MATH 567: Mathematical Techniques in Data Science
Clustering I

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Supervised and unsupervised learning

Supervised learning problems:

- Data (X, Y) is "labelled" (input/output) with joint density $P(X, Y)$.
- We are mainly interested by the conditional density $P(Y|X)$.
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Unsupervised learning problems:

- Data X is **not** labelled and has density $P(X)$.
- We want to infer properties of $P(X)$ without the help of a "supervisor" or "teacher".
- Examples: Density estimation, PCA, ICA, sparse autoencoder, clustering, etc..

Clustering

Wikipedia - Chire.

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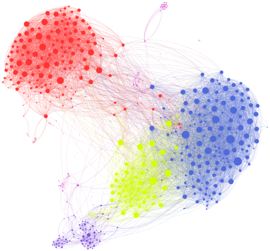
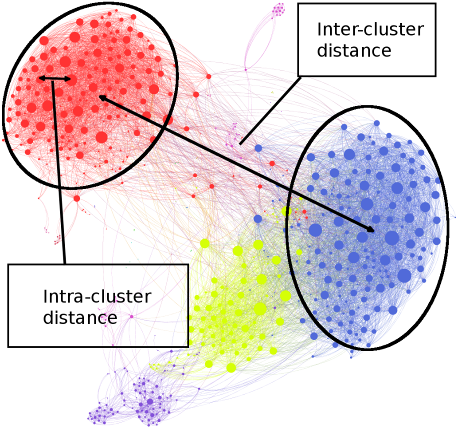


- Unsupervised problem.
- Work only with features/independent variables.
- Want to label points according to a measure of their similarity.

What is a cluster?

We try to partition observations into "clusters" such that:

- Intra-cluster distance is minimized.
- Inter-cluster distance is maximized.



For graphs, we want vertices in the same cluster to be highly connected, and vertices in different clusters to be mostly disconnected.

The K-means algorithm

- Goes back to Hugo Steinhaus (of the Banach–Steinhaus theorem) in 1957.

Source: Wikipedia.

Steinhaus authored over 170 works. Unlike his student, Stefan Banach, who tended to specialize narrowly in the field of functional analysis, Steinhaus made contributions to a wide range of mathematical sub-disciplines, including geometry, probability theory, functional analysis, theory of trigonometric and Fourier series as well as mathematical logic. He also wrote in the area of applied mathematics and enthusiastically collaborated with engineers, geologists, economists, physicians, biologists and, in Kac's words, "even lawyers".

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- We want a partition $\hat{S} = \{S_1, \ldots, S_K\}$ of $\{x_1, \ldots, x_n\}$ such that

$$\hat{S} = \underset{S}{\operatorname{argmin}} \sum_{i=1}^{K} \sum_{x_j \in S_i} \|x_j - \mu_i\|^2,$$

  where $\mu_i = \frac{1}{|S_i|} \sum_{x_j \in S_i} x_j$ is the mean of the points in S_i (the "center" of S_i).

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- Efficient approximation algorithms exist (converge to a local minimum though).

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1. Assign each point x_j to the cluster whose mean is closest to x_j:

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3. $t \leftarrow t + 1$.

Until convergence.

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Note that Lloyds's algorithm uses a greedy approach to sequentially minimize:

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1. **The Forgy method:** Pick K observations at random from $\{x_1, \dots, x_n\}$ and use these as the initial means.
2. **Random partition:** Randomly assign a cluster to each observation and compute the mean of each cluster.

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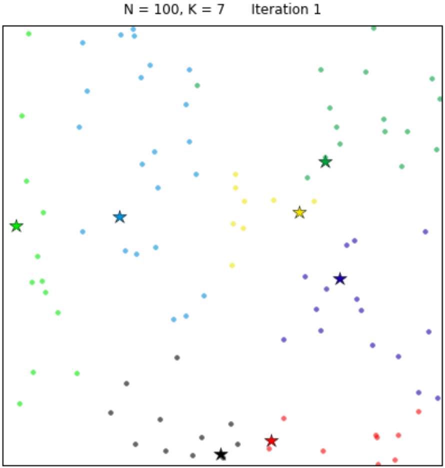

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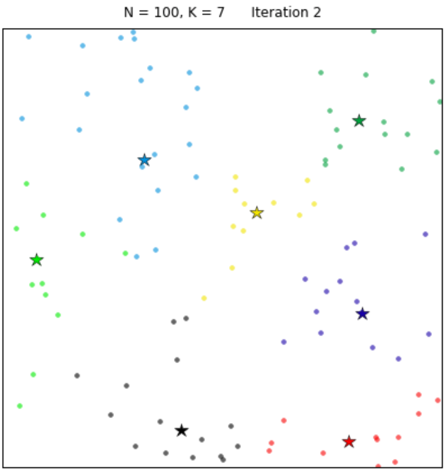

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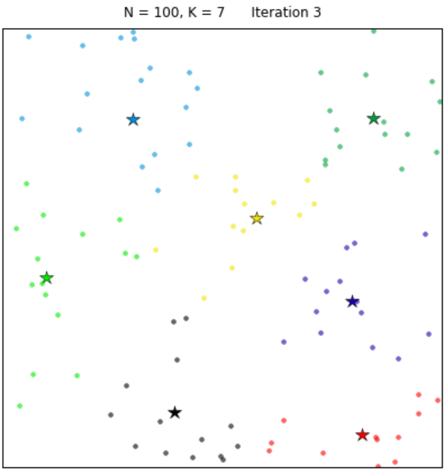

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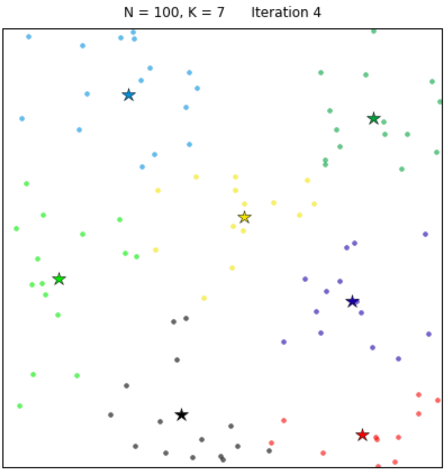

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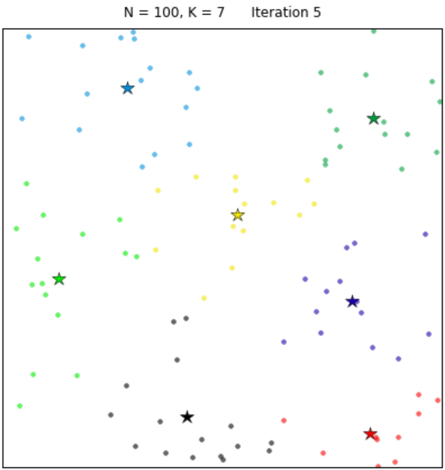

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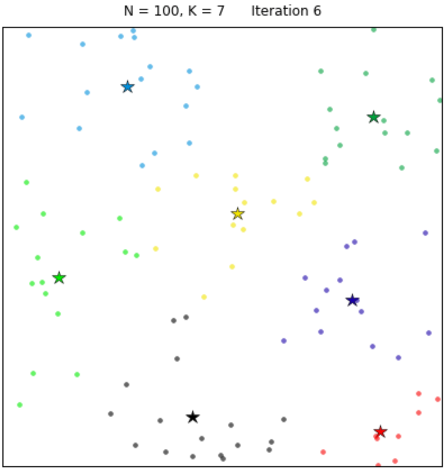

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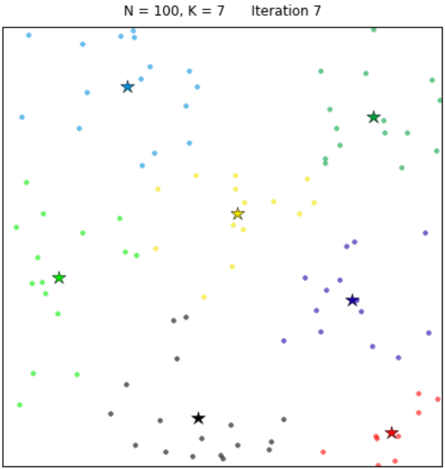

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Example: clustering the zip data

Is there a nice cluster structure in the zip dataset?

Experiment:

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$$p_{ij} = \begin{pmatrix}
0.00 & 0.00 & 2.45 & 0.38 & 0.94 & 0.57 & 0.00 & \mathbf{83.96} & 0.19 & 11.51 \\
14.78 & 0.00 & 0.77 & 0.26 & 0.77 & 14.40 & \mathbf{68.64} & 0.00 & 0.39 & 0.00 \\
1.08 & 0.46 & 7.57 & 11.13 & 0.77 & 10.66 & 0.31 & 0.62 & \mathbf{66.46} & 0.93 \\
\mathbf{90.37} & 0.00 & 2.28 & 0.18 & 0.18 & 1.23 & 5.08 & 0.00 & 0.70 & 0.00 \\
\mathbf{88.96} & 0.00 & 0.51 & 0.34 & 0.00 & 2.72 & 7.13 & 0.00 & 0.34 & 0.00 \\
1.08 & 0.00 & \mathbf{86.15} & 1.85 & 2.15 & 1.38 & 5.54 & 0.31 & 1.54 & 0.00 \\
1.41 & 0.00 & 5.66 & 1.13 & \mathbf{62.23} & 5.66 & 1.41 & 3.25 & 1.41 & 17.82 \\
1.63 & 0.00 & 3.69 & \mathbf{59.22} & 0.00 & 32.00 & 0.00 & 0.00 & 3.25 & 0.22 \\
0.00 & \mathbf{93.03} & 0.37 & 0.09 & 3.90 & 0.00 & 0.84 & 0.28 & 1.02 & 0.46 \\
0.00 & 0.12 & 1.10 & 1.46 & 16.93 & 0.61 & 0.24 & 20.46 & 4.99 & \mathbf{54.08}
\end{pmatrix}$$

Spectral clustering: overview

We saw how K-means can be used to cluster points in $\mathbb{R}^p$.

Spectral clustering:

- Very popular clustering method.
- Often outperforms other methods such as K-means.
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4. Cluster the graph using the eigenvectors of the graph Laplacian using the K-means algorithm.

Notation

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- If $A \subset V$, then we let $\mathbb{1}_A = (f_1, \ldots, f_n)^T \in \mathbb{R}^n$, where $f_i = 1$ if $v_i \in A$ and 0 otherwise.

Similarity graphs

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- We will discuss 3 popular ways of building a similarity graph.

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2. **The k-nearest neighbor graph:** The goal is to connect v_i to v_j if x_j is among the k nearest neighbords of x_i. However, this leads to a directed graph. We therefore define:

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1. **The ϵ-neighborhood graph:** Connect all points whose pairwise distances are smaller than some $\epsilon > 0$. We usually don't weight the edges. The graph is thus a simple graph (unweighted, undirected graph containing no loops or multiple edges).
2. **The k-nearest neighbor graph:** The goal is to connect v_i to v_j if x_j is among the k nearest neighbords of x_i. However, this leads to a directed graph. We therefore define:
   - the k-nearest neighbor graph: v_i is adjacent to v_j iff x_j is among the k nearest neighbords of x_i **OR** x_i is among the k nearest neighbords of x_j.

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   We weight the edges by the similarity of their endpoints.

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All graphs mentioned above are regularly used in spectral clustering.

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We will see in the next lecture how these Laplacians can be used to cluster graphs.