MATH 829: Introduction to Data Mining and Analysis
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 $P(Y|X)$.
- Example: regression problems, classification problems, etc..

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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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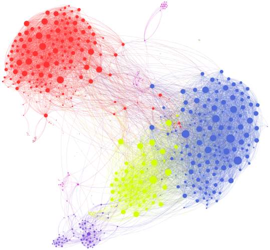
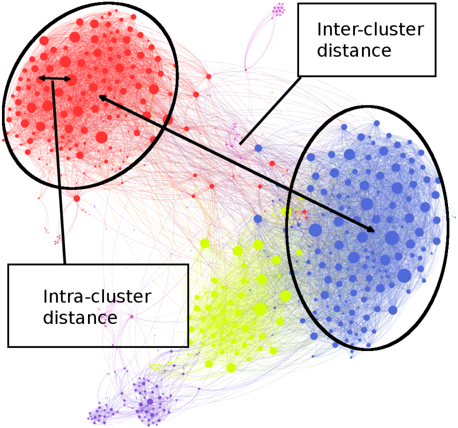


- Unsupervised problem.
- Work only with features/independent variables.
- Want to label points according to a measure of their similarity.

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.

- 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

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

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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- The above problem is NP hard.
- Efficient approximation algorithms exist (converge to a local minimum though).

Some equivalent formulations

- Note that

$$\frac{1}{2}\sum_{i=1}^{K}\sum_{x_j\in S_i}\sum_{x_k\in S_i}\|x_j-x_k\|^2=\sum_{i=1}^{K}|S_i|\sum_{x_j\in S_i}\|x_j-\mu_i\|^2$$

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- Other equivalent problem: solve

$$\operatorname*{argmin}_{(m_l)_{l=1}^K}\sum_{j=1}^{n}\min_{1\le i\le K}\|x_j-m_i\|^2,$$

and let $S_i:=\{x_j:\|x_j-m_i\|^2\le\|x_j-m_k\|^2\ \forall k=1,\ldots,K\}$.

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2. Compute the average $m_i^{(t+1)}$ of the observations in cluster i:
$$m_i^{(t+1)} := \frac{1}{|S_i^{(t)}|} \sum_{x_j \in S_i^{(t)}} x_j.$$

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3. $t \leftarrow t + 1$.

Until convergence.

Convergence of Lloyds's algorithm

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1. **The Forgy method:** Pick K observations at random from $\{x_1, \ldots, x_n\}$ 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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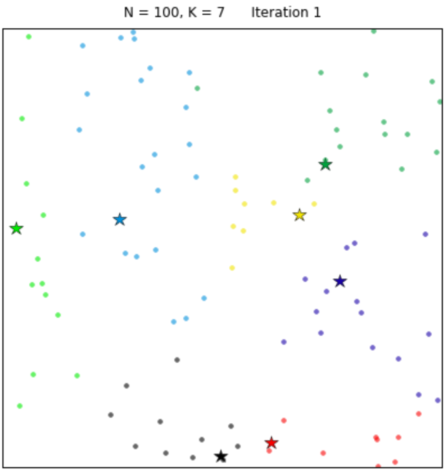

Source: https://datasciencelab.wordpress.com

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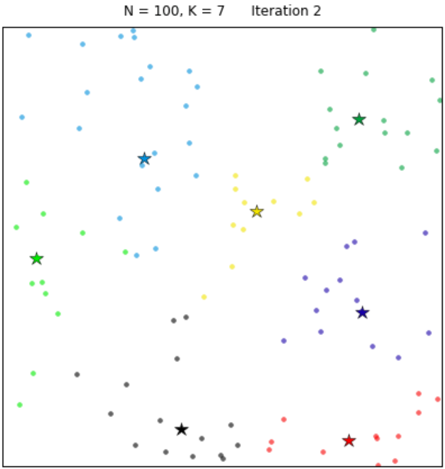

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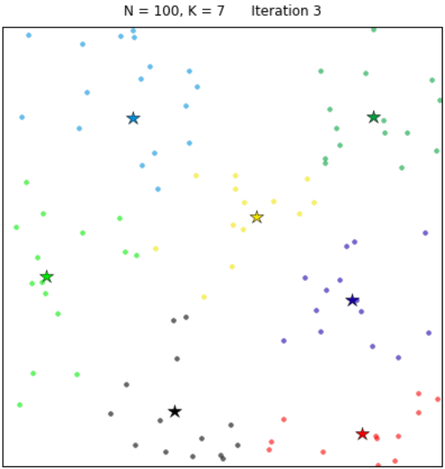

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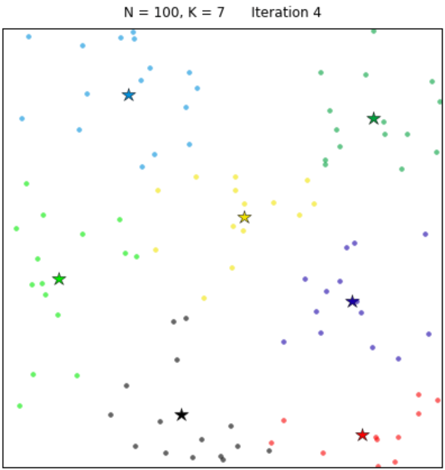

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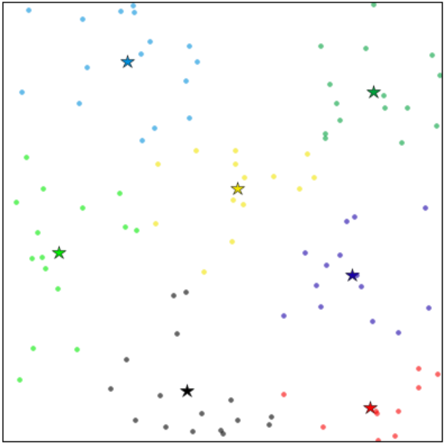
N = 100, K = 7 Iteration 5



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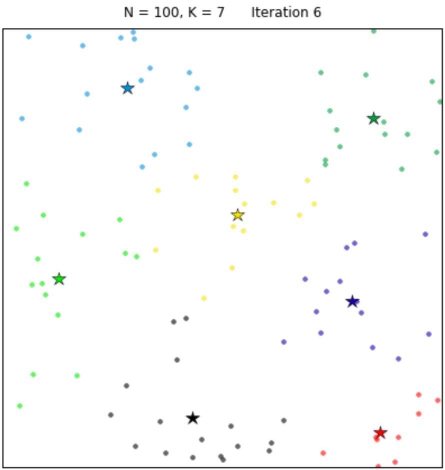

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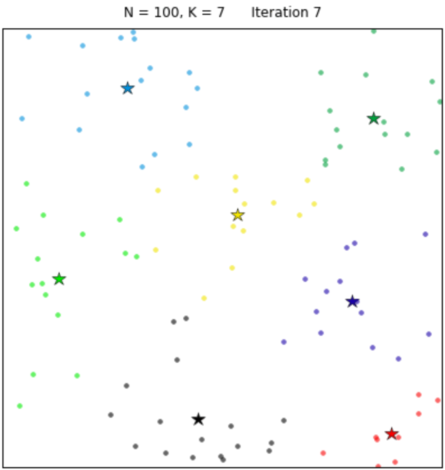

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- Let $\overline{A} = \overline{A}(k)$ satisfy

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Consistency of K-means (cont.)

Theorem:(Pollard, 1981)

Suppose:

- $\int \|x\|^2 \, dP(x) < \infty$ and
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- Pollard's theorem guarantees consistency under mild assumptions.
- Note however, that the theorem assumes that the clustering was obtain by **globally** minimizing the K-means objective function (not true in applications).

Example: clustering the zip data

Is there a nice cluster structure in the zip dataset?

```
# Load zip data
est = KMeans(n_clusters=10, verbose=1)  # Note: verbose=1 is just to
                                        # see what sklearn is doing...
est.fit(X_train)

Prop_mat = np.zeros((10,10))  # Percentage of label i that is digit j


for i in range(10):
    N_i = np.sum(est.labels_ == i) # Number of samples with label i
    for j in range(10):
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Prop_mat =

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