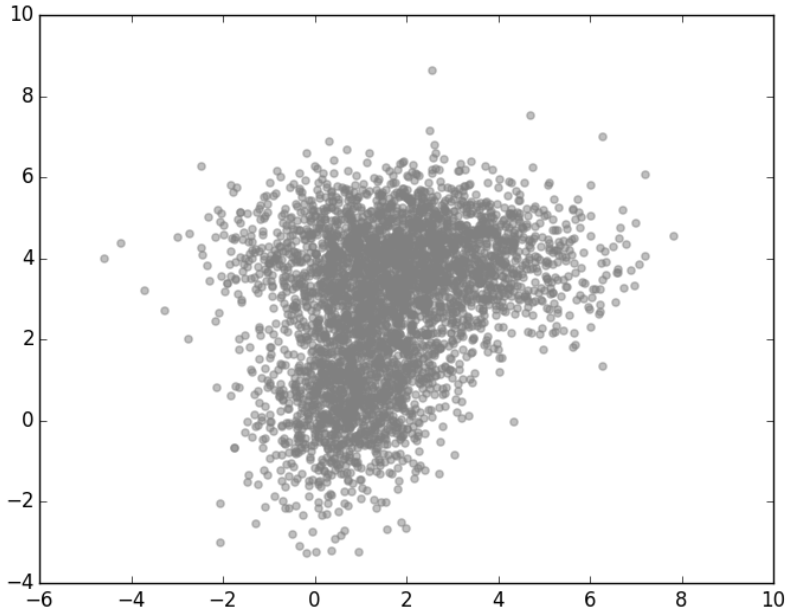

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- An alternative is hierarchical [agglomerative] clustering (HAC), which gives a tree-based representation of the dataset

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EM algorithm for GMM clustering

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$$r_{ik} = \frac{\pi_k \mathcal{N}(\boldsymbol{x}_i | \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)}{\sum_{j=1}^{K} \pi_j \mathcal{N}(\boldsymbol{x}_i | \boldsymbol{\mu}_j, \boldsymbol{\Sigma}_j)} \tag{6}$$

- **M-step:** Update parameters

$$\pi_k = \frac{N_k}{N} \tag{7}$$

$$\boldsymbol{\mu}_k = \frac{1}{N_k} \sum_{i=1}^{N} r_{ik} \boldsymbol{x}_i \tag{8}$$

$$\boldsymbol{\Sigma}_k = \frac{1}{N_k} \sum_{i=1}^{N} r_{ik} (\boldsymbol{x}_i - \boldsymbol{\mu}_k)(\boldsymbol{x}_i - \boldsymbol{\mu}_k)^\top \tag{9}$$

where $N_k = \sum_{i=1}^{N} r_{ik}$ is the effective number of points assigned to cluster k.

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- Ultimately,

$$\boldsymbol{\mu}_k = \frac{1}{N_k} \sum_{i=1}^{N} r_{ik} \boldsymbol{x}_i \tag{10}$$

where $r_{ik} \in \{0, 1\}$ indicates hard assignment of point i to cluster k.

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$$D(U, V) = \frac{|U| \cdot |V|}{|U| + |V|} ||\bar{u}_i - \bar{v}_j||^2 \tag{15}$$

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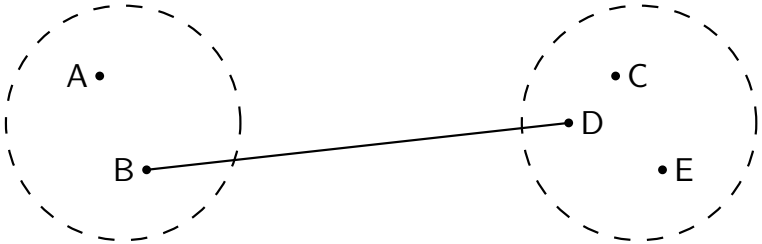

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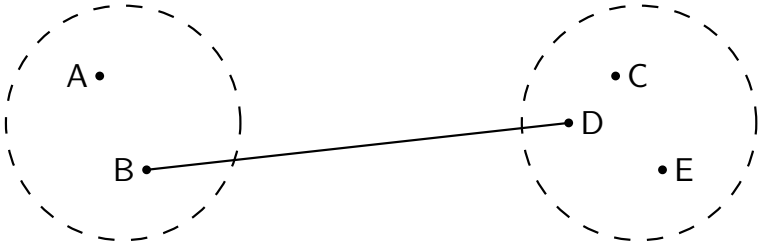

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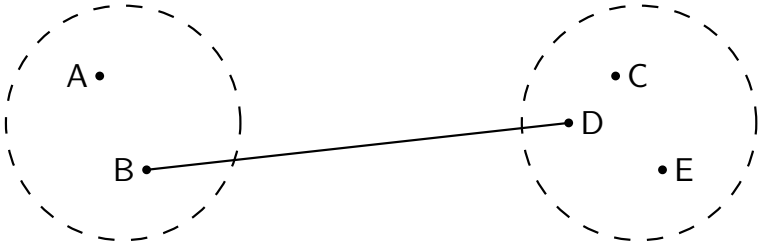

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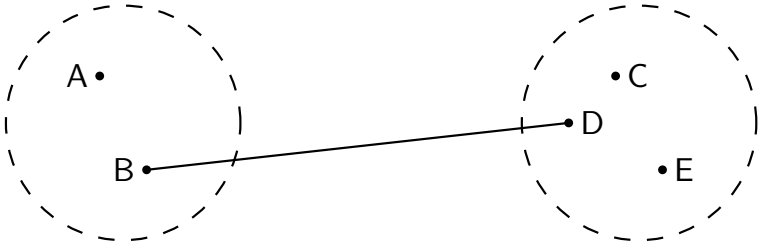

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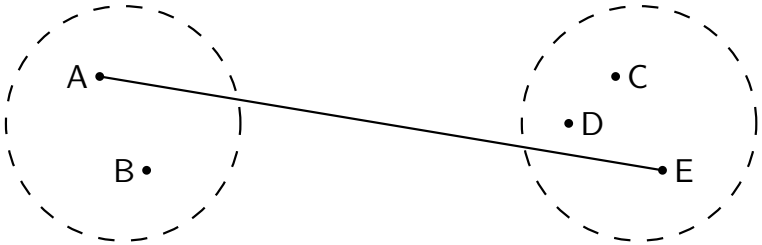

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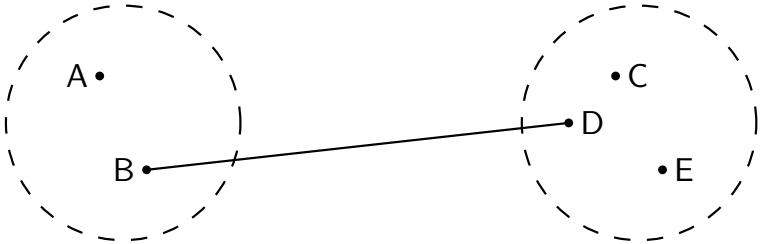

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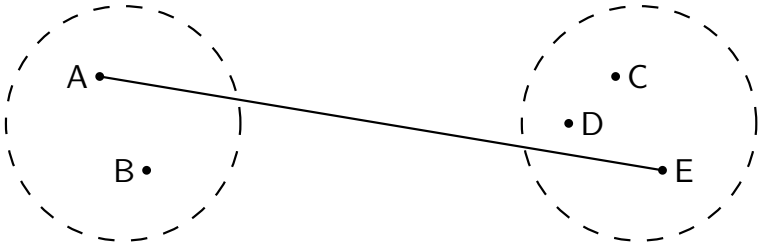

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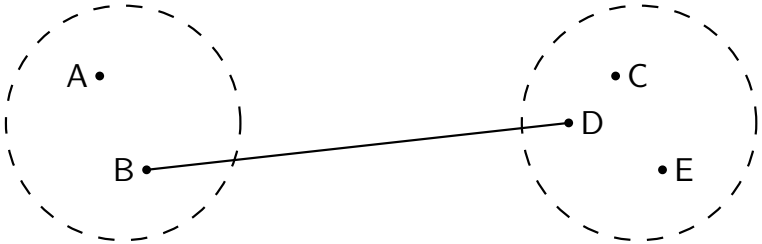

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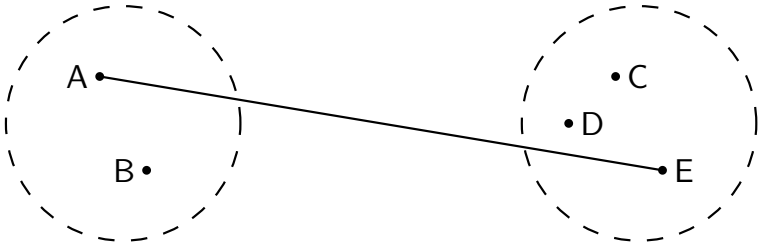

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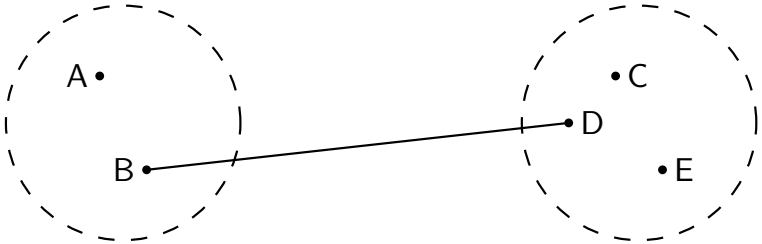

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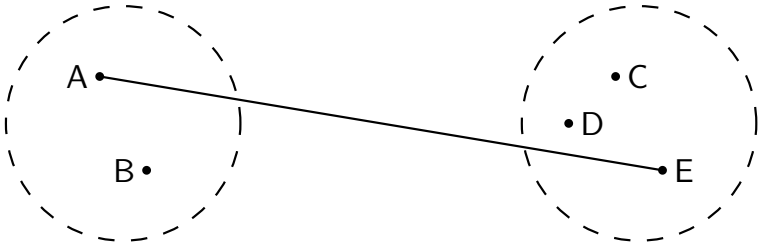

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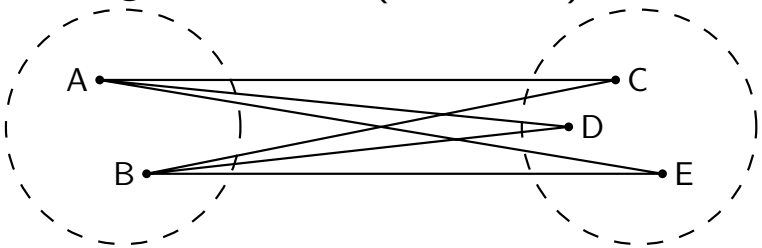

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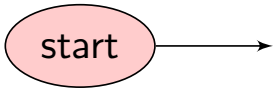

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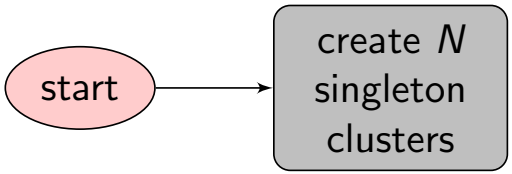

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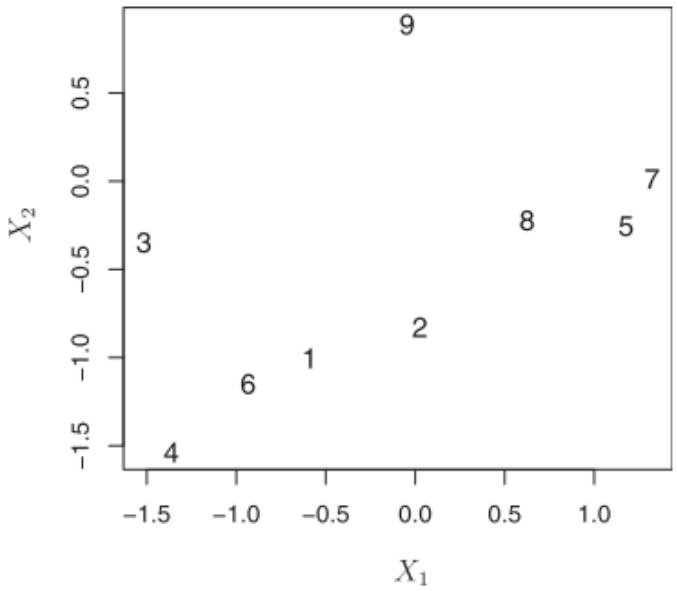

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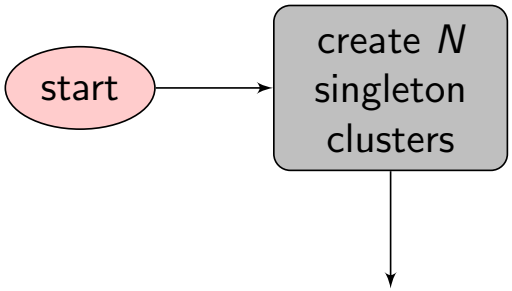

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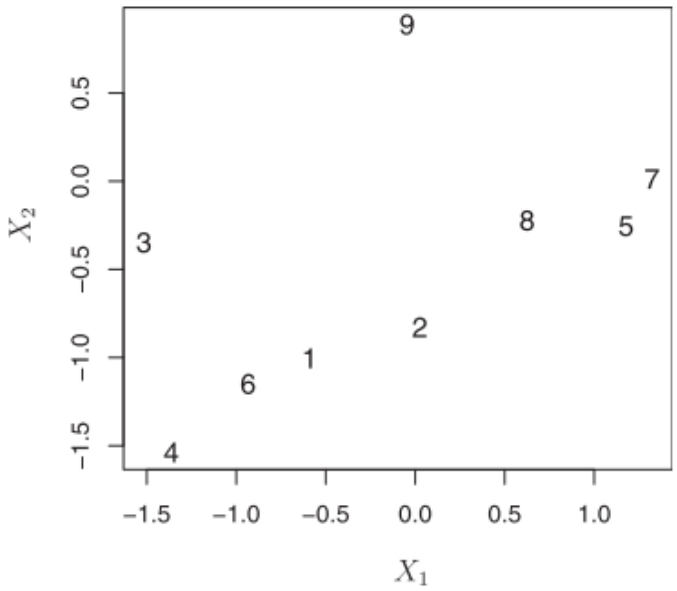

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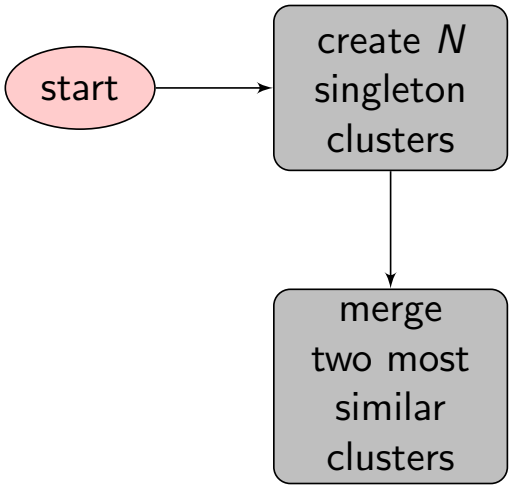

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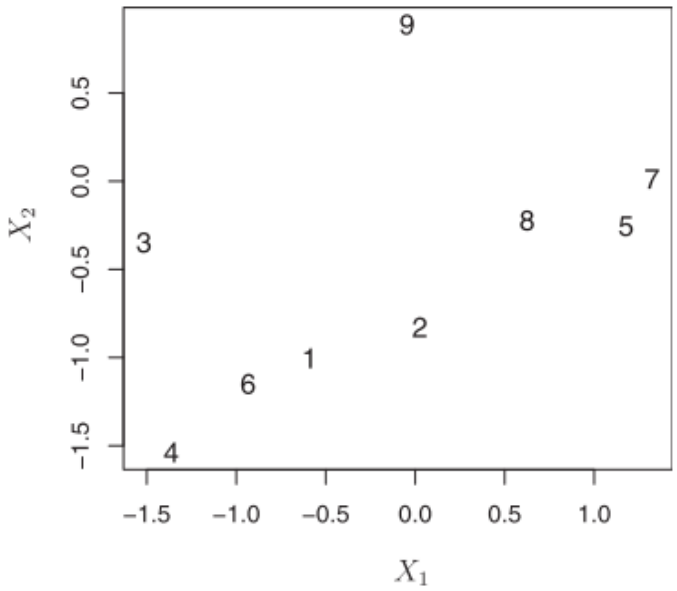

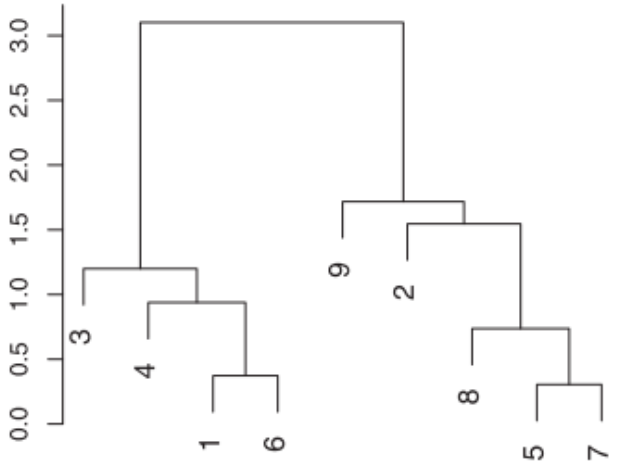

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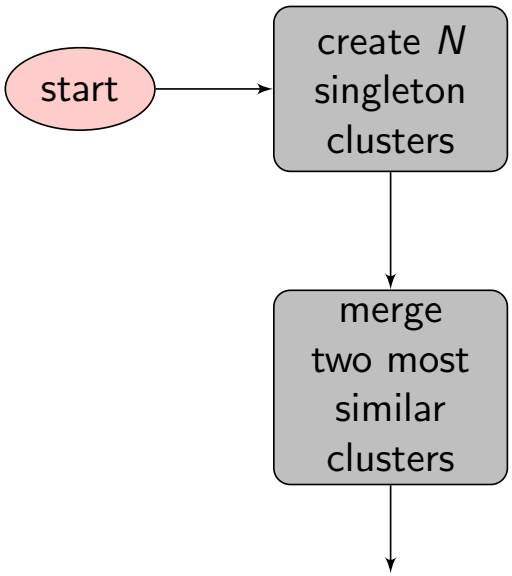

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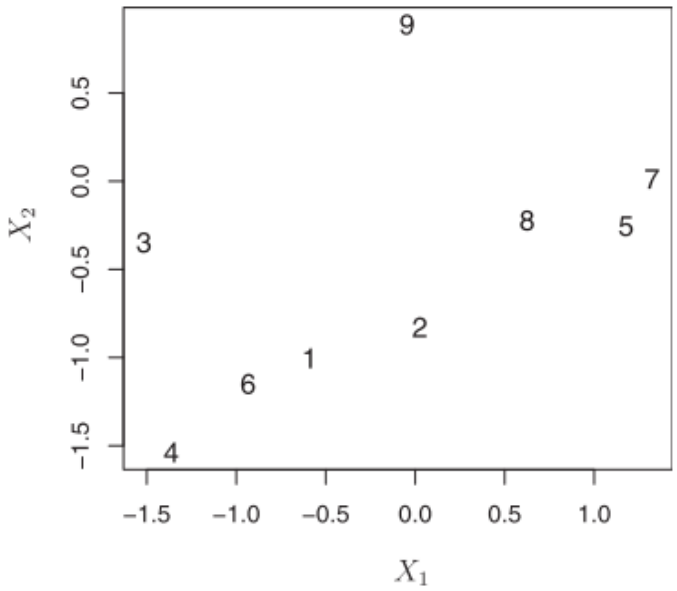

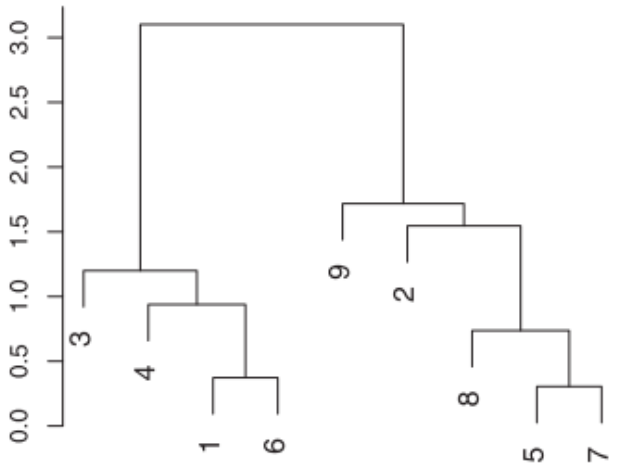

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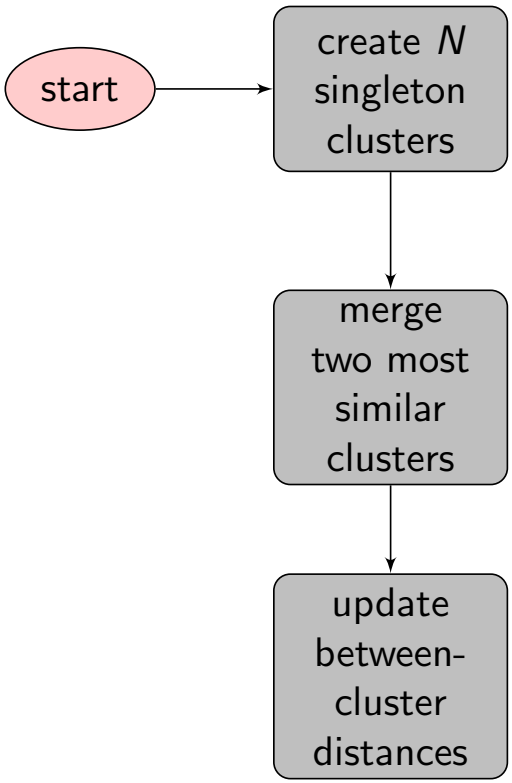

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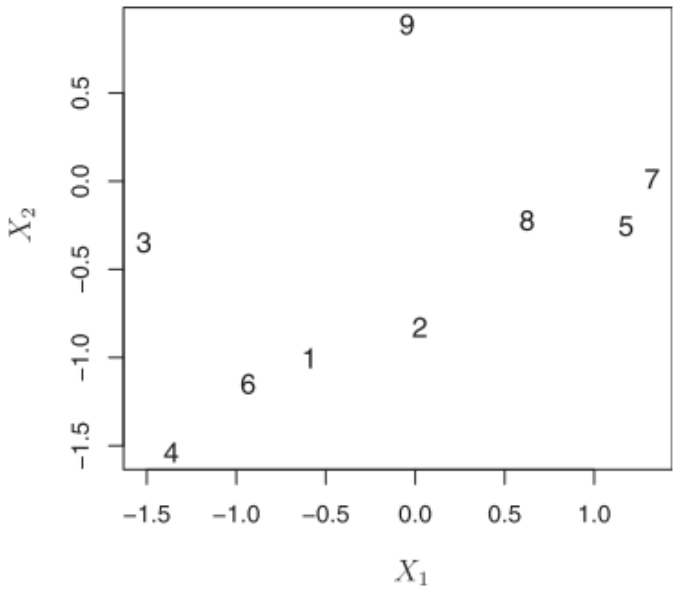

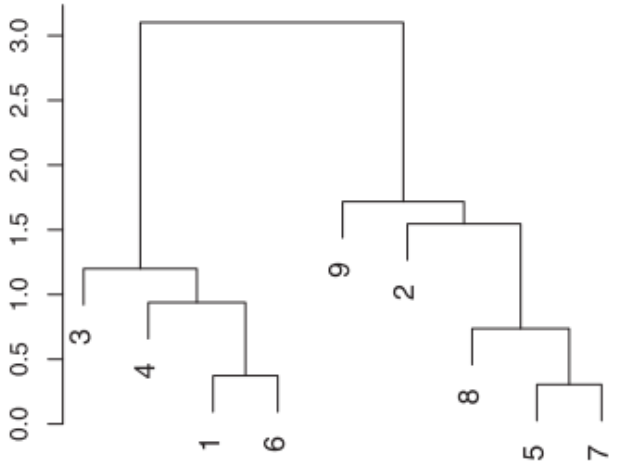

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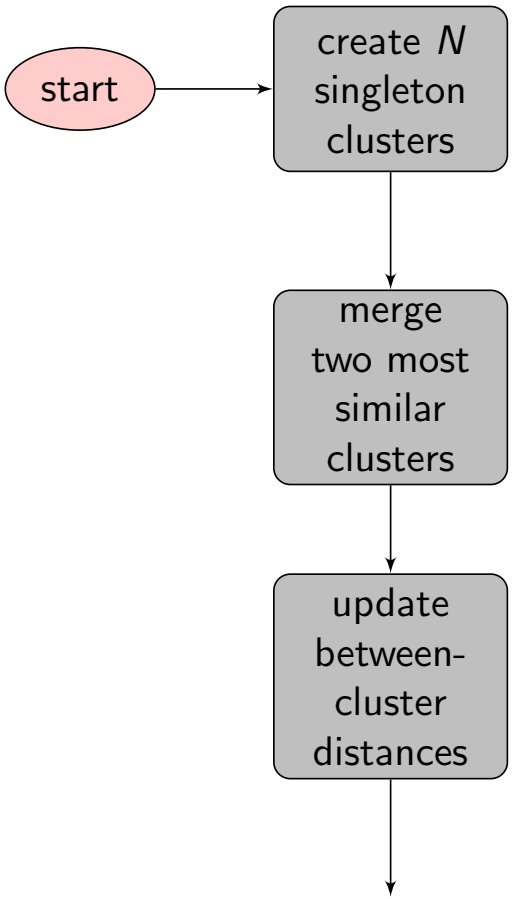

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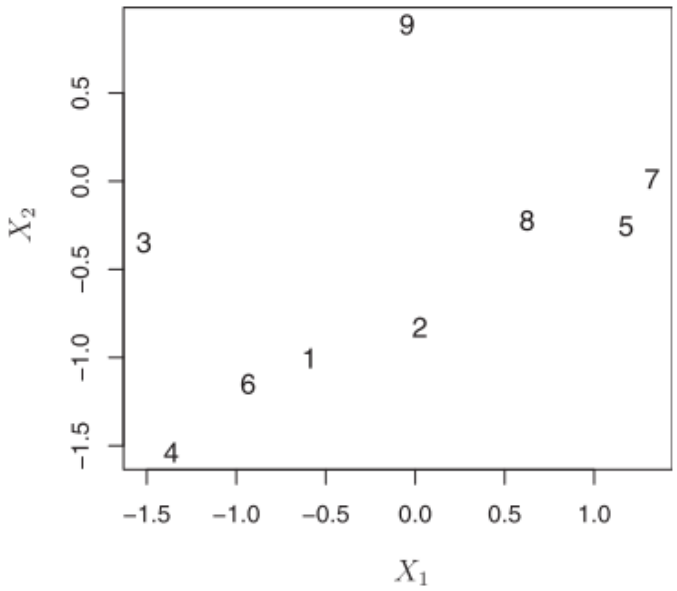

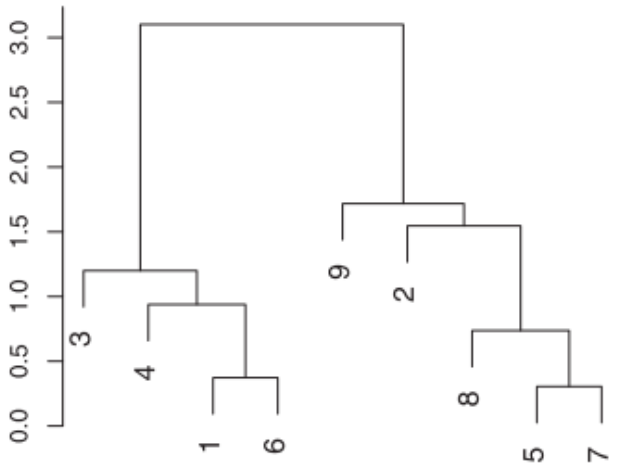

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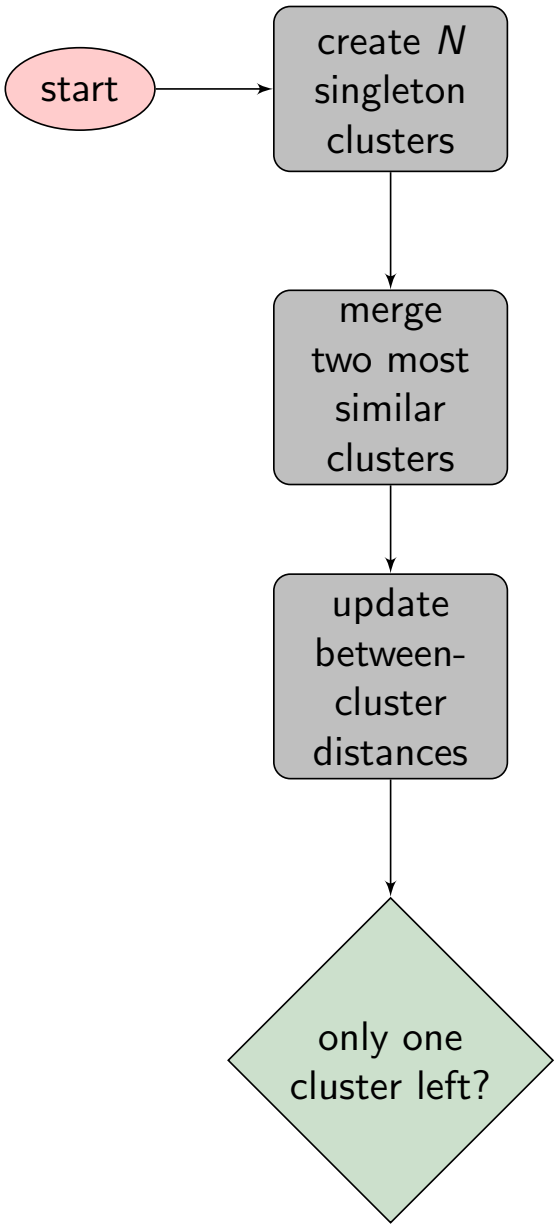

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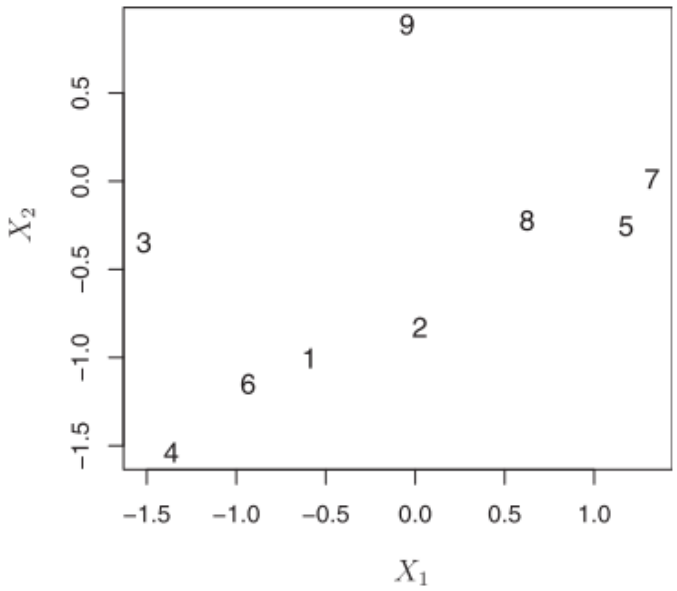

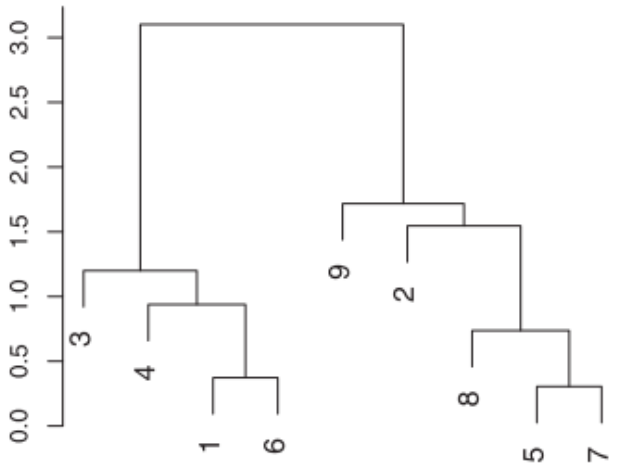

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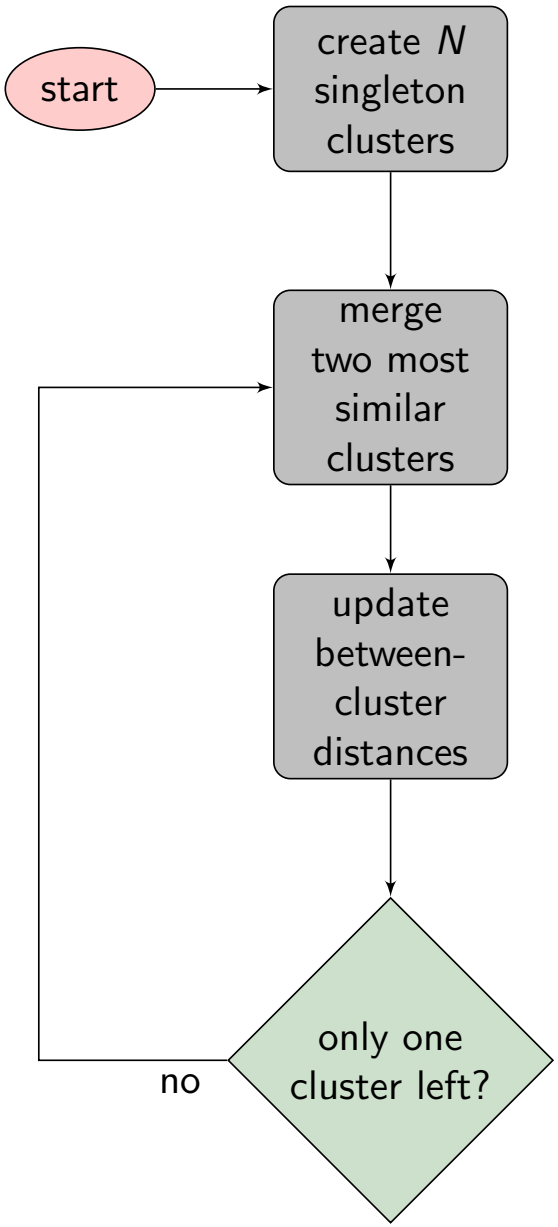

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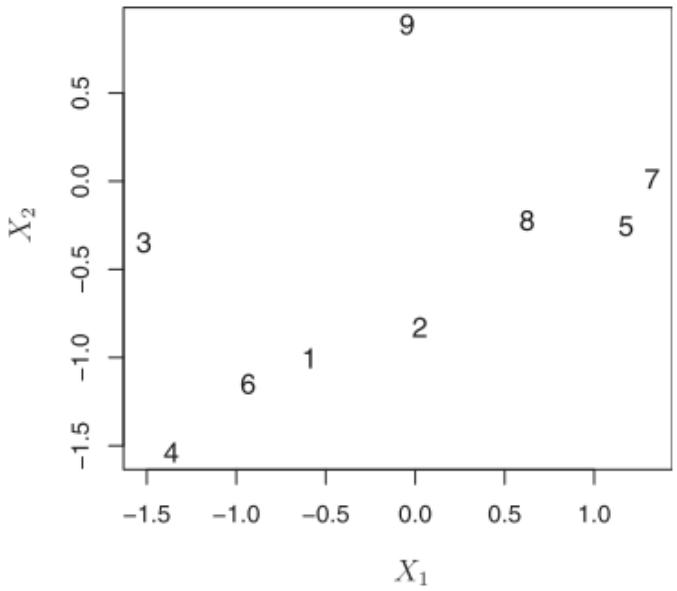

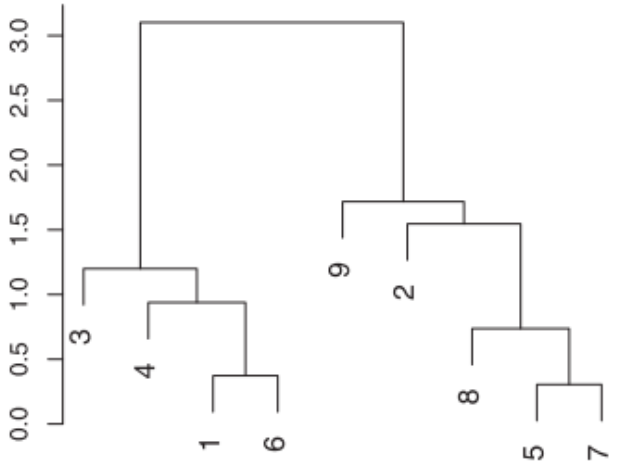

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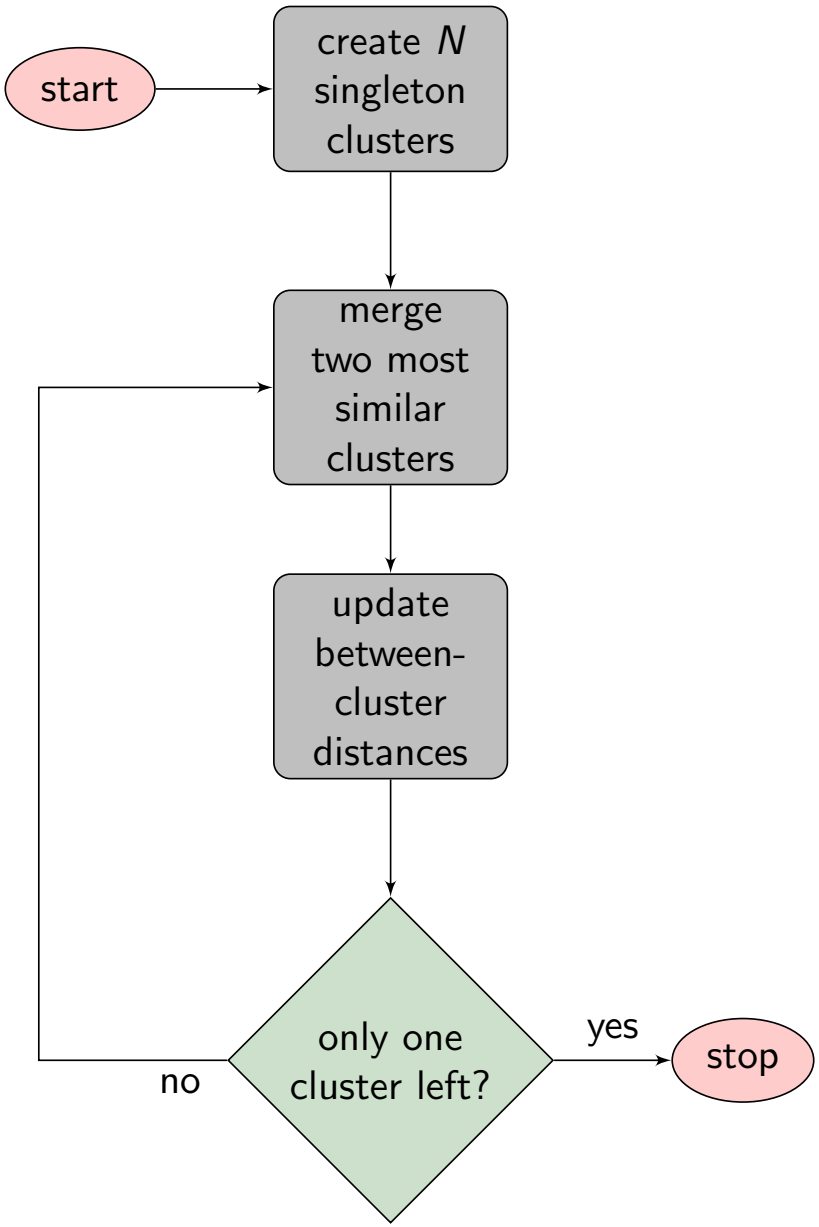

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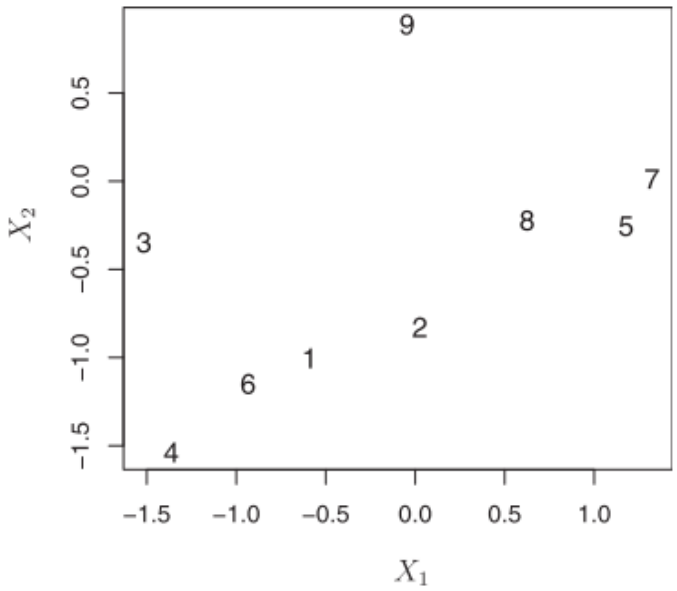
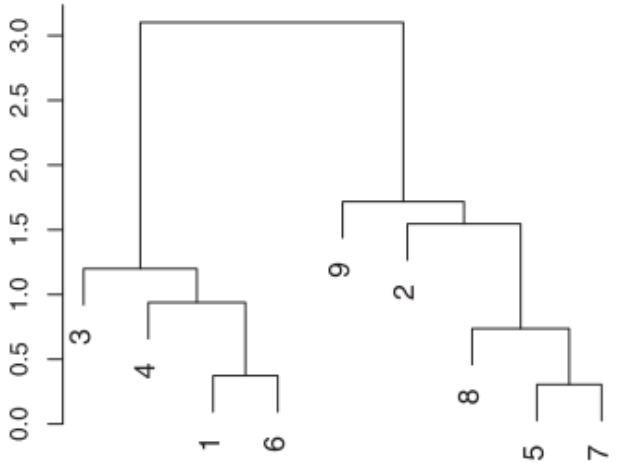
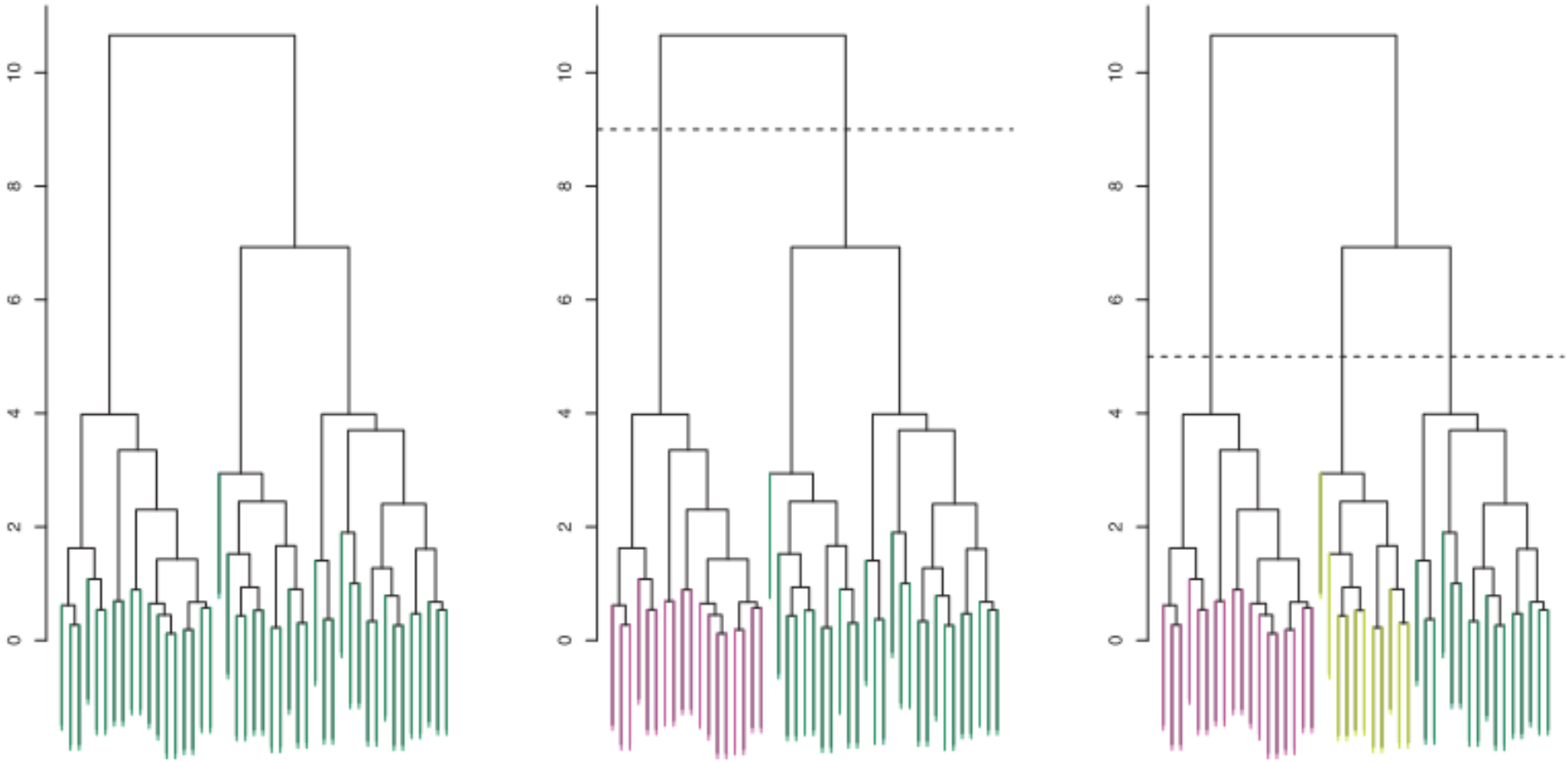




Choosing the clusters

We decide a Cut



Source: James et Al., Introduction to Statistical Learning

Practical Considerations

Advantages

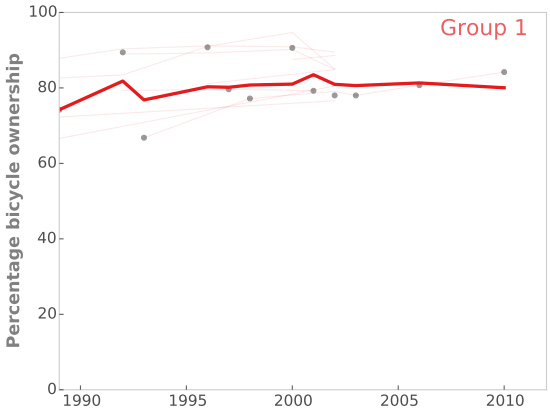
- No apriori number of clusters required
- Simple algorithms
- Self-organized structural view of data

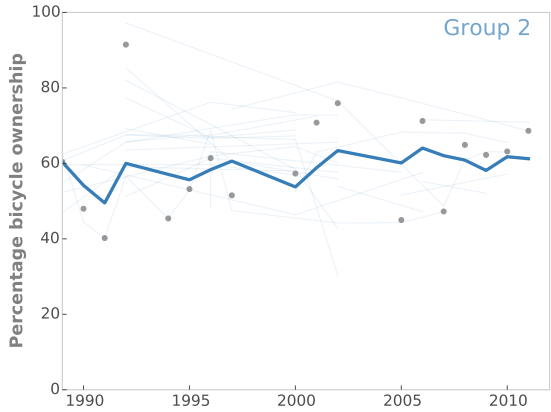
Disadvantages

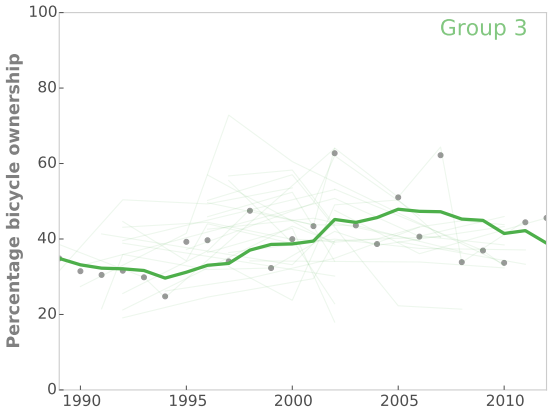
- Dendrogram often difficult to visualize
- Sometimes the inherent clusters in our data are not hierarchical by nature (K-means performs better in these cases)

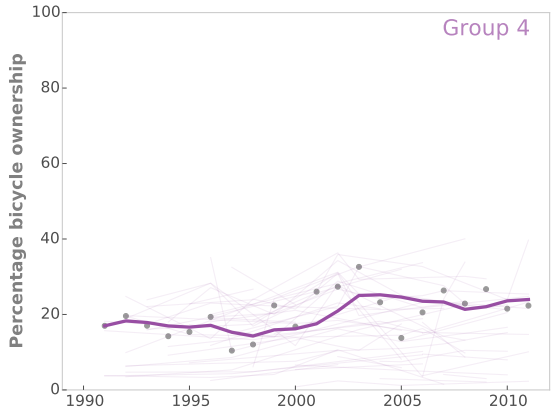
HAC example: Bicycle ownership trends

Pattern discovery from survey data in 150 countries spanning 30 years [1]



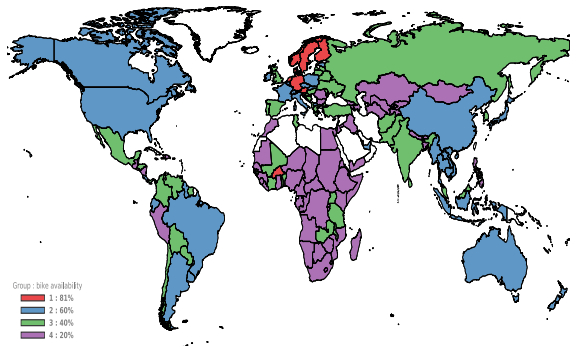






Key findings

- To cluster time-series data of varying lengths, the dynamic time warping (DTW) algorithm can be used to compute the dissimilarity matrix



[1] Oke et al., 2015
https://www.sciencedirect.com/science/article/abs/pii/S2214140515006787

Density-based clustering

Density-based clustering approaches are based on these hypotheses:

- Clusters are dense spatial regions
- Clusters are separated by low-density regions
- The density of points in a cluster are greater than a given minimum

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Examples of density-based clustering algorithms:

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- Clusters are dense spatial regions
- Clusters are separated by low-density regions
- The density of points in a cluster are greater than a given minimum

Examples of density-based clustering algorithms:

- DBSCAN
- OPTICS

Density-based spatial clustering of applications with noise

[2] https://citeseerx.ist.psu.edu/viewdoc/summary?doi=10.1.1.121.9220

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Source: https://www.nature.com/articles/srep34406

Figure: Example of clusters generated by DBSCAN on a dataset

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DBSCAN: key definitions

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- Epsilon neighborhood, N_ε: set of all observations within distance ε
- Core point: has at least `minPoint` observations within its N_ε
- DDR: An observation j is **directly density reachable** from a core point i if $j \in N_\varepsilon$
- DR: Two observations are **density reachable** if there exists a chain of DDR observations linking them
- Boundary/border points: these are DDR but not core points
- Noise/outlier points: do not belong to any observations N_ε

Source: Giacoumidis et al. (2019)

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Figure: DBSCAN example with minpoints = 4

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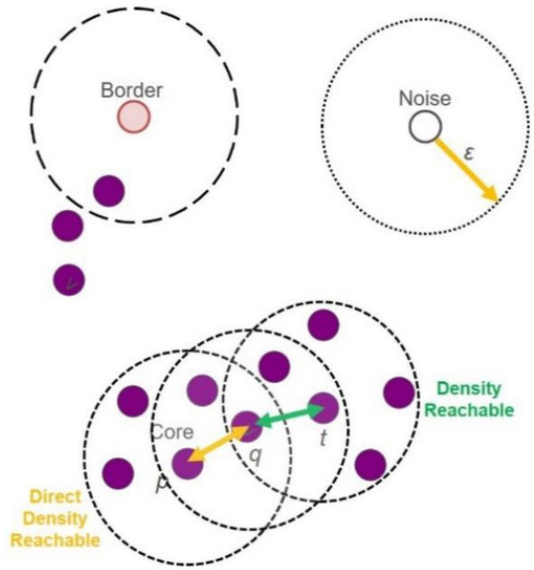

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Figure: DBSCAN example with minpoints = 4

DBSCAN serial algorithm

DBSCAN serial algorithm

procedure DBSCAN(X, ε, minPoints)
  for each unvisited point $x \in X$ **do**
    mark x as visited
    $N \leftarrow$ FindNeighbors(x, ε)
    if $|N| <$ minPoints **then**
      mark x as noise
    else
      $C \leftarrow \{x\}$
    end if
    for each point $x' \in N$ **do**
      $N \leftarrow N \setminus x'$
      if x' is not visited **then**
        mark x' as visited
        $N' \leftarrow$ FindNeighbors(x', ε)
        if $|N'| \geq$ minPoints **then**
          $N \leftarrow N \cup N'$
        end if
      end if
      if x' is not yet a member of any cluster **then**
        $C \leftarrow C \cup \{x'\}$
      end if
    end for
  end for
end procedure

DBSCAN example: stop detection

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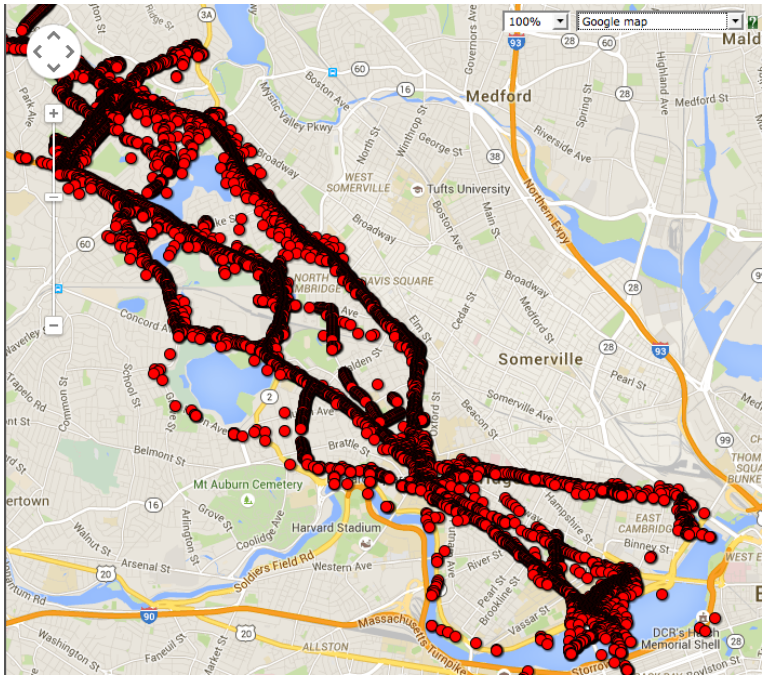

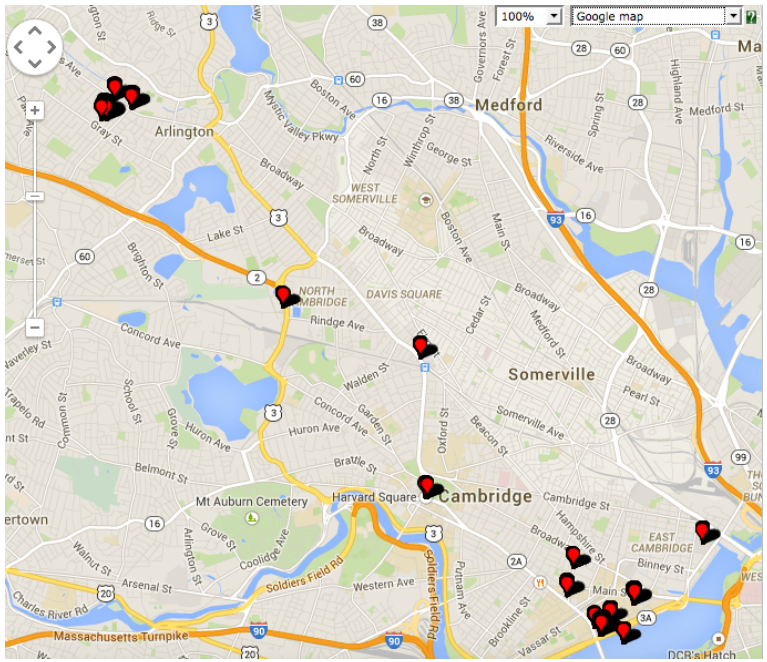

DBSCAN considerations

DBSCAN considerations

- Performs well on geographical data
- Requires careful selection of two parameters (can be computationally intensive)
- Several improvements and updates to the original DBSCAN algorithm have been made (e.g. OPTICS: "Ordering points to identify the clustering structure")

Fitness of clustering solution

Good clustering should:

- Minimize within-cluster (inter-cluster) variability ($\mathbf{W}$)
- Maximize the silhouette (Rousseeuw, 1987)
- Several other goodness-of-fit measures can be used:
  - Krzanowski-Lai (KL) index
  - Gap statistic (Tibshirani et al., 2001)
- We consider the silhouette metric in detail

Silhouette

- Silhouette of observation $\mathbf{x}_j$, $s(\mathbf{x}_j)$:

$$s(\mathbf{x}_j) = \frac{b(\mathbf{x}_j) - a(\mathbf{x}_j)}{\max\{a(\mathbf{x}_j), b(\mathbf{x}_j)\}} \tag{16}$$

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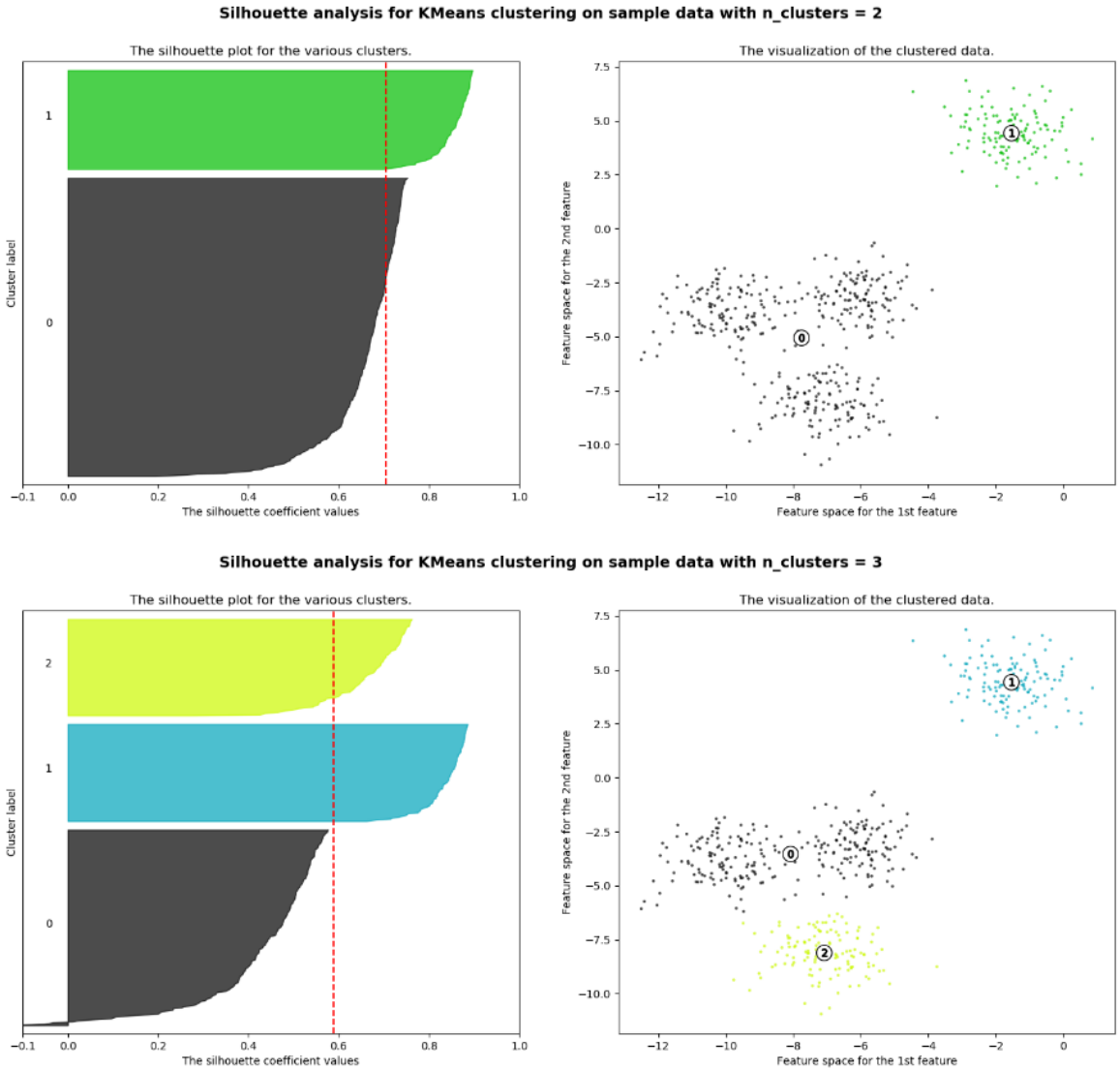
Silhouette: visualization



source:Scikit-learn: scikit-learn.org/stable/auto/examples/cluster/plot_kmeans_silhouette_analysis.html

Outlook

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- Assigned reading: ISLR 10.3, 10.4

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- Further recommended reading: ESL 14.3