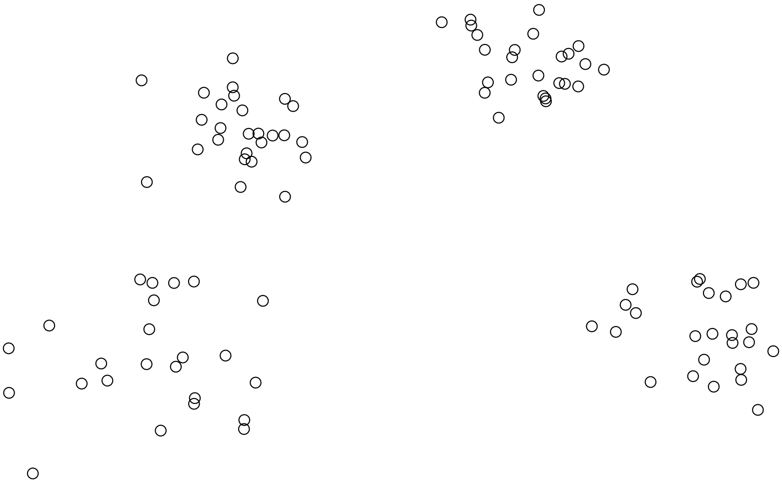
Mini lecture

k-means clustering

Arthur Van Camp

Monday 15 May 2023

Introduction



Course information: arthurvancamp.github.io/mini-lecture

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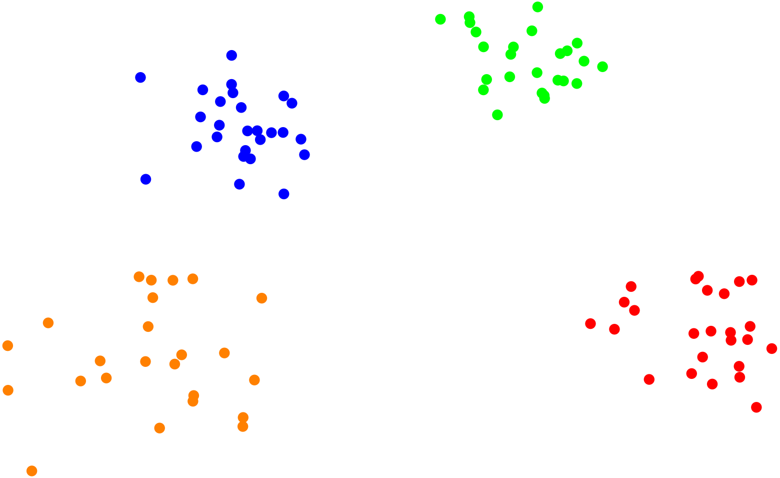

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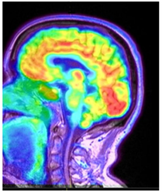
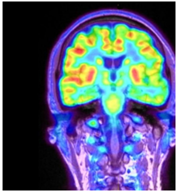
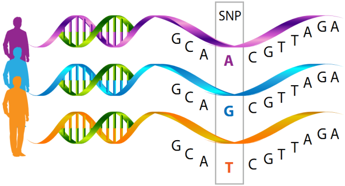
Clustering is widely used

- Social networks
- (Medical) imaging
- Market analysis
- Chemistry
- Gene sequencing

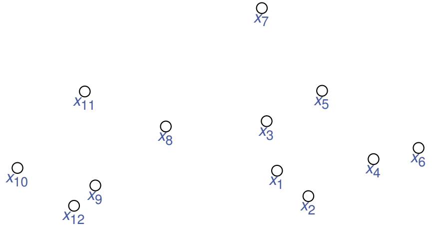




Clustering

Given: $x_1, \ldots, x_n$ vectors,
and k: number of clusters, with $n \gg k$.

Required: Partition $\{x_1, \ldots, x_n\}$ into $\{C_1, \ldots, C_k\}$
such that each group (cluster) C_ℓ contains vectors
that are close to each other.

$\{C_1, \ldots, C_k\}$ is a **partition** of $\{x_1, \ldots, x_n\}$ if
$C_1 \cup C_2 \cup \cdots \cup C_k = \{x_1, \ldots, x_n\}$ and
$C_i \cap C_j = \emptyset$ for all $i \neq j$.



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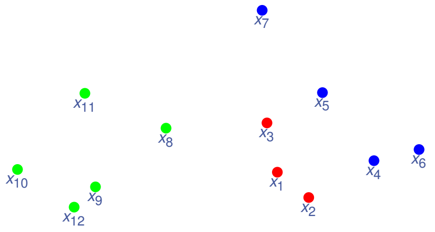

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We will study k-means clustering.

k-means clustering

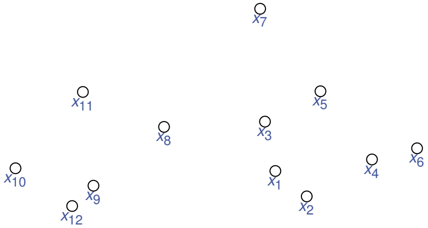
Idea: Find a partition $\{C_1, \ldots, C_k\}$ such that

$$\sum_{\ell=1}^{k} \frac{1}{|C_\ell|} \sum_{x,y \in C_\ell} \|x - y\|^2$$

is as small as possible.

$\|\bullet\|$ is the **Euclidean norm**: $\|x\| = \sqrt{\sum_{i=1}^{d} x_i^2}$.

Exercise 1: Why is there a factor $\frac{1}{|C_\ell|}$?



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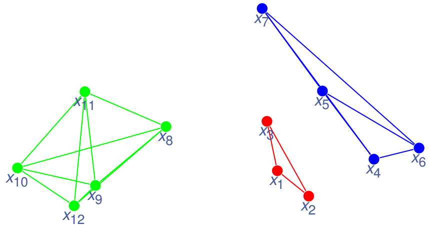

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A useful alternative expression

Find a partition $\{C_1, \ldots, C_k\}$ that minimises $\sum_{\ell=1}^{k} \frac{1}{|C_\ell|} \sum_{x,y \in C_\ell} \|x - y\|^2$.

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Define $\mu_\ell = \sum_{x \in C_\ell} \frac{x}{|C_\ell|}$, the centroid of cluster C_ℓ. Then the same $\{C_1, \ldots, C_k\}$ minimises

$$\sum_{\ell=1}^{k} \sum_{x \in C_\ell} \|x - \mu_\ell\|^2.$$

(Exercise 2)

However, finding a partition that minimises $\sum_{\ell=1}^{k} \sum_{x \in C_\ell} \|x - \mu_\ell\|^2$ is NP-hard.

Exercise 2: solution

Compare

$$\sum_{x,y\in C_\ell} \|x-y\|^2 = \sum_{x,y\in C_\ell} \left(\|x\|^2 + \|y\|^2 - 2\langle x,y\rangle\right)$$

$$= 2|C_\ell| \sum_{x\in C_\ell} \|x\|^2 - 2\sum_{x,y\in C_\ell} \langle x,y\rangle = 2|C_\ell| \sum_{x\in C_\ell} \|x\|^2 - 2\sum_{x\in C_\ell} \langle x,\mu_\ell\rangle |C_\ell| = 2|C_\ell| \Big(\sum_{x\in C_\ell} \|x\|^2\Big) - 2|C_\ell|^2 \|\mu_\ell\|^2$$

with

$$\sum_{x\in C_\ell} \|x-\mu_\ell\|^2 = \sum_{x\in C_\ell} \left(\|x\|^2 + \|\mu_\ell\|^2 - 2\langle x,\mu_\ell\rangle\right)$$

$$= \sum_{x\in C_\ell} \|x\|^2 + |C_\ell| \|\mu_\ell\|^2 - 2\sum_{x\in C_\ell} \langle x,\mu_\ell\rangle = 2\sum_{x\in C_\ell} \|x\|^2 + |C_\ell|\|\mu_\ell\|^2 - 2|C_\ell|\|\mu_\ell\|^2 = \Big(\sum_{x\in C_\ell} \|x\|^2\Big) - |C_\ell|\|\mu_\ell\|^2$$

to infer that $\sum_{x\in C_\ell} \|x-\mu_\ell\|^2 = \frac{1}{2|C_\ell|} \sum_{x,y\in C_\ell} \|x-y\|^2$. Therefore minimising $\sum_{\ell=1}^{k} \sum_{x\in C_\ell} \|x-\mu_\ell\|^2$ is tantamount to minimising $\sum_{\ell=1}^{k} \frac{1}{|C_\ell|} \sum_{x,y\in C_\ell} \|x-y\|^2$, as the former is a factor 2 larger than the latter.

A heuristic: Lloyd's algorithm

Reformulation: Find a partition $\{C_1, \ldots, C_k\}$ such that

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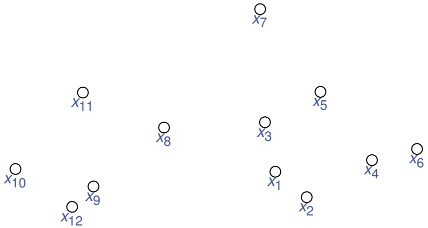

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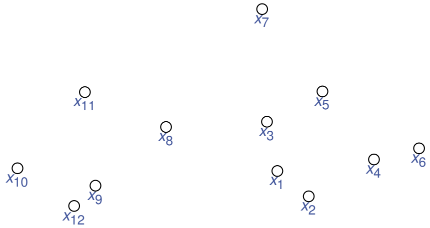
Step 1: Choose k points (centroids) $\mu_1, \ldots, \mu_k$ from $\{x_1, \ldots, x_n\}$.



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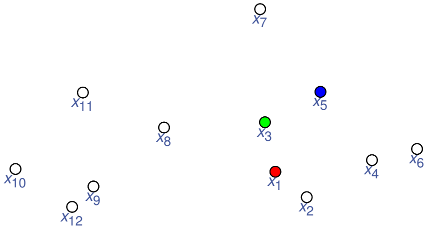

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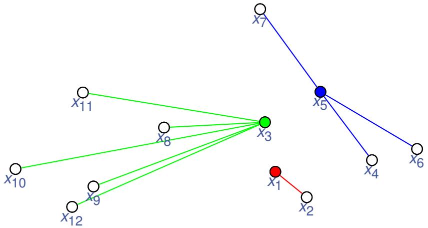
Step 2: While centroids are not stable:

a. Define clusters: add x_i to cluster C_ℓ if μ_ℓ is the centroid closest to x_i.

b. Update μ_ℓ by computing the new centroid of C_ℓ.



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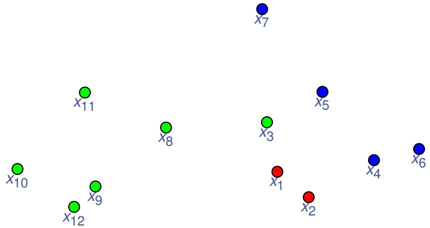

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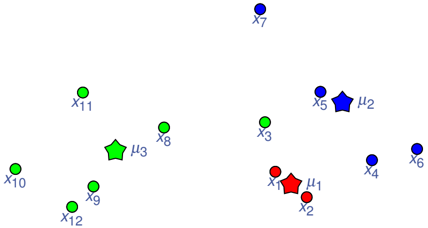

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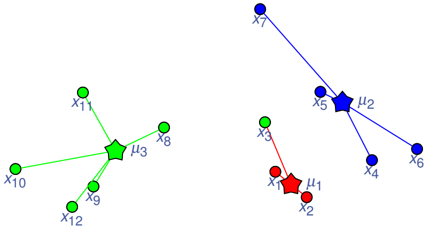

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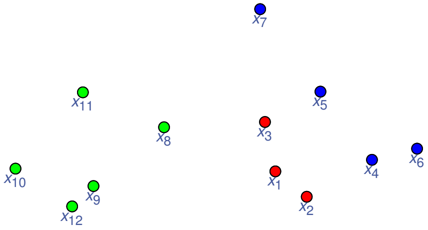

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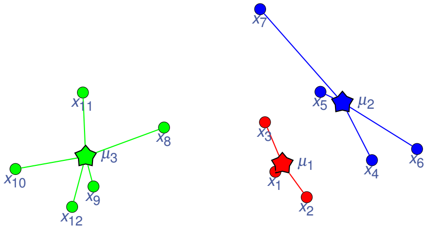

Exercise 3: Implement Lloyd's algorithm

Implement Lloyd's algorithm in Python in two dimensions ($d = 2$).

Given an input `X` of the form `X=[X[0], X[1], ..., X[n]]` and a `k`, implement Lloyd's algorithm.

Create some data sets to test your implementation on.

See arthurvancamp.github.io/mini-lecture/k-means.py