MATH 637: 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 $P(Y|X)$.
- Example: regression problems, classification problems, etc..

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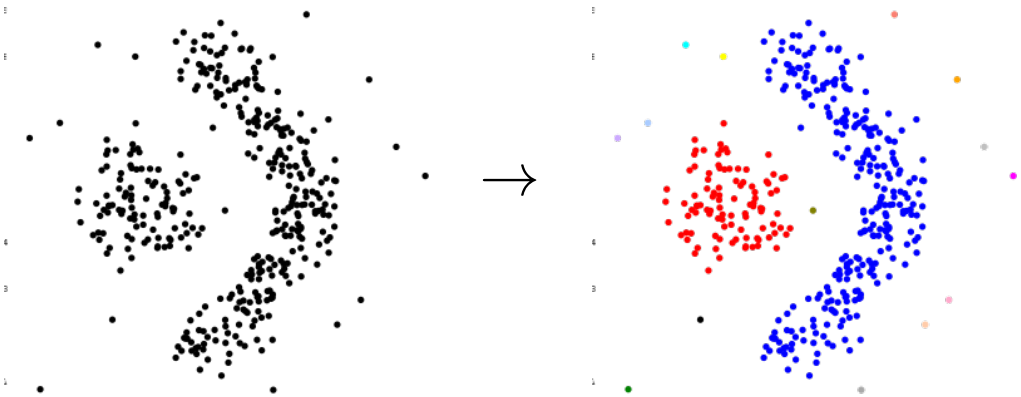
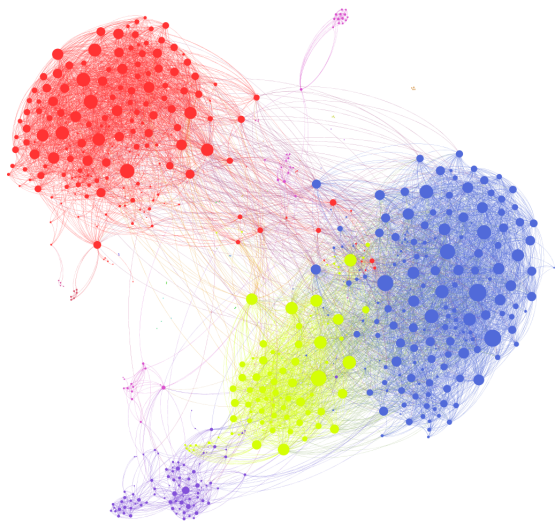
Unsupervised learning problems:

- 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.

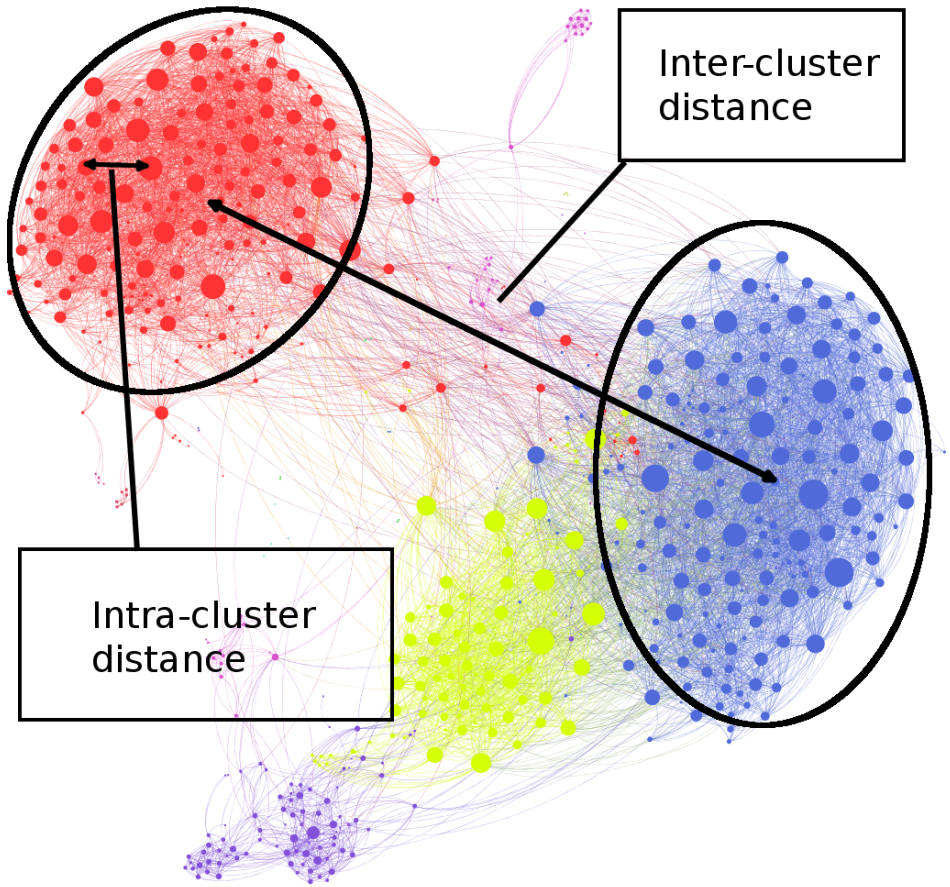


- Unsupervised problem.
- Work only with features/independent variables.
- Want to label points according to a measure of their similarity.

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

Some equivalent formulations

- For any $S \subset \{x_1, \ldots, x_n\}$,

$$\mu_S := \frac{1}{|S|} \sum_{x_i \in S} x_i = \operatorname*{argmin}_m \sum_{x_i \in S} \|x_i - m\|^2.$$

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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

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

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Common initialization methods:

1. **The Forgy method:** Pick K observations at random from $\{x_1, \ldots, x_n\}$ and use these as the initial means.

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Common initialization methods:

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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- 100 random points in $\mathbb{R}^2$.

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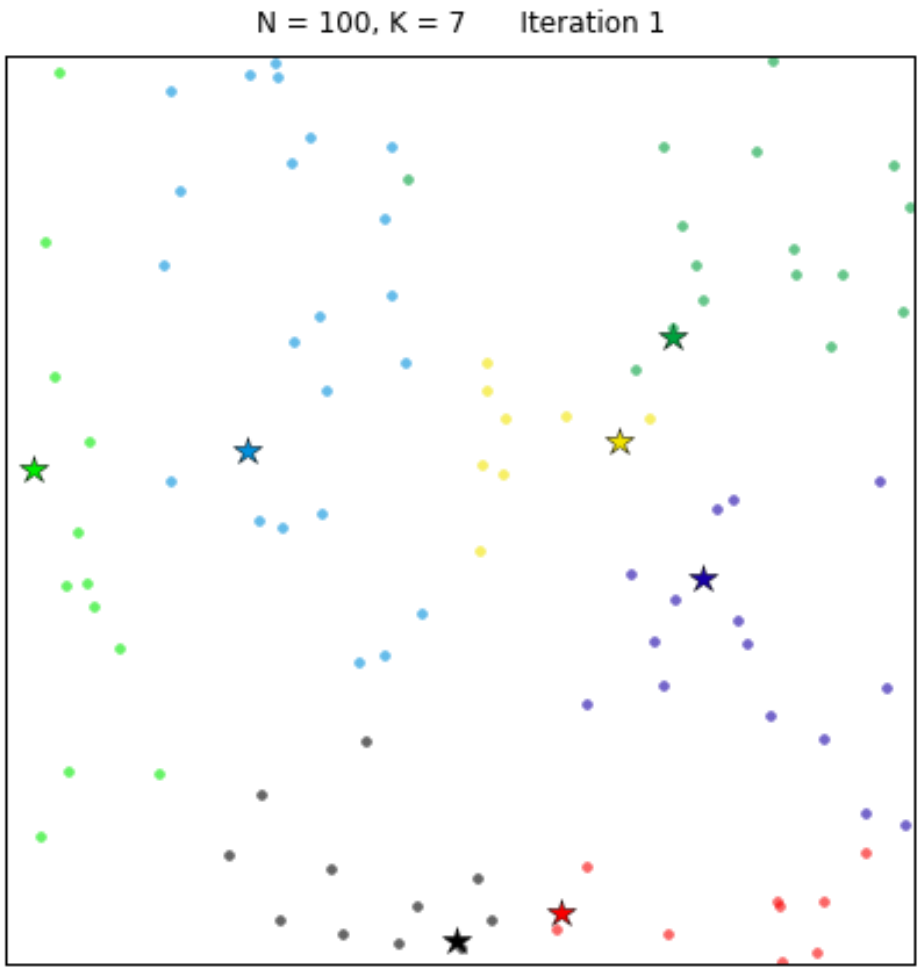

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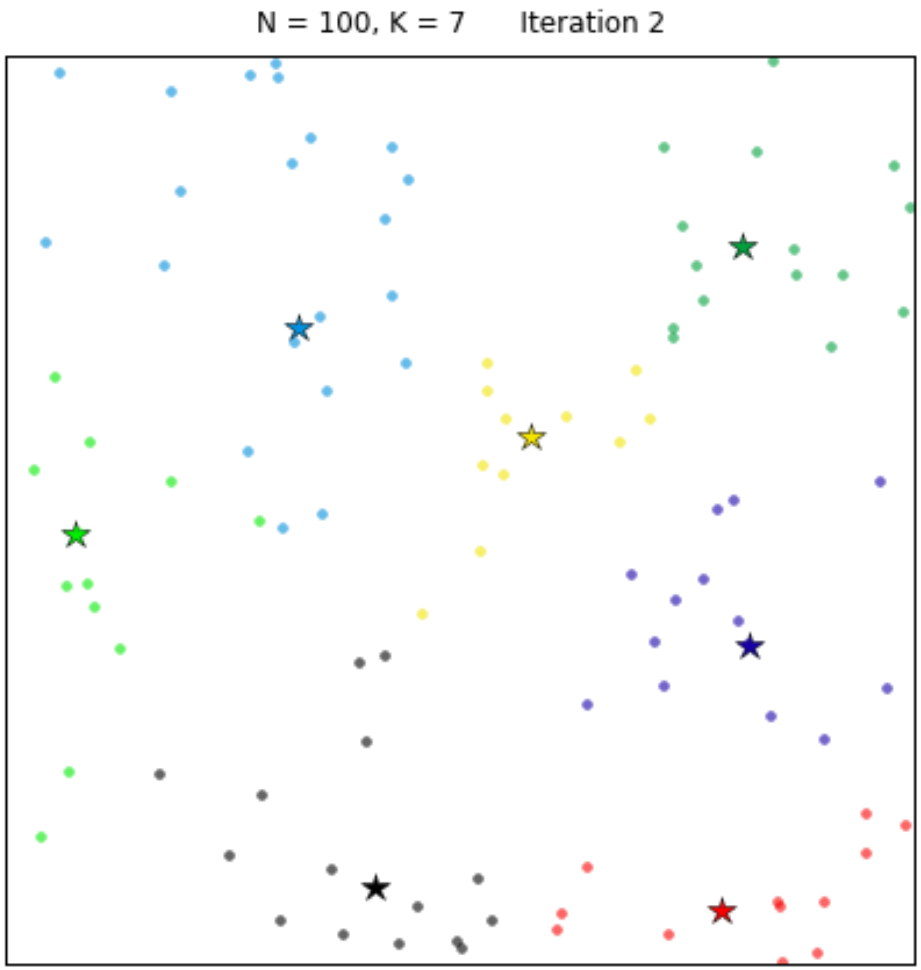

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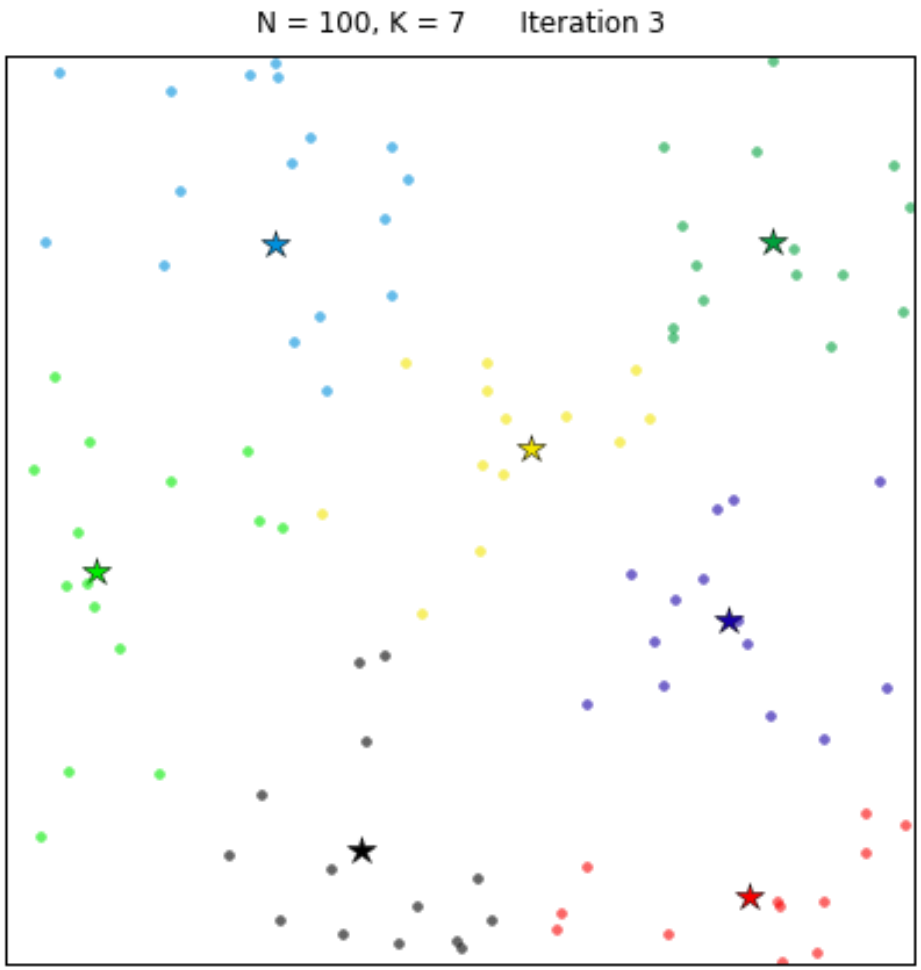

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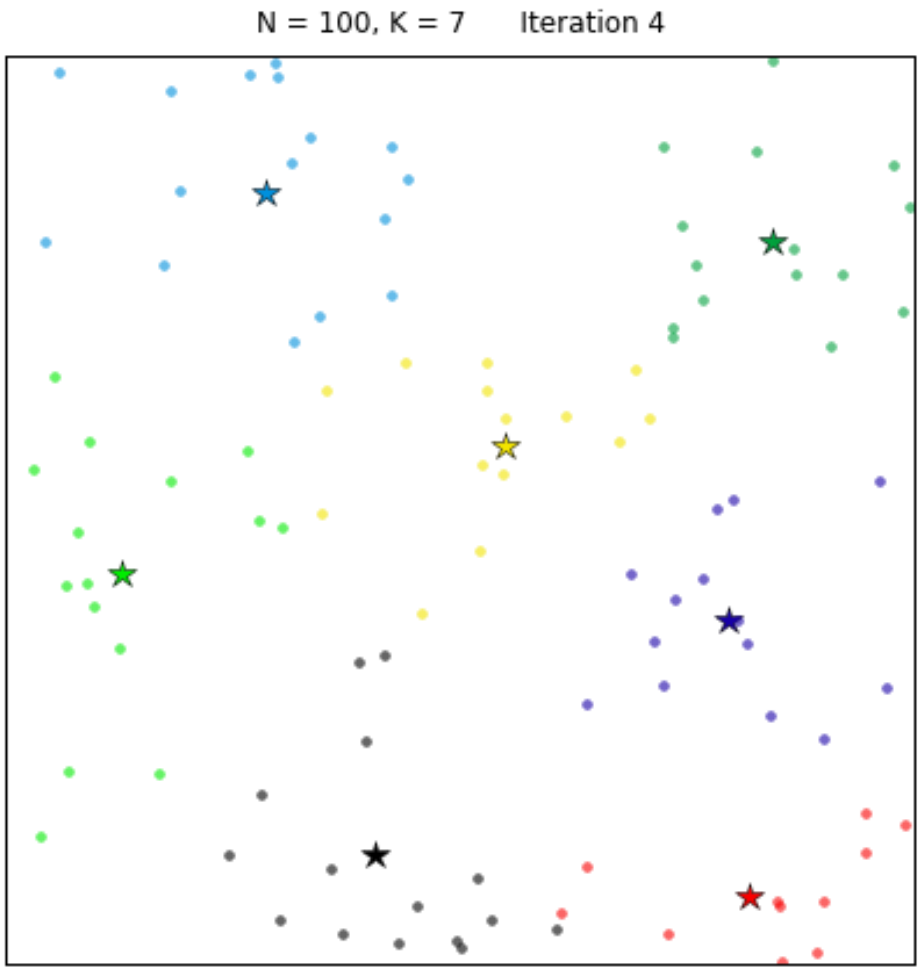

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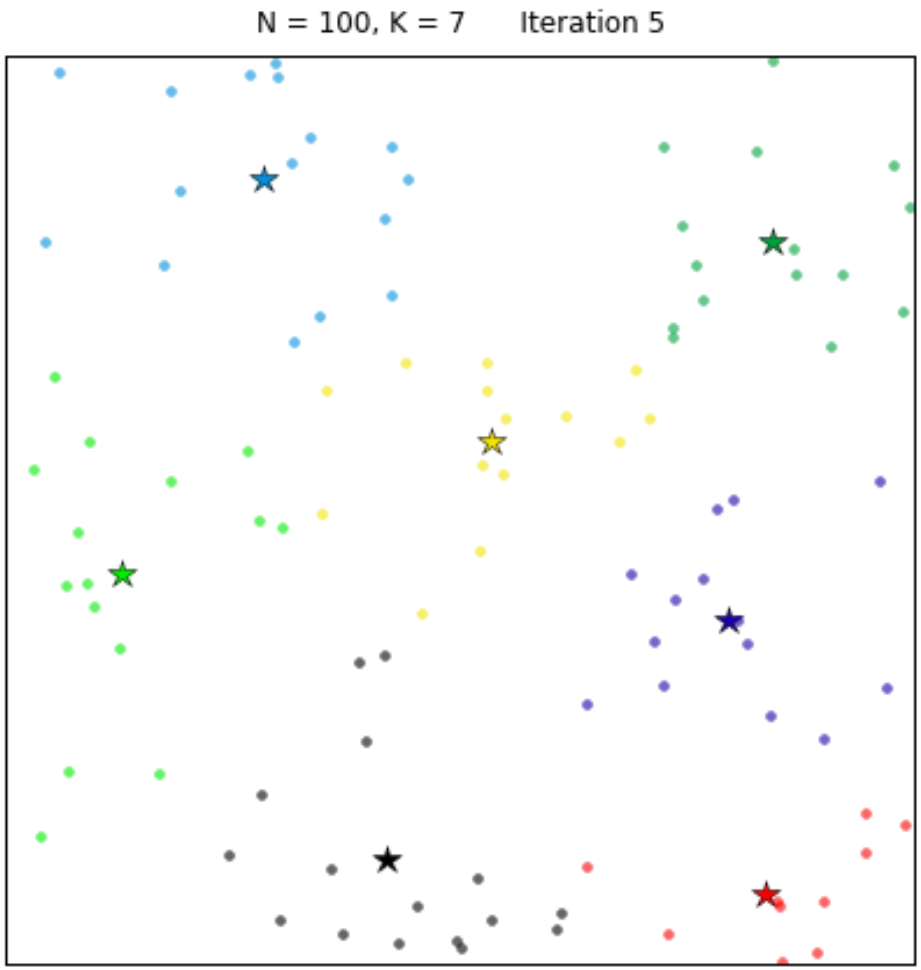

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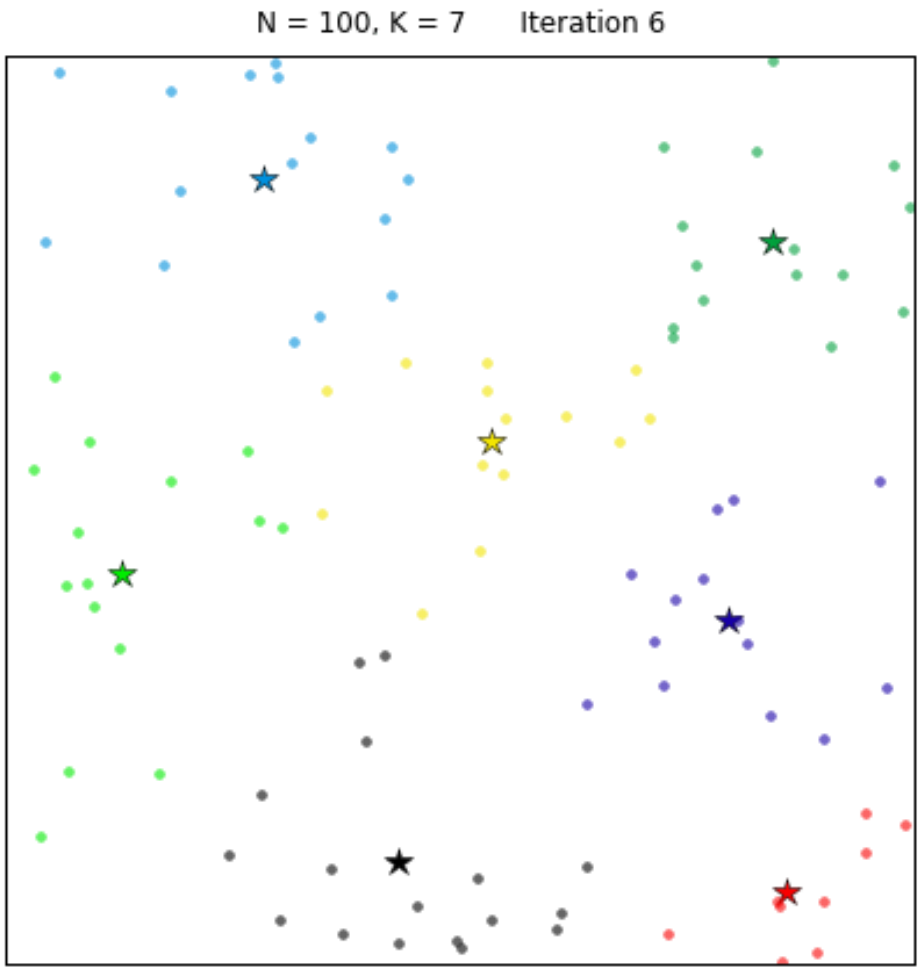

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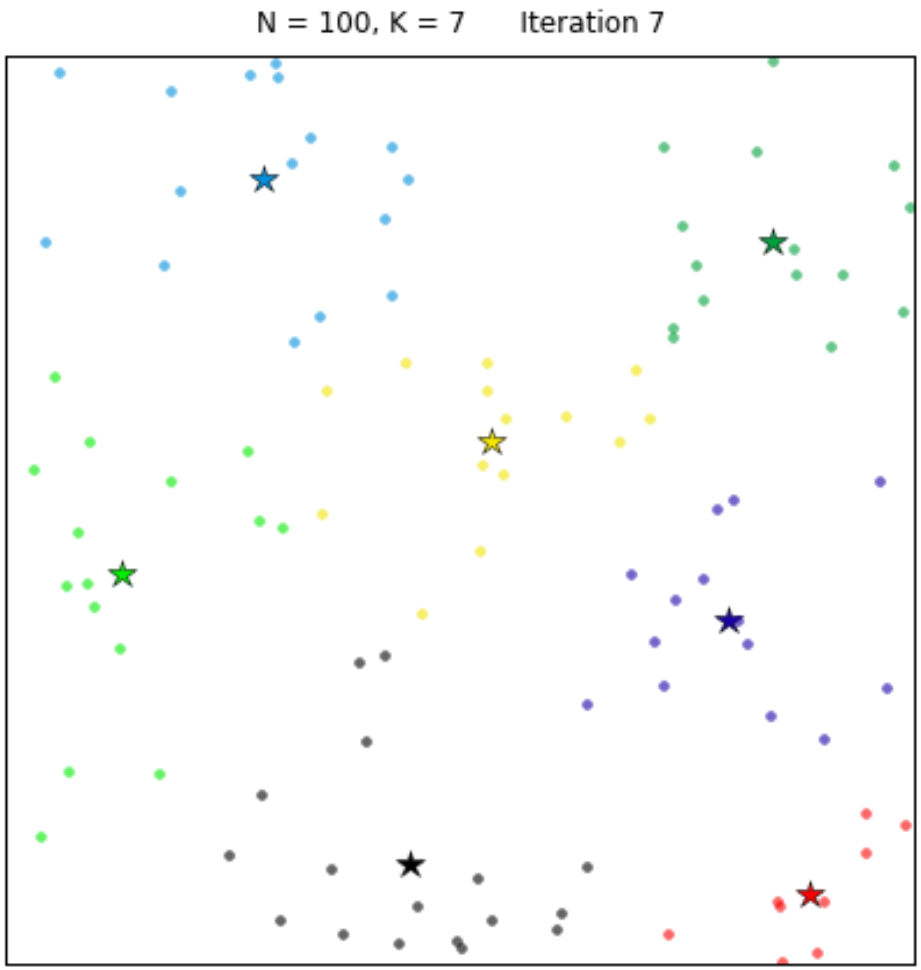

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Consistency of K-means

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- Assume $\{x_1, \ldots, x_n\} \subset \mathbb{R}^p$ are iid from a distribution P on $\mathbb{R}^p$.
- Let P_n denote the *empirical measure* for a sample of size n.
- For a given probability measure Q on $\mathbb{R}^p$, and any set $A \subset \mathbb{R}^p$, let

$$\Phi(A, Q) := \int \min_{a \in A} \|x - a\|^2 \, dQ(x),$$

and let

$$m_k(Q) := \inf\{\Phi(A, Q) : A \text{ contains } k \text{ or fewer points}\}.$$

- For a given k, the set $A_n = A_n(k)$ of optimal cluster centers is chosen to satisfy

$$\Phi(A_n, P_n) = m_k(P_n).$$

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

$$\Phi(\overline{A}, P) = m_k(P).$$

Consistency of K-means (cont.)

Theorem:(Pollard, 1981)

Suppose:

- $\int \|x\|^2 \, dP(x) < \infty$ and
- for $j = 1, 2, \ldots, k$ there is a unique set $\overline{A}(j)$ for which $\Phi(\overline{A}(j), P) = m_j(P)$.

Then $A_n \to \overline{A}(k)$ a.s. (in the Hausdorff distance), and $\Phi(A_n, P_n) \to m_k(P)$ a.s..

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

Spectral clustering: overview

We discussed 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.
- Can be used for various "types" of data (not only points in $\mathbb{R}^p$).
- Easy to implement. Only uses basic linear algebra.

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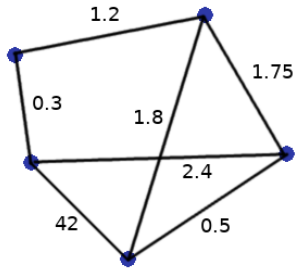
2. Use the similarity matrix to construct a (weighted or unweighted) graph.
3. Compute eigenvectors of the *graph Laplacian*.
4. Cluster the graph using the eigenvectors of the graph Laplacian using the K-means algorithm.

Notation

We will use the following notation/conventions:

- $G = (V, E)$ a graph with vertex set $V = \{v_1, \ldots, v_n\}$ and edge set $E \subset V \times V$.
- Each edge carries a *weight* $w_{ij} \geq 0$.



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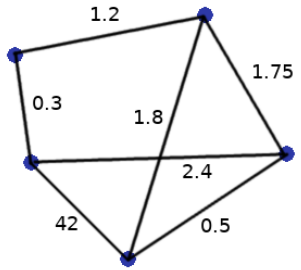

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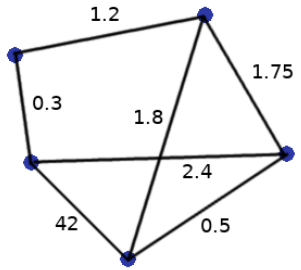

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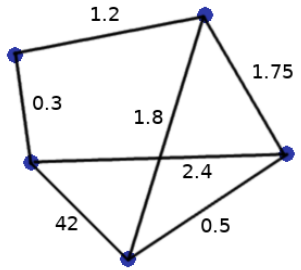

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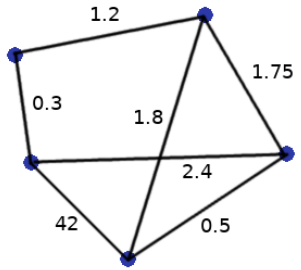

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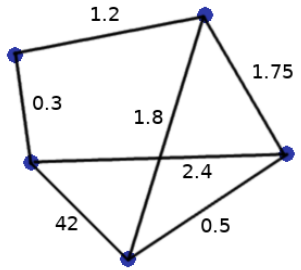

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- If $A \subset V$, then we let $\mathbb{1}_A = (f_1, \ldots, f_n)^T \in \mathbb{R}^n$, where $f_i = 1$ if $v_i \in A$ and 0 otherwise.

Similarity graphs

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

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All graphs mentioned above are regularly used in spectral clustering.

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Proof: To prove (1),

$$\begin{aligned} f^T L f = f^T D f - f^T W f &= \sum_{i=1}^{n} d_i f_i^2 - \sum_{i,j=1}^{n} w_{ij} f_i f_j \\ &= \frac{1}{2}\left(\sum_{i=1}^{n} d_i f_i^2 - 2 \sum_{i,j=1}^{n} w_{ij} f_i f_j + \sum_{j=1}^{n} d_j f_j^2 \right) \\ &= \frac{1}{2} \sum_{i,j=1}^{n} w_{ij}(f_i - f_j)^2. \end{aligned}$$

(2) follows from (1). (3) is easy. □

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Proof: If f is an eigenvector associated to $\lambda = 0$, then

$$0 = f^T L f = \sum_{i,j=1}^{n} w_{ij}(f_i - f_j)^2.$$

It follows that $f_i = f_j$ whenever $w_{ij} > 0$. Thus f is constant on the connected components of G. We conclude that the eigenspace of 0 is contained in $\mathrm{span}(\mathbb{1}_{A_1}, \ldots, \mathbb{1}_{A_k})$. Conversely, it is not hard to see that each $\mathbb{1}_{A_i}$ is an eigenvector associated to 0 (write L in block diagonal form). □

The normalized Laplacians

Proposition: The normalized Laplacians satisfy the following properties:

1. For every $f \in \mathbb{R}^n$, we have

$$f^T L_{\mathrm{sym}} f = \frac{1}{2} \sum_{i,j=1}^{n} w_{ij} \left(\frac{f_i}{\sqrt{d_i}} - \frac{f_j}{\sqrt{d_j}} \right)^2 .$$

2. λ is an eigenvalue of L_{rw} with eigenvector u if and only if λ is an eigenvalue of L_{sym} with eigenvector $w = D^{1/2} u$.
3. λ is an eigenvalue of L_{rw} with eigenvector u if and only if λ and u solve the generalized eigenproblem $Lu = \lambda D u$.

Proof: The proof of (1) is similar to the proof of the analogous result for the unnormalized Laplacian. (2) and (3) follow easily by using appropriate rescalings.

The normalized Laplacians (cont.)

Proposition: Let G be an undirected graph with non-negative weights. Then:

1. The multiplicity k of the eigenvalue 0 of both L_{sym} and L_{rw} equals the number of connected components $A_1, \ldots, A_k$ in the graph.
2. For L_{rw}, the eigenspace of eigenvalue 0 is spanned by the indicator vectors $\mathbb{1}_{A_i}$, $i = 1, \ldots, k$.
3. For L_{sym}, the eigenspace of eigenvalue 0 is spanned by the vectors $D^{1/2}\mathbb{1}_{A_i}$, $i = 1, \ldots, k$.

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