

Computational Tools for Data Science

Week 6: Clustering

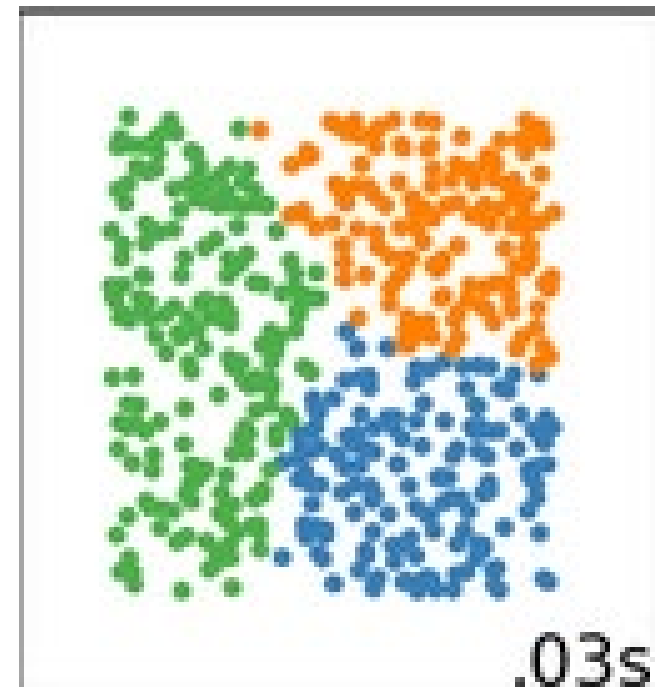
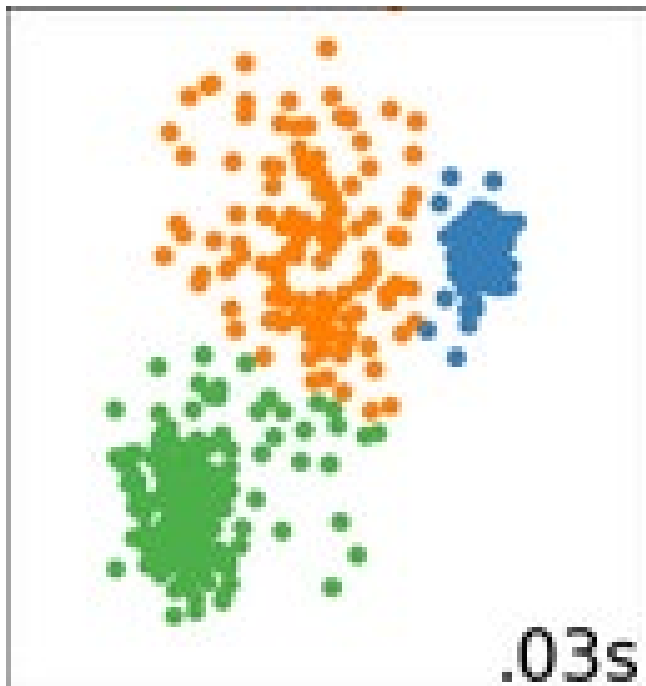
Motivation: Clustering

- **What is it:** Task of **grouping** objects s.t. objects of the same group are more “similar” to each other than objects from different ones. The groups are called “**clusters**”. In general they may overlap.
- **For which data:** numerical, usually a lot of data and high-dimensional
- **Usually:**
 - Objects are points (or vectors) in a high-dimensional (vector) space.
 - “Similarity” is defined via some distance measure, e.g.:
 - » vectors: Euclidean distance, Cosine
 - » Jaccard similarity (for sets), edit distance (strings)

Reminder: Distance

- **Definition (distance d):** Let V be a (top.) space. A map $d: V \times V \rightarrow \mathbb{R}$ is called a *distance* if the following properties hold:
 - 1) For all $u, v \in V$: $d(u, v) \geq 0$ and $d(u, v) = 0$ iff $u = v$.
 - 2) For all $u, v \in V$: $d(u, v) = d(v, u)$
 - 3) For all $u, v, w \in V$: $d(u, v) + d(v, w) \geq d(u, w)$. [Triangular inequality]

Motivation: Clustering



Motivation: Clustering

Examples:

- In general: categorisation, classification and segmentation
 - » But also: finding anomalies, recognition
- Clustering stellar objects (clusters of stars)
- Group people by interest in social media (via #s, followers, topics)
- Group people / customer by consumed goods (e.g. music, movies, food)
- Find categories for goods by customers who bought them
- Identify topics for documents via shared words

Motivation: Clustering

Example: Categorise goods, say **movies**, via some set $\mathcal{C}$ of customers

- Represent each movie as $|\mathcal{C}|$ dimensional 0-1 vector, one dimension per customer from $\mathcal{C}$.
- An entry / component in this vector is 1 iff the corresponding customer has watched / purchased the movie.
- → This yields thousands or even millions of dimensions (e.g. Amazon)
- Idea behind: Taste in movies causes us to buy / watch similar movies.

Hierarchical Clustering

A) Agglomerative (bottom up):

1. Initialise each data point as a (singleton) cluster.
2. Repeatedly combine two “most similar / closest” clusters to a new one.
3. Stop w.r.t. certain criterion (e.g. # of clusters, density of clusters, ...)

Hierarchical Clustering

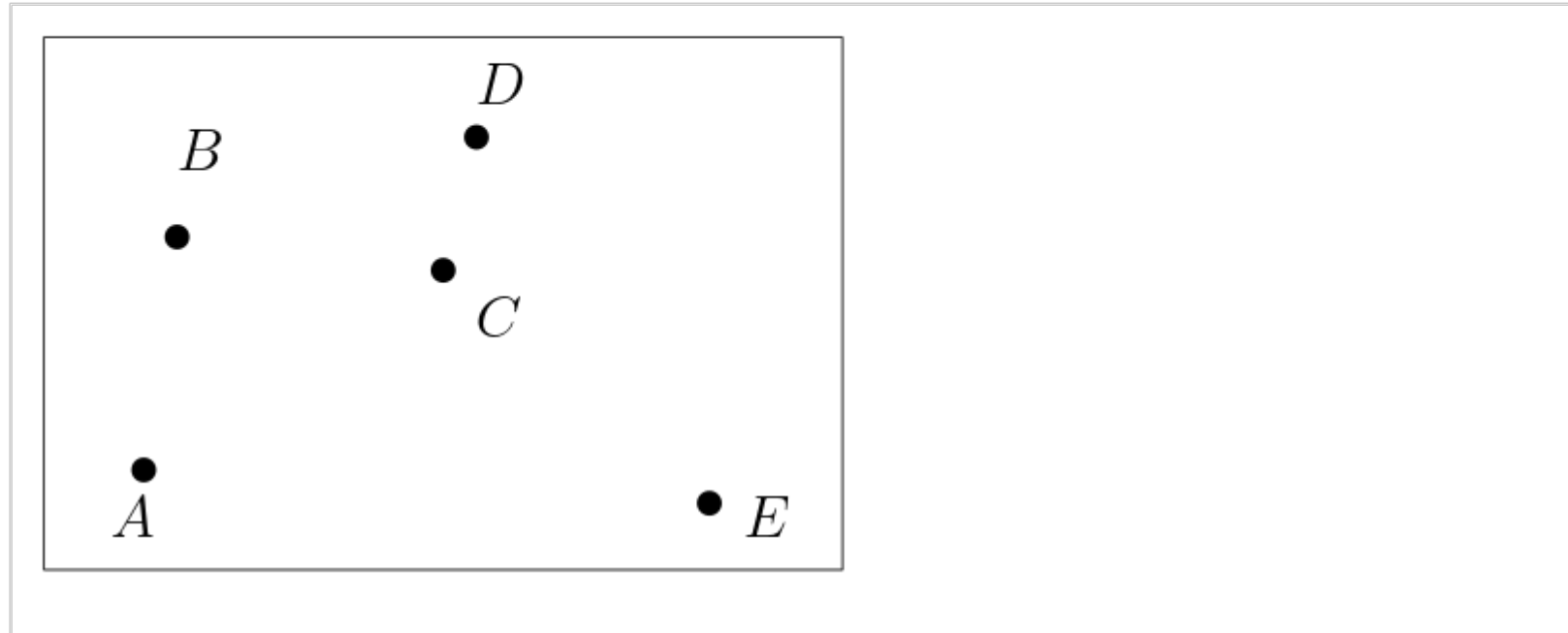
A) Agglomerative (bottom up):

1. Initialise each data point as a (singleton) cluster.
2. Repeatedly combine two “most similar / closest” clusters to a new one.
3. Stop w.r.t. certain criterion (e.g. # of clusters, density of clusters, ...)

B) Divisive (top down):

1. Initialise the whole data set as one big cluster.
2. Recursively split up cluster which is least “dense / connected”.
3. Stop w.r.t. certain criterion (e.g. # of clusters, density of clusters, ...)

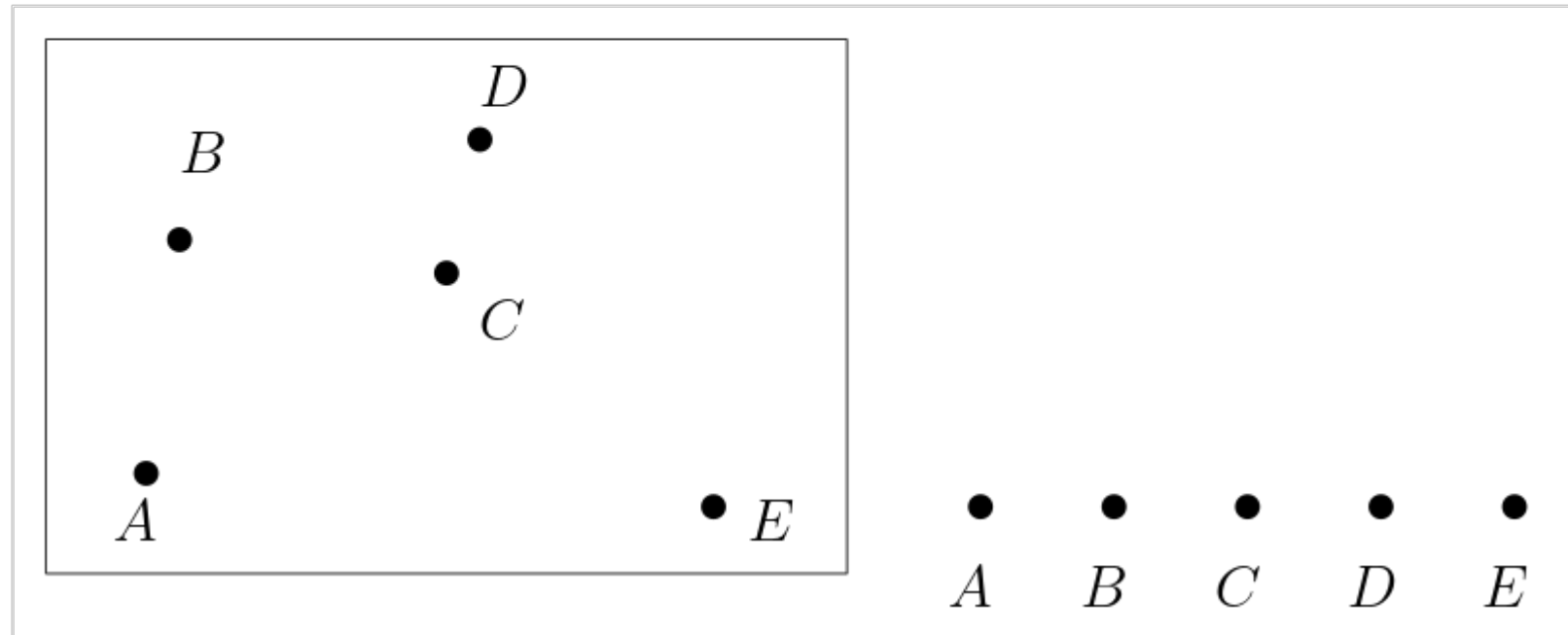
Small example



Resulting **tree structure** called ***dendrogram***.

Use case: E.g. in **phylogenetics** with no huge data (**phylogenetic tree**)

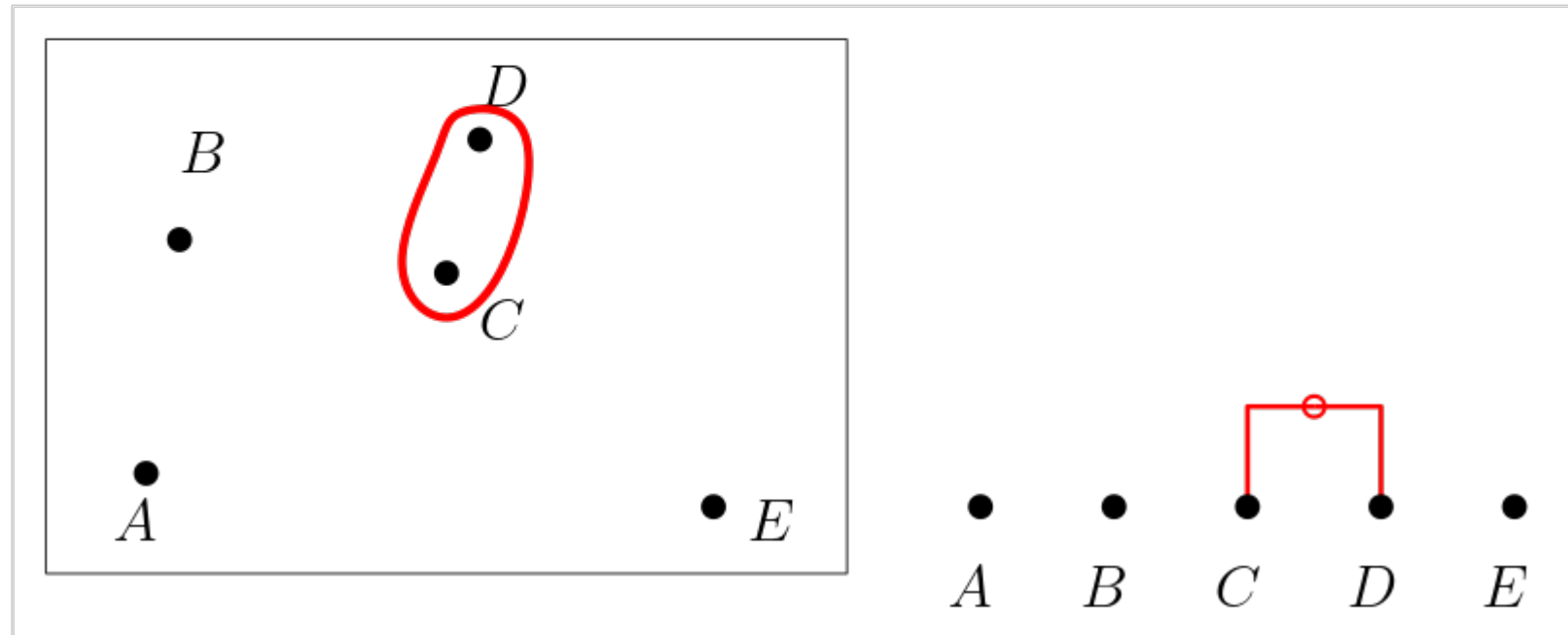
Small example



Resulting **tree structure** called ***dendrogram***.

Use case: E.g. in **phylogenetics** with no huge data (**phylogenetic tree**)

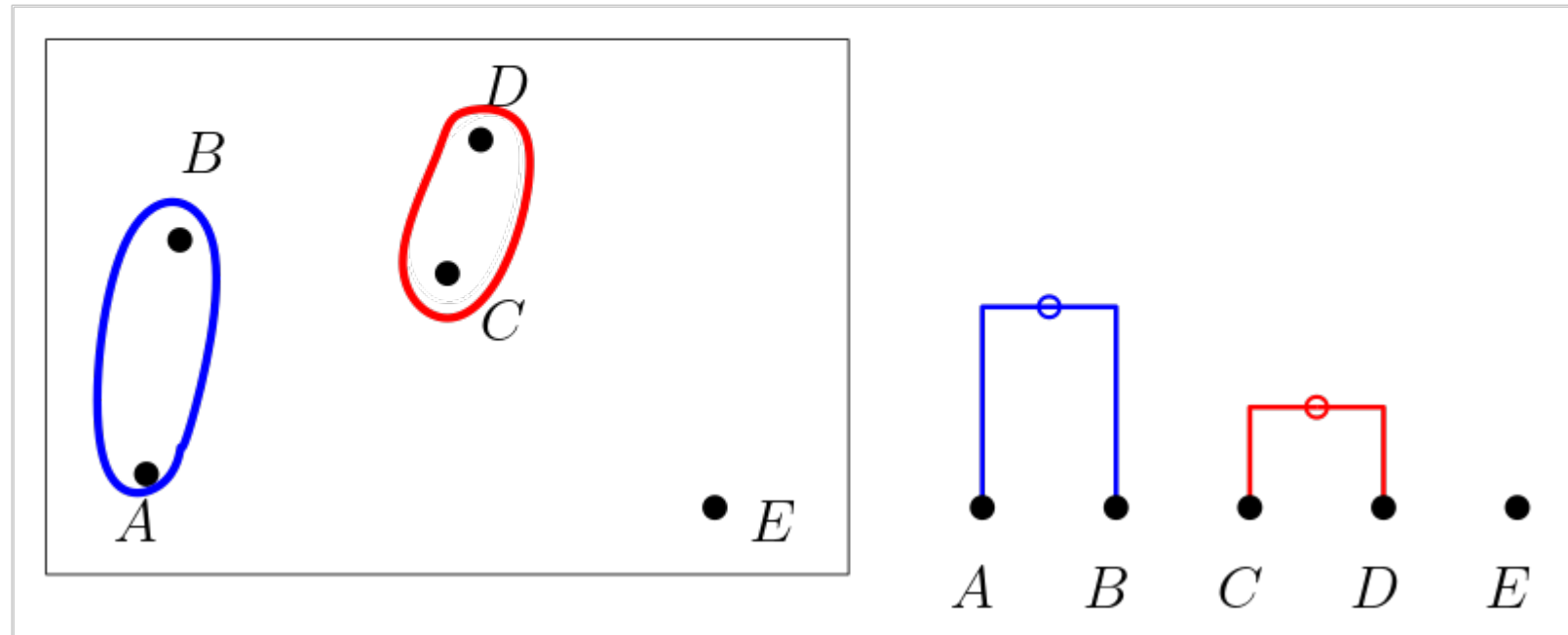
Small example



Resulting **tree structure** called ***dendrogram***.

Use case: E.g. in **phylogenetics** with no huge data (**phylogenetic tree**)

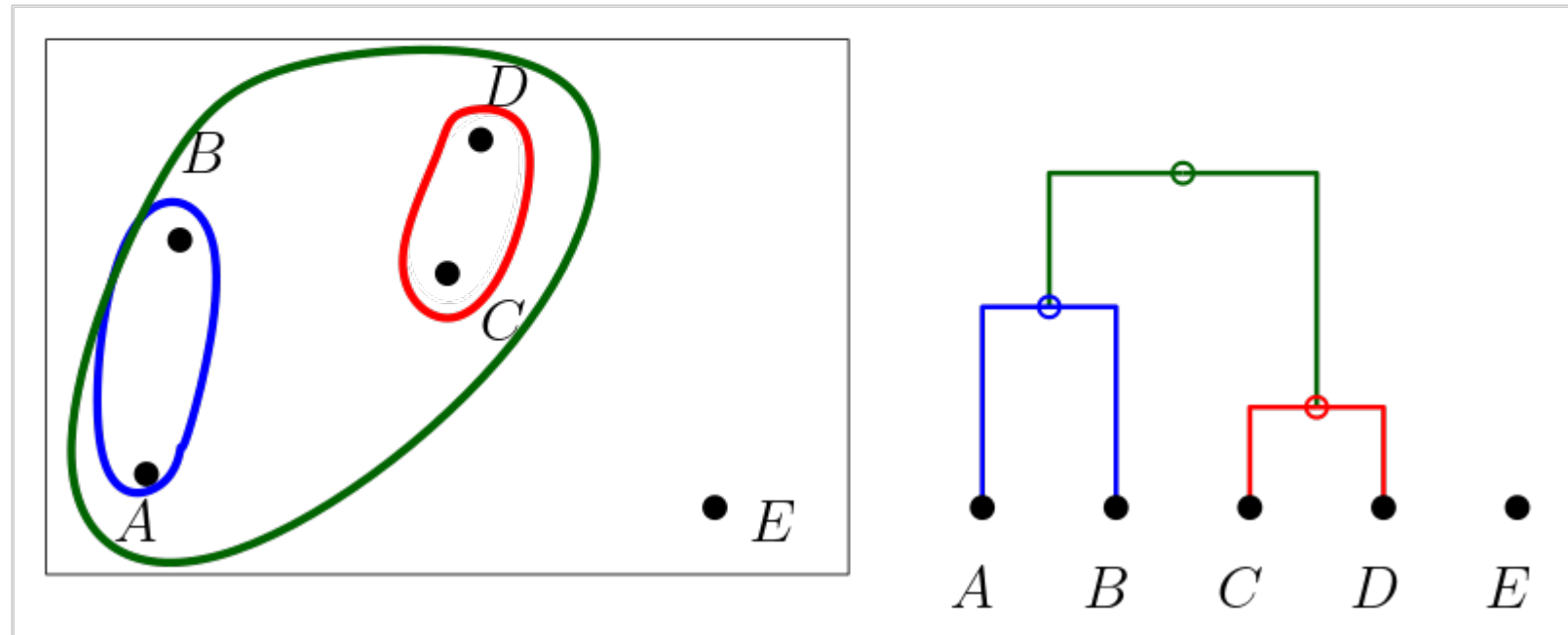
Small example



Resulting **tree structure** called ***dendrogram***.

Use case: E.g. in **phylogenetics** with no huge data (**phylogenetic tree**)

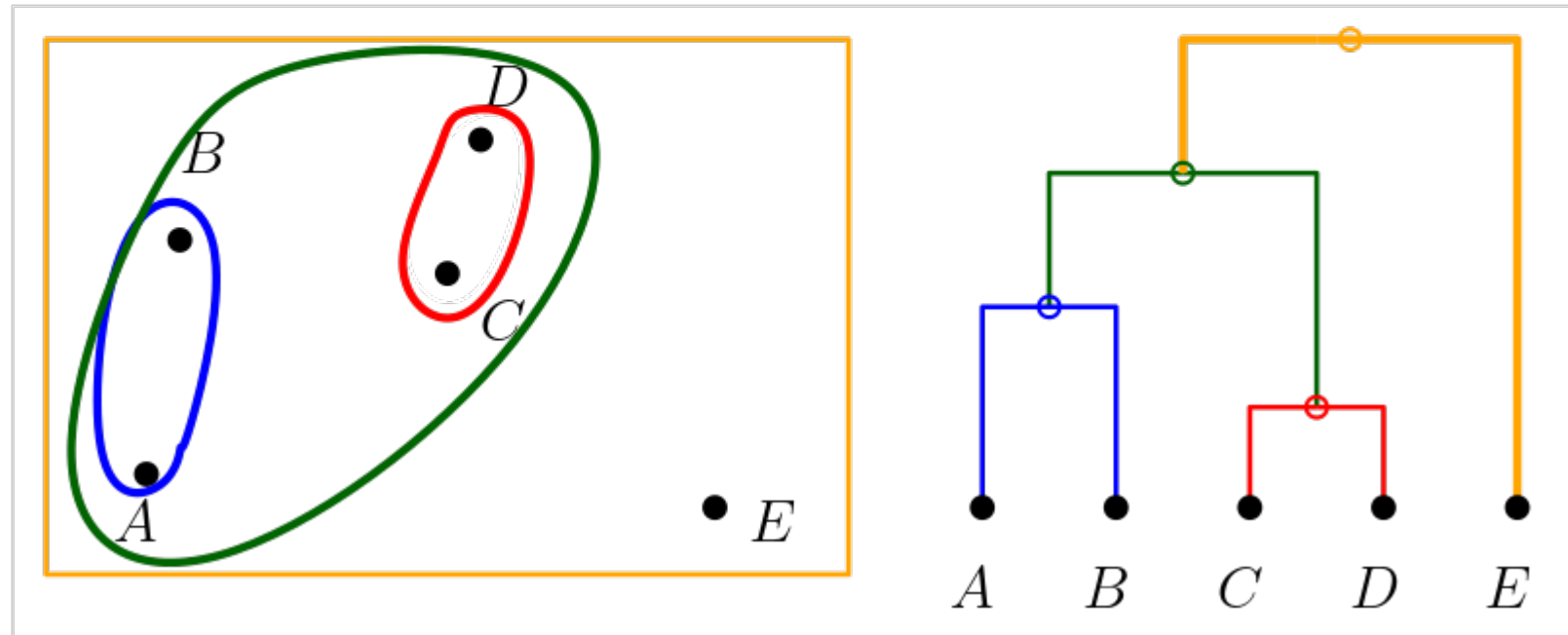
Small example



Resulting **tree structure** called ***dendrogram***.

Use case: E.g. in **phylogenetics** with no huge data (**phylogenetic tree**)

Small example



Resulting **tree structure** called ***dendrogram***.

Use case: E.g. in **phylogenetics** with no huge data (**phylogenetic tree**)

(Hierarchical) Clustering

3 important questions to answer:

- a) How do we represent clusters?
- b) How do we determine “similarity / closeness” of clusters?
- c) When do we stop the algorithm?

Representation of clusters

Euclidean case:

Let C be a cluster of n many d -dimensional data points, say in $\mathbb{R}^d$. We define the **centroid** $cent(C)$ of C as follows:

$$cent(C) = \frac{1}{n} \sum_{c \in C} c$$

Think of **centroid** as a **centre of gravity**.

Representation of clusters

Non-Euclidean case:

Let C be a cluster of n many data points.

Define the **clustroid** $clust(C)$ of C as a data point (from C) that is “closest” to the other points in C .

Some possible meanings of “closest”:

Representation of clusters

Non-Euclidean case:

Let C be a cluster of n many data points.

Define the **clustroid** $clust(C)$ of C as a data point (from C) that is “closest” to the other points in C .

Some possible meanings of “closest”:

- Smallest maximum distance to other points in C . $\rightarrow \min_{c \in C} \max_{v \in C} d(c, v)$

Representation of clusters

Non-Euclidean case:

Let C be a cluster of n many data points.

Define the **clustroid** $clust(C)$ of C as a data point (from C) that is “closest” to the other points in C .

Some possible meanings of “closest”:

- Smallest maximum distance to other points in C . $\rightarrow \min_{c \in C} \max_{v \in C} d(c, v)$
- Smallest average distance to other points in C . $\rightarrow \min_{c \in C} \frac{1}{n} \sum_{v \in C} d(c, v)$

Representation of clusters

Non-Euclidean case:

Let C be a cluster of n many data points.

Define the **clustroid** $clust(C)$ of C as a data point (from C) that is “closest” to the other points in C .

Some possible meanings of “closest”:

- Smallest maximum distance to other points in C . $\rightarrow \min_{c \in C} \max_{v \in C} d(c, v)$
- Smallest average distance to other points in C . $\rightarrow \min_{c \in C} \frac{1}{n} \sum_{v \in C} d(c, v)$
- Smallest sum of squared distances to other points in C .

$$\rightarrow \min_{c \in C} \sum_{v \in C} d^2(c, v)$$

Similarity / closeness of clusters

Idea: Replace each cluster by its centroid (Euclidean) or clustroid (Non-Euclidean).

Measure distance of two clusters C and C' to each other by:

Euclidean setting: $d(\text{cent}(C), \text{cent}(C'))$

Non-Euclidean setting: $d(\text{clust}(C), \text{clust}(C'))$

Similarity / closeness of clusters

Other ways to measure:

- Define distance between two clusters C and C' as the minimum distance between **any** data **point from** C and **any** data **point in** C' .
- Set a notion of “**cohesion**” (or connectivity, density, ...)
 - Merge two cluster whose union is most cohesive.

Similarity / closeness of clusters

Set a notion of “**cohesion**” (or connectivity, density, ...)

→ Merge two cluster whose union is most cohesive.

Possible notions of “cohesion”:

A) Minimum **diameter**

For a cluster C define its diameter $diam(C)$ as:

$$diam(C) = \max_{c, c' \in C} d(c, c')$$

Similarity / closeness of clusters

Set a notion of “**cohesion**” (or connectivity, density, ...)

→ Merge two cluster whose union is most cohesive.

Possible notions of “cohesion”:

B) Minimum **average distance** (between two points in the cluster)

Let C be a cluster with $n := |C|$ many points in it. Further let $\binom{C}{2}$ denote the set of all pairs of points in C . Then the average distance $avd(C)$ of C is:

$$avd(C) := \frac{2}{n(n-1)} \sum_{\{c, c'\} \in \binom{C}{2}} d(c, c')$$

Similarity / closeness of clusters

Set a notion of “**cohesion**” (or connectivity, density, ...)

→ Merge two cluster whose union is most cohesive.

Possible notions of “cohesion”:

C) Minimum **density**

E.g. define the density of a cluster C by: $\frac{\text{diam}(C)}{|C|}$ or $\frac{\text{avd}(C)}{|C|}$

Evaluating the clustering (Davies-Bouldin index)

Definition (Davies-Bouldin index):

Let $k \in \mathbb{N}$ and $C_1, \dots, C_k$ be the clusters of some data set.

Let $c_i := \text{cent}(C_i)$ for all $i \in \{1, \dots, k\}$.

Define the **average radius** r_i of a cluster C_i as:

$$r_i := \frac{1}{|C_i|} \sum_{c \in C_i} d(c_i, c)$$

Define the **Davies-Bouldin index** $DB(C_1, \dots, C_k)$ for $C_1, \dots, C_k$ as:

$$DB(C_1, \dots, C_k) := \frac{1}{k} \sum_{i=1}^k \max_{j \neq i} \frac{r_i + r_j}{d(c_i, c_j)}$$

Note: Index is low if average radii are small and clusters are far apart.

(Naive) Hierarchical clustering algorithm

Agglomerative (bottom up):

1. Initialise each data point as a (singleton) cluster.
AND initialise representatives for clusters (centroid / clustroid).
2. Repeatedly combine two “most similar / closest” clusters to a new one.
BY computing in each turn **distances** between **all pairs** of clusters.
3. Stop w.r.t. certain criterion (e.g. # of clusters, density of clusters, ...)
BY computing abort parameter each turn.

(Naive) Hierarchical clustering algorithm

2. Repeatedly combine two “most similar / closest” clusters to a new one.

BY computing in each turn **distances** between **all pairs** of clusters.

If we have n data points in total. This part of the algorithm takes $O(n^3)$ much time.

Conclusion: Hierarchical clustering takes too long for large data sets!

The (naive) k -means algorithm

- Sometimes also called **Lloyd's algorithm**, named after Stuart P. Lloyd.
- During the algorithm, the **number of clusters** is **fixed** and equal to k .
- **Point assignment method**, no hierarchical approach.
 - Every data point will be assigned to precisely one cluster.
- **Iterative algorithm** that assumes **Euclidean setting**.
- The algorithm alternates between two steps:
 - **Assignment step**
 - **Update step**

The (naive) k -means algorithm

Step 0: Initialisation

- Choose k data points as representatives (centroids), one for each (singleton) cluster $C_1, \dots, C_k$.
 - e.g. all at random, or
 - one at random and each next as far away from former(s) as possible

Assignment step:

(Re)assign each data point p to the cluster C_i for which the distance between p and the centroid of C_i is minimal, i.e. to the cluster C_i that minimises: $d(p, \text{cent}(C_i))$.

The (naive) k -means algorithm

Assignment step:

(Re)assign each data point p to the cluster C_i for which the distance between p and the centroid of C_i is minimal, i.e. to the cluster C_i that minimises: $d(p, \text{cent}(C_i))$.

Update step:

Recalculate the centroids for all clusters.

Termination rule:

- E.g. run until the process converges / stabilises, or
- stop if only a few / tiny proportion of data points were reassigned.

(Naive) k -means algorithm: running time

Let $k \in \mathbb{N}$ be fixed

Let n be the **total number of data points** we want to cluster.

Let I denote the **number of iteration** the k -means algorithm needs **until convergence** / it stabilises (abort criterion: no changes anymore).

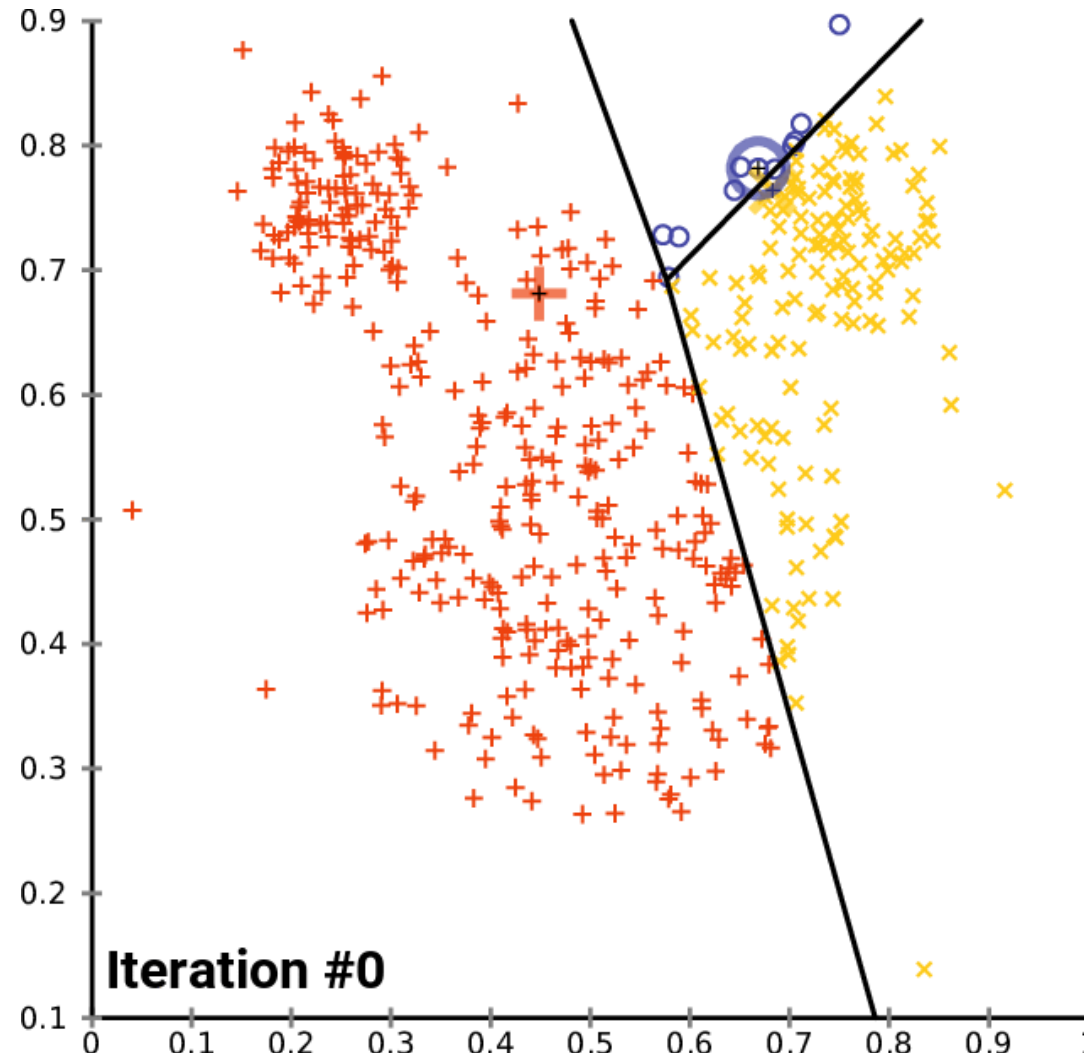
Then the **running time** is: $O(knI)$.

How big is I ?

Worst case: $I = 2^{\Omega(\sqrt{n})}$

In practice: I can often be considered **constant**.

The k -means Algorithm



GIF published on Wikipedia under
[CC BY-SA 4.0](#) license by Chire.
See this [link](#).

What might the right k be?

Let $k \in \mathbb{N}$ and $C_1, \dots, C_k$ be the clusters of some data set.

Let $c_i := \text{cent}(C_i)$ for all $i \in \{1, \dots, k\}$.

Define the **average radius** r_i of a cluster C_i as:

$$r_i := \frac{1}{|C_i|} \sum_{c \in C_i} d(c_i, c)$$

Often: Average radii get rapidly smaller while we increase k , up to some value from where on changes are relatively small.

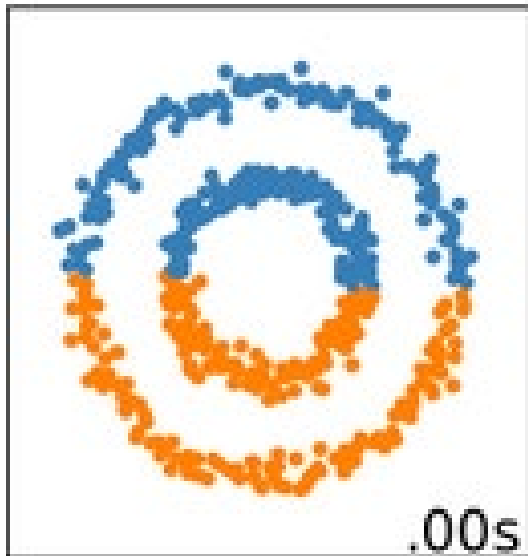
Compute evaluation score: (e.g. Davies-Bouldin index)

Problem with k -means

In general, k -means (tries) to minimise the following term:

$$\sum_{i=1}^k \sum_{c \in C_i} d(c, \text{cent}(C_i))$$

Problematic, if (actual) clusters differ a lot in size or are not well-distributed.



CURE (Clustering Using REpresentatives) algorithm

An algorithm “between” agglomerative and k -means clustering.

Step 0: Pick **random sample** of data points fitting into main memory.

Step 1: Cluster the sample set, e.g. via agglomerative clustering.

Step 2:

- Within each cluster C_i , pick a sample set S_i of data points which is as “***dispersed***” as possible.
- Define **set of representatives** R_i of C_i as those points we get by moving each point of S_i by some fraction towards $cent(C_i)$.

Note: Points in R_i are not necessarily actual data points.

CURE (Clustering Using REpresentatives) algorithm

Next: Merge two clusters if there are two representatives, one from each cluster, whose distance from each other is below some fixed threshold.

→ pick new scattered representatives

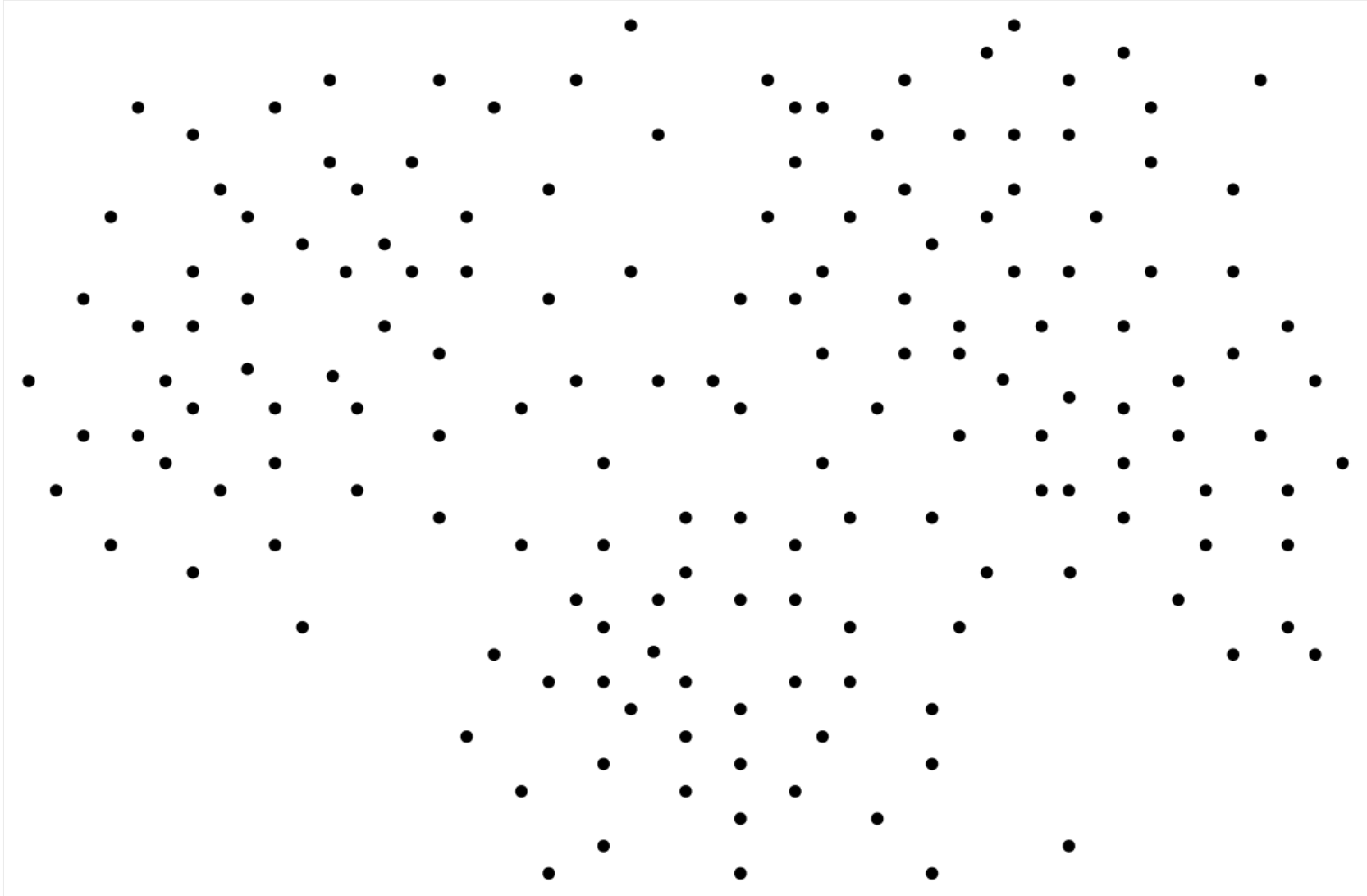
Now start clustering of the whole data by the following rule:

Assignment rule: Place data point p into cluster C_i if p is closest to a representative of C_i among representatives of all clusters.

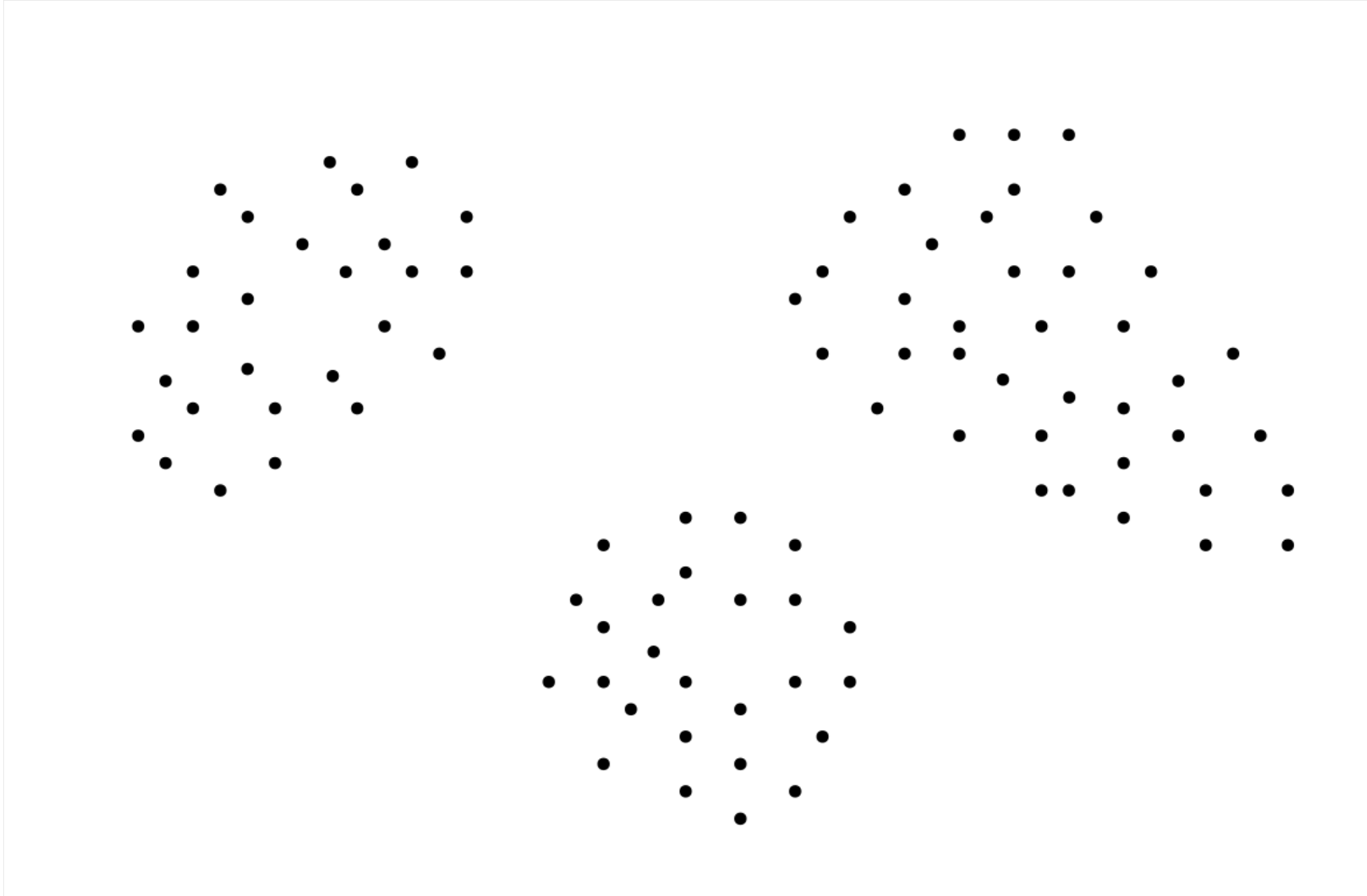
Advantage: Robust for data that is not well-distributed.

Disadvantage: Relatively costly with respect to running time.

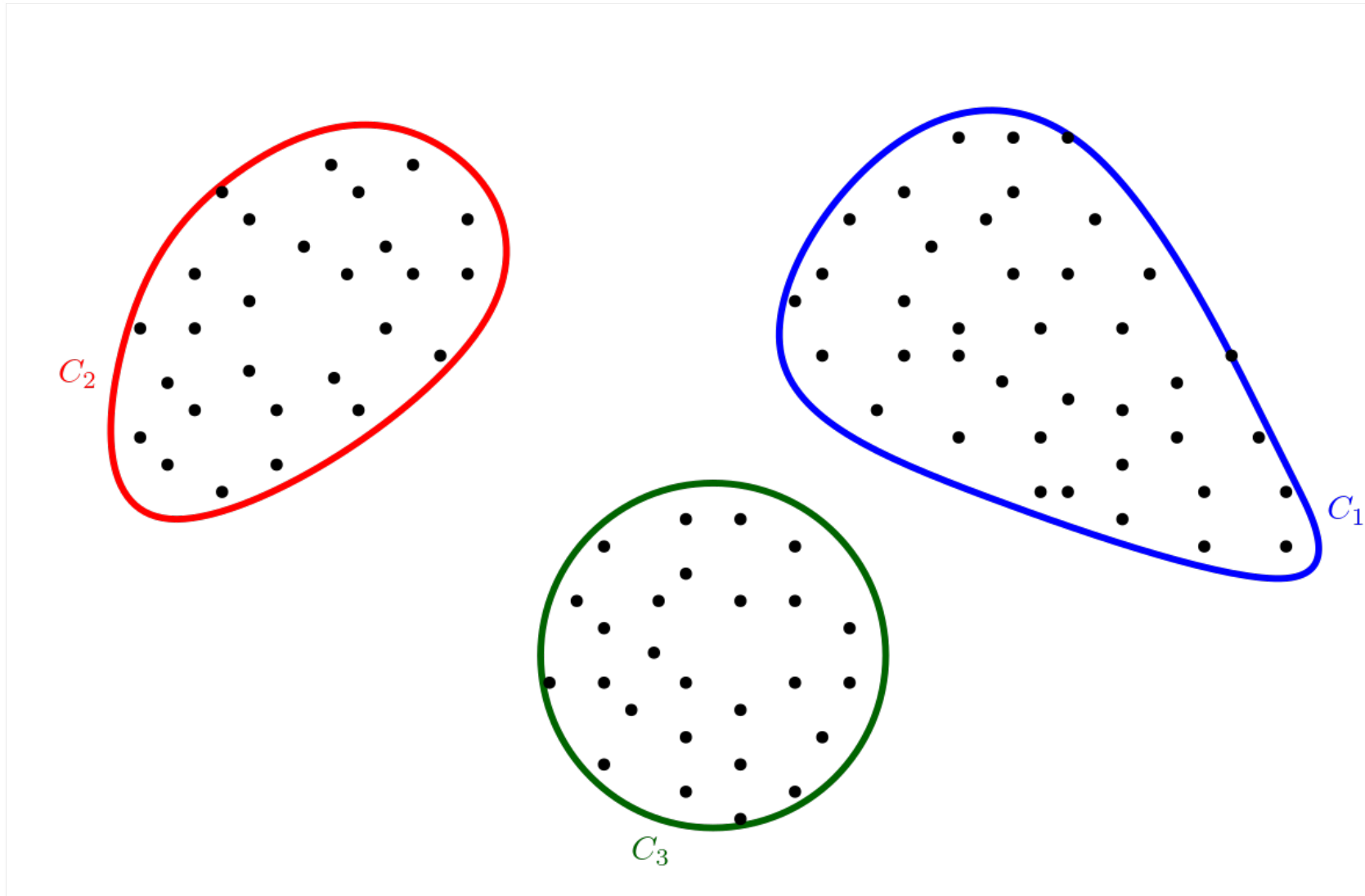
CURE (Clustering Using REpresentatives) algorithm



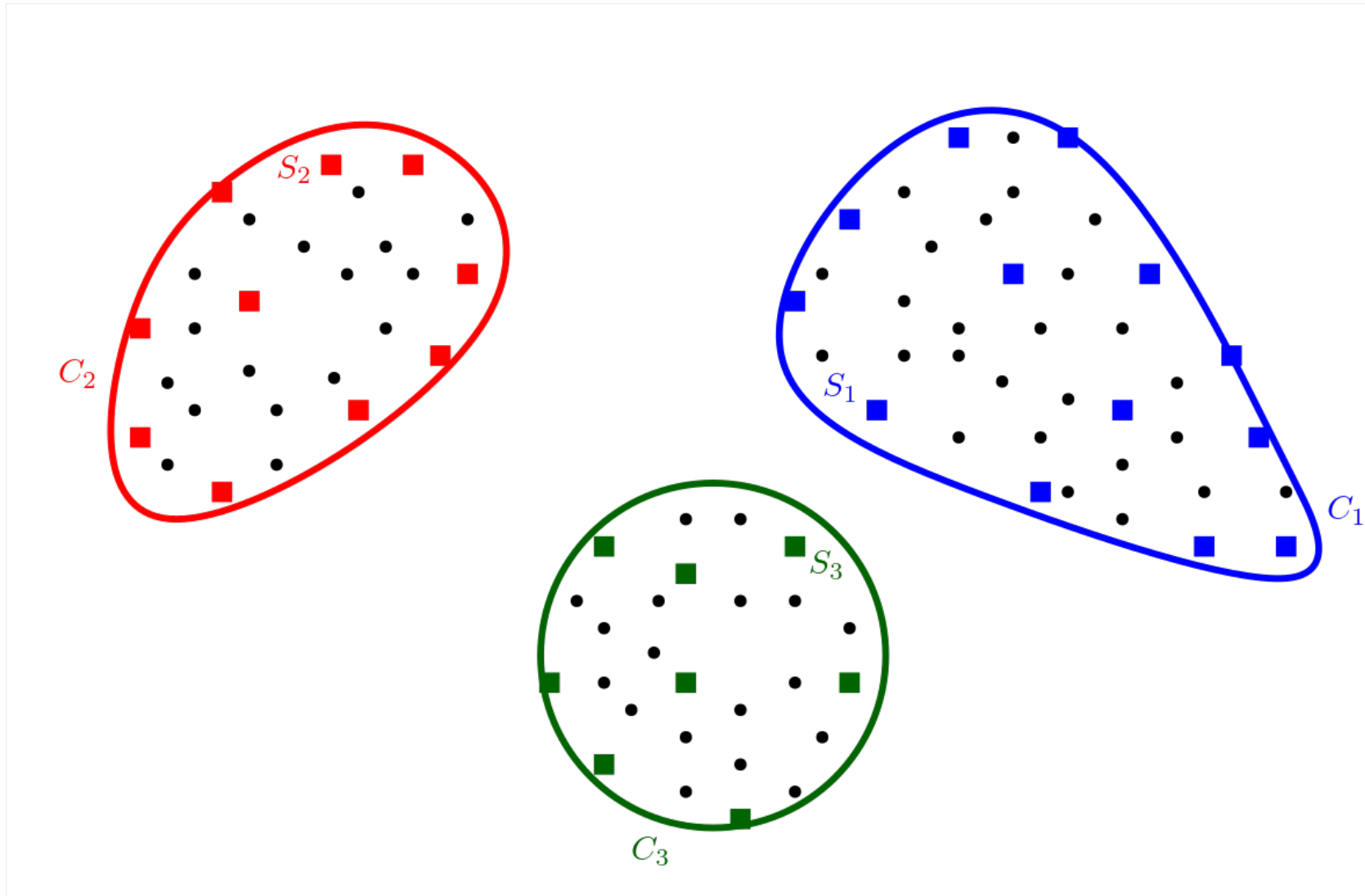
CURE (Clustering Using REpresentatives) algorithm



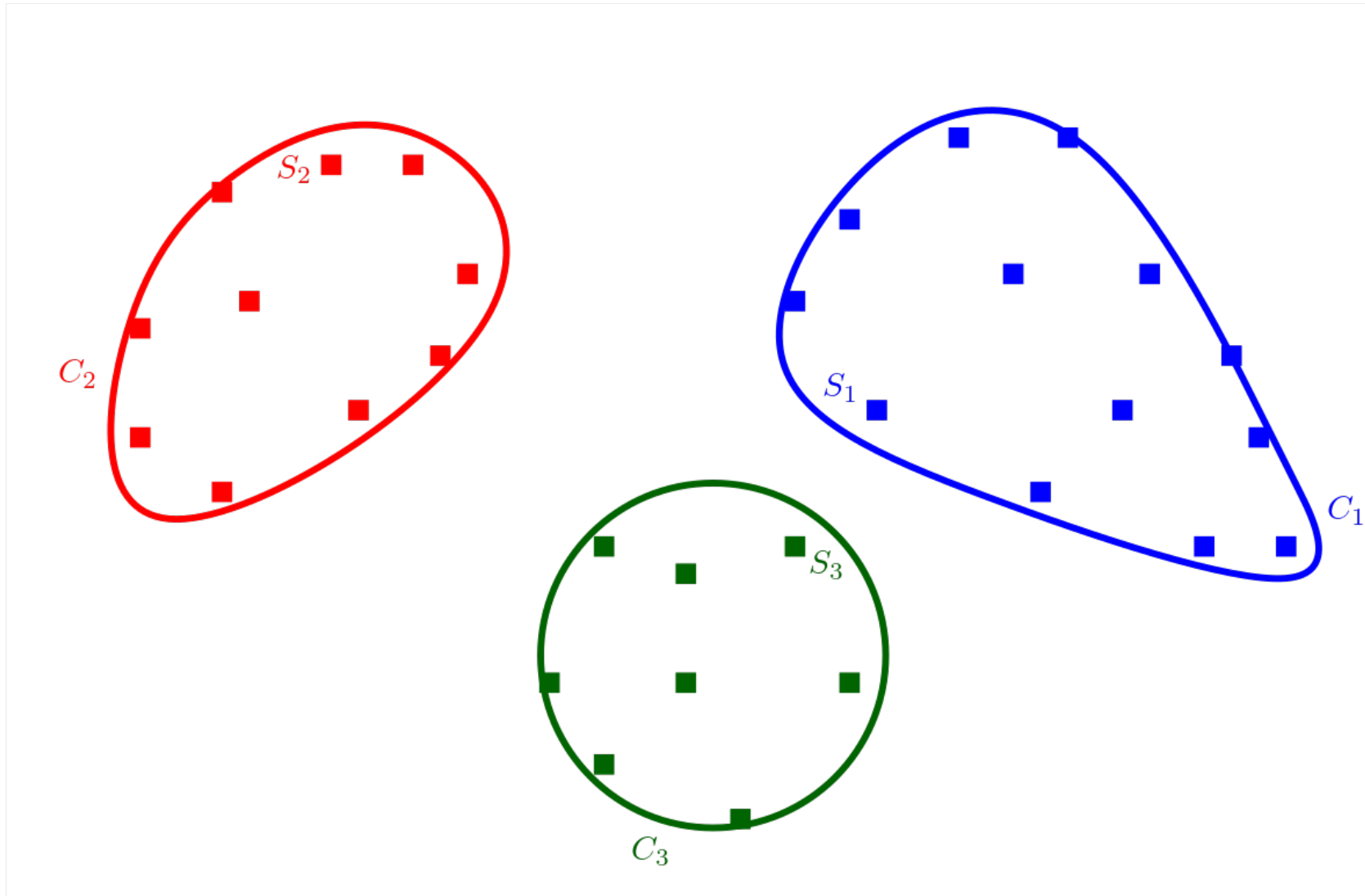
CURE (Clustering Using REpresentatives) algorithm



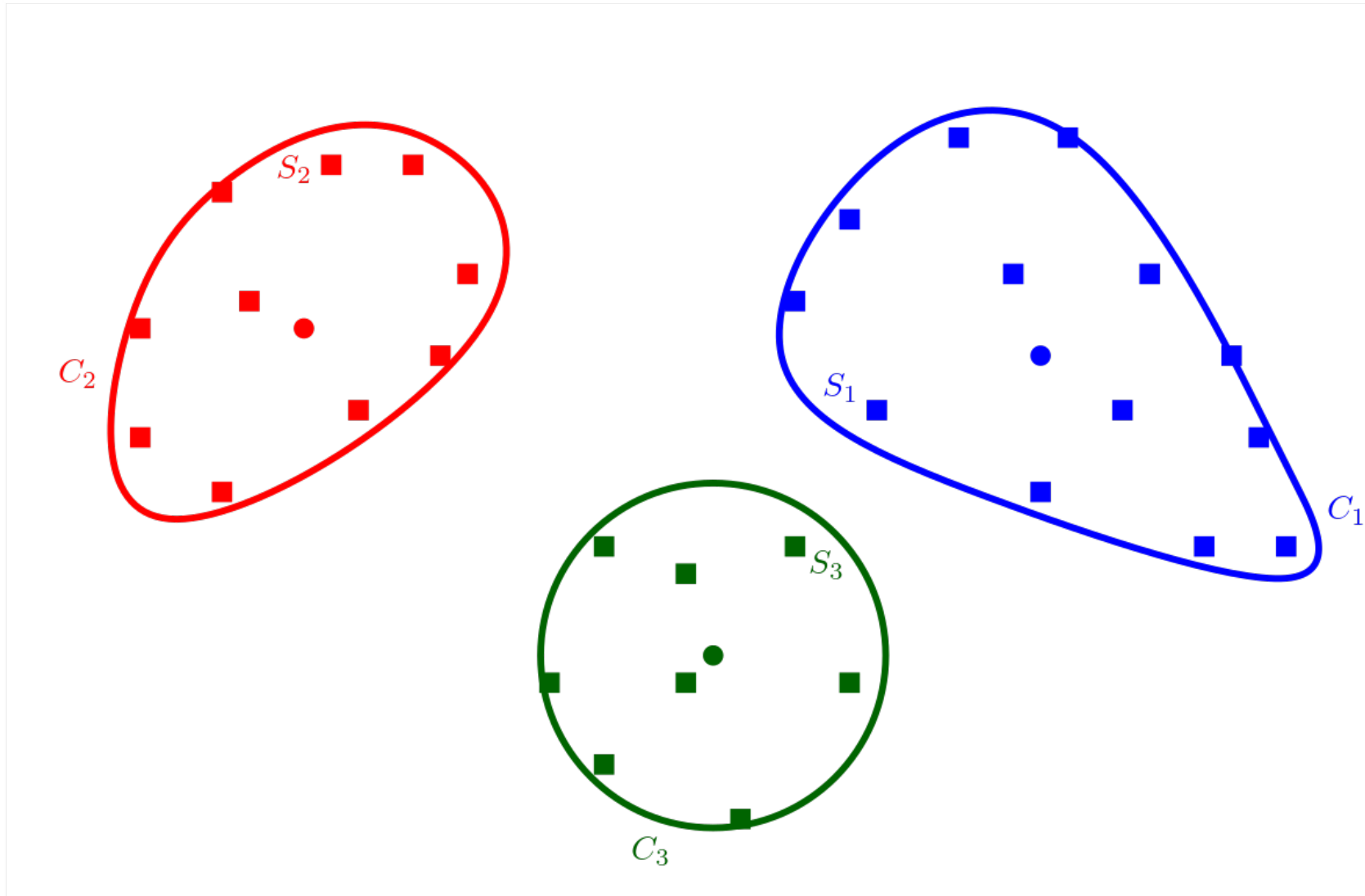
CURE (Clustering Using REpresentatives) algorithm



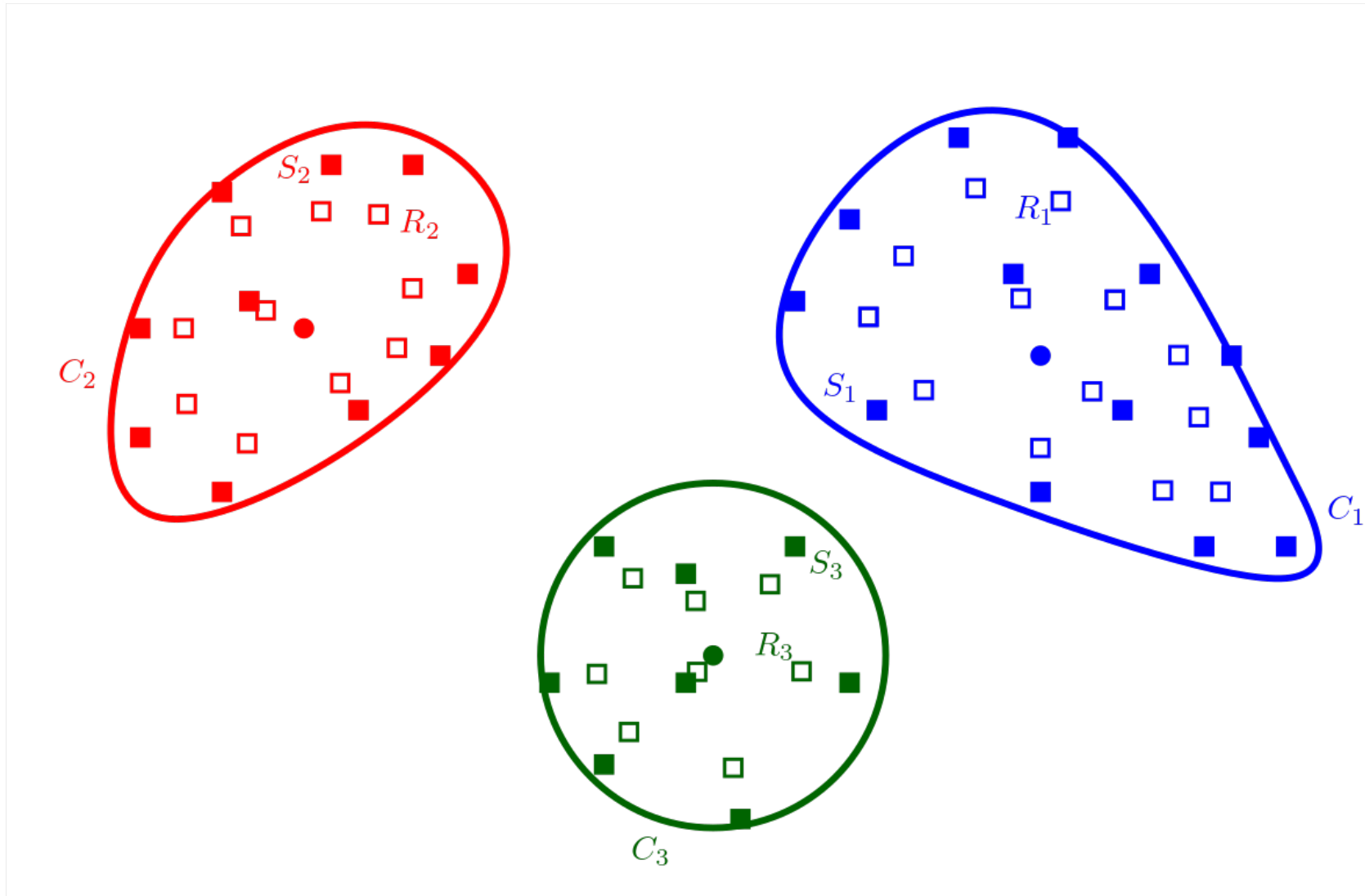
CURE (Clustering Using REpresentatives) algorithm



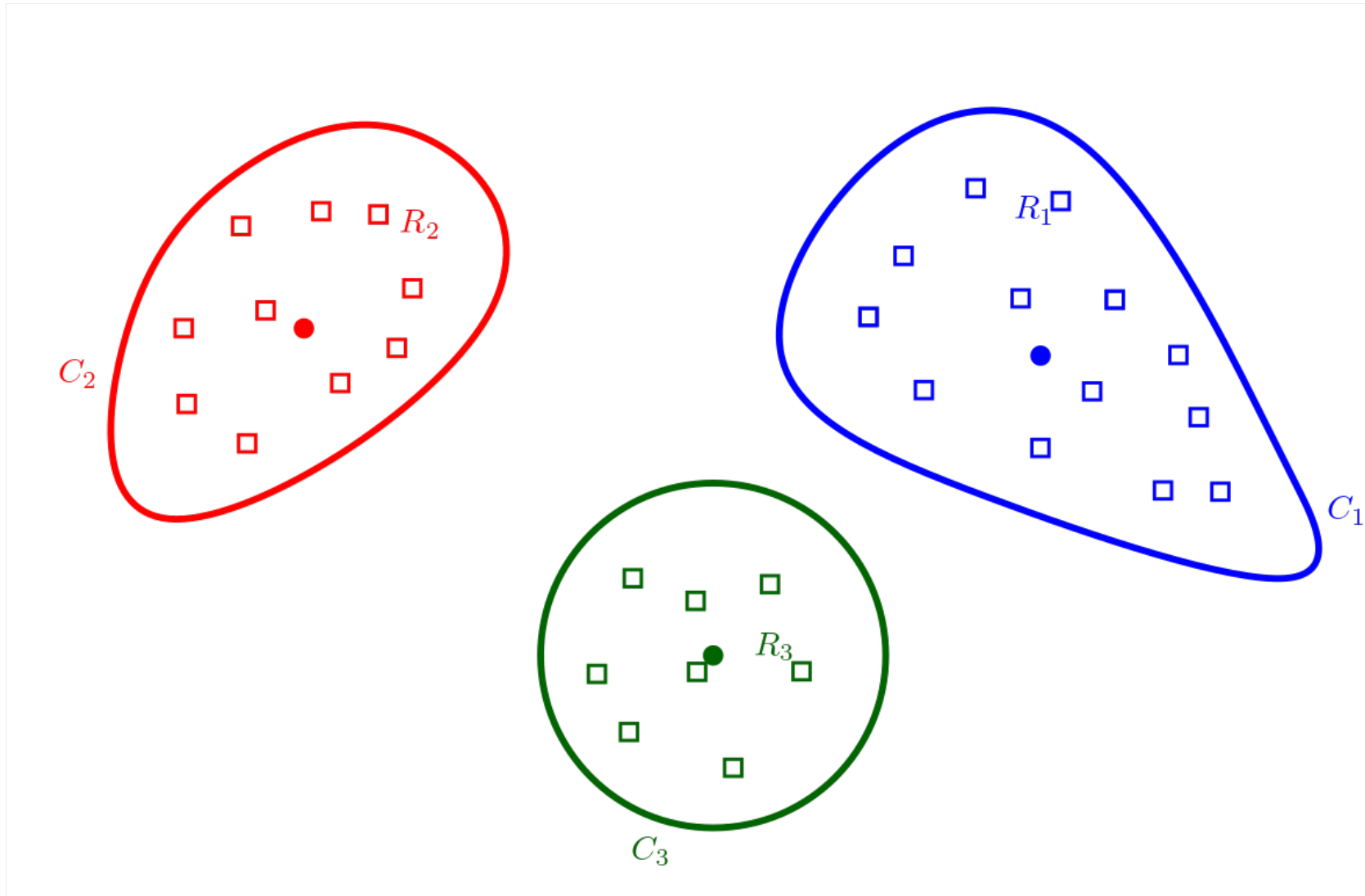
CURE (Clustering Using REpresentatives) algorithm



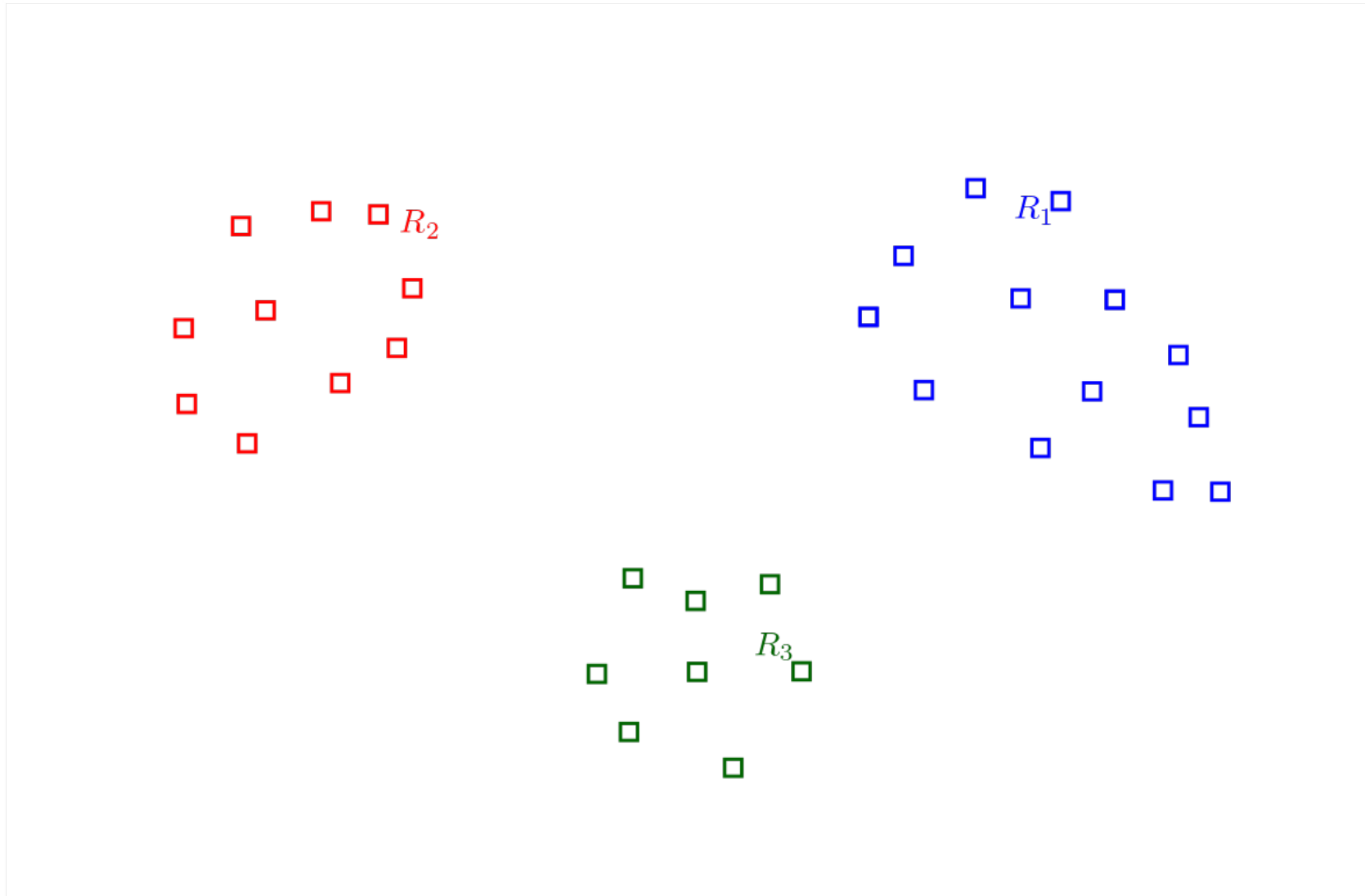
CURE (Clustering Using REpresentatives) algorithm



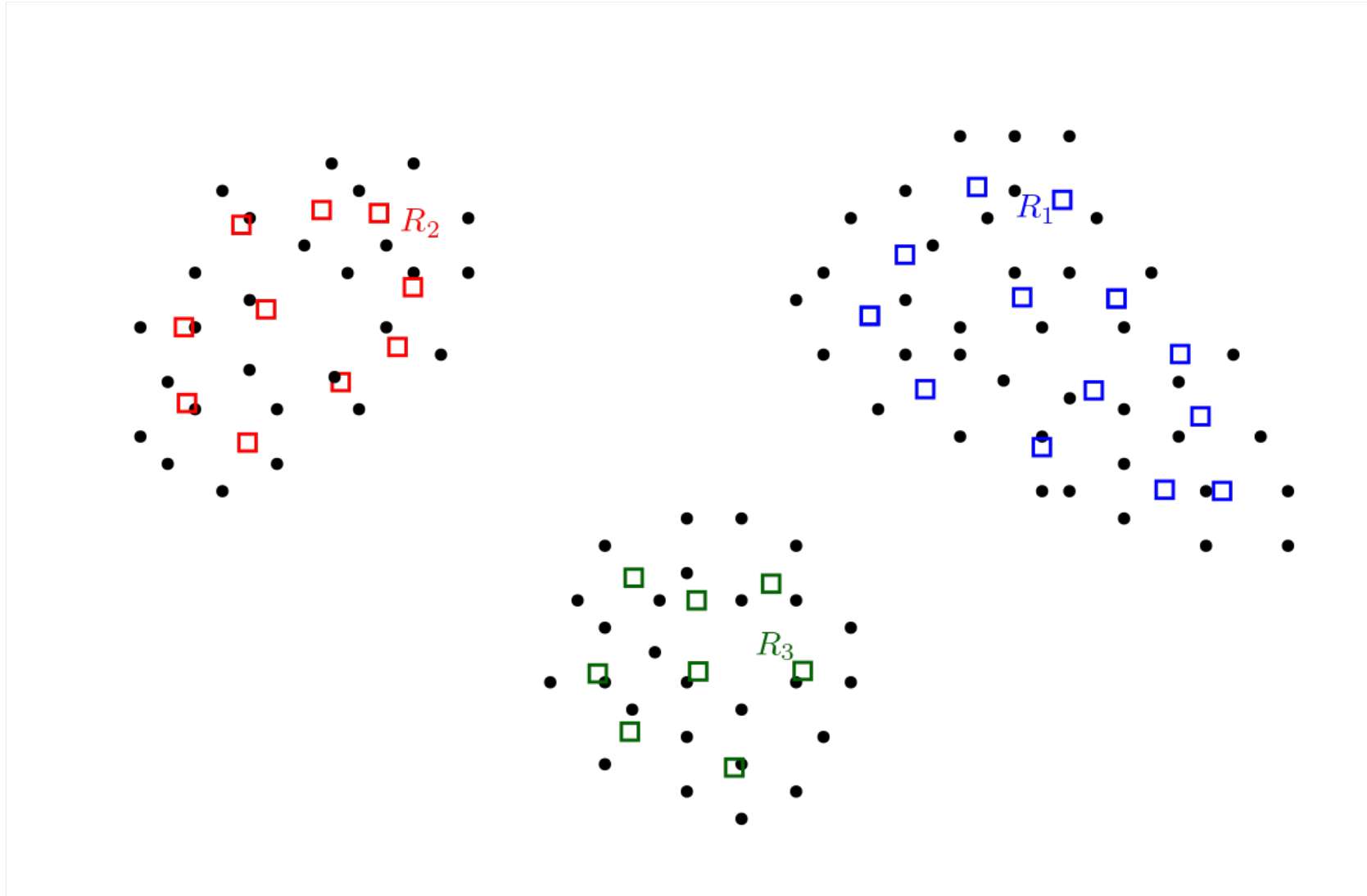
CURE (Clustering Using REpresentatives) algorithm



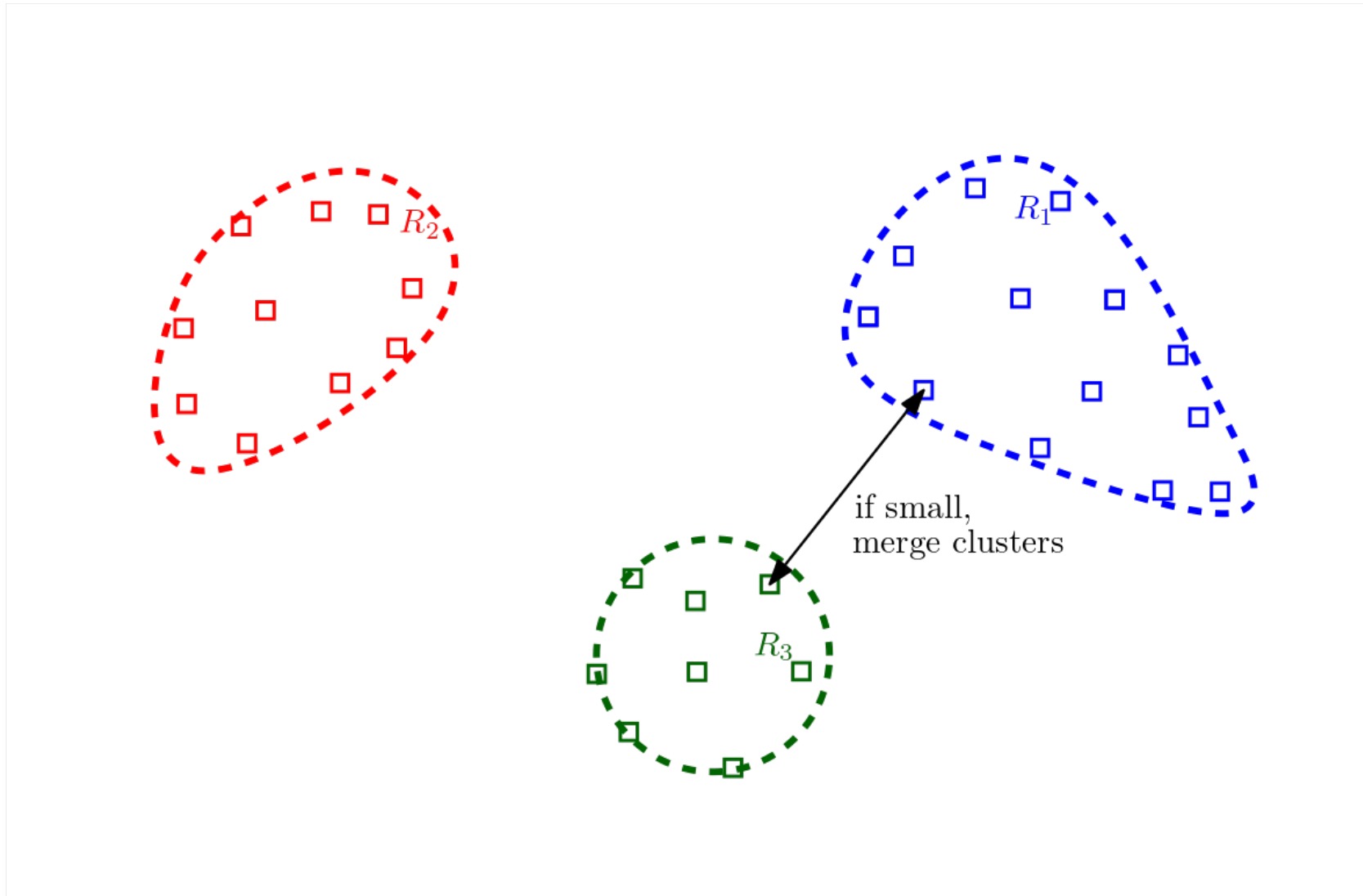
CURE (Clustering Using REpresentatives) algorithm



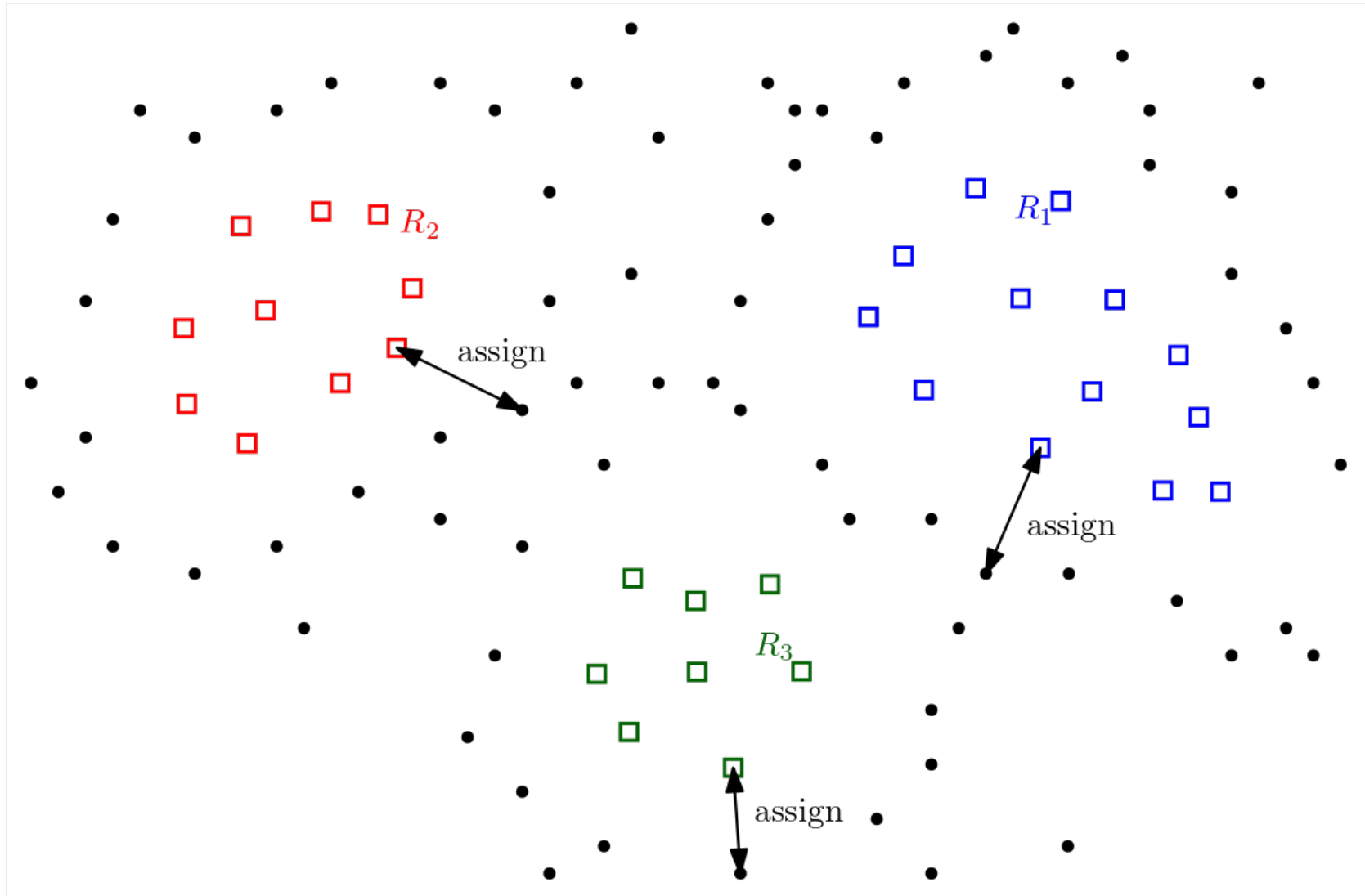
CURE (Clustering Using REpresentatives) algorithm



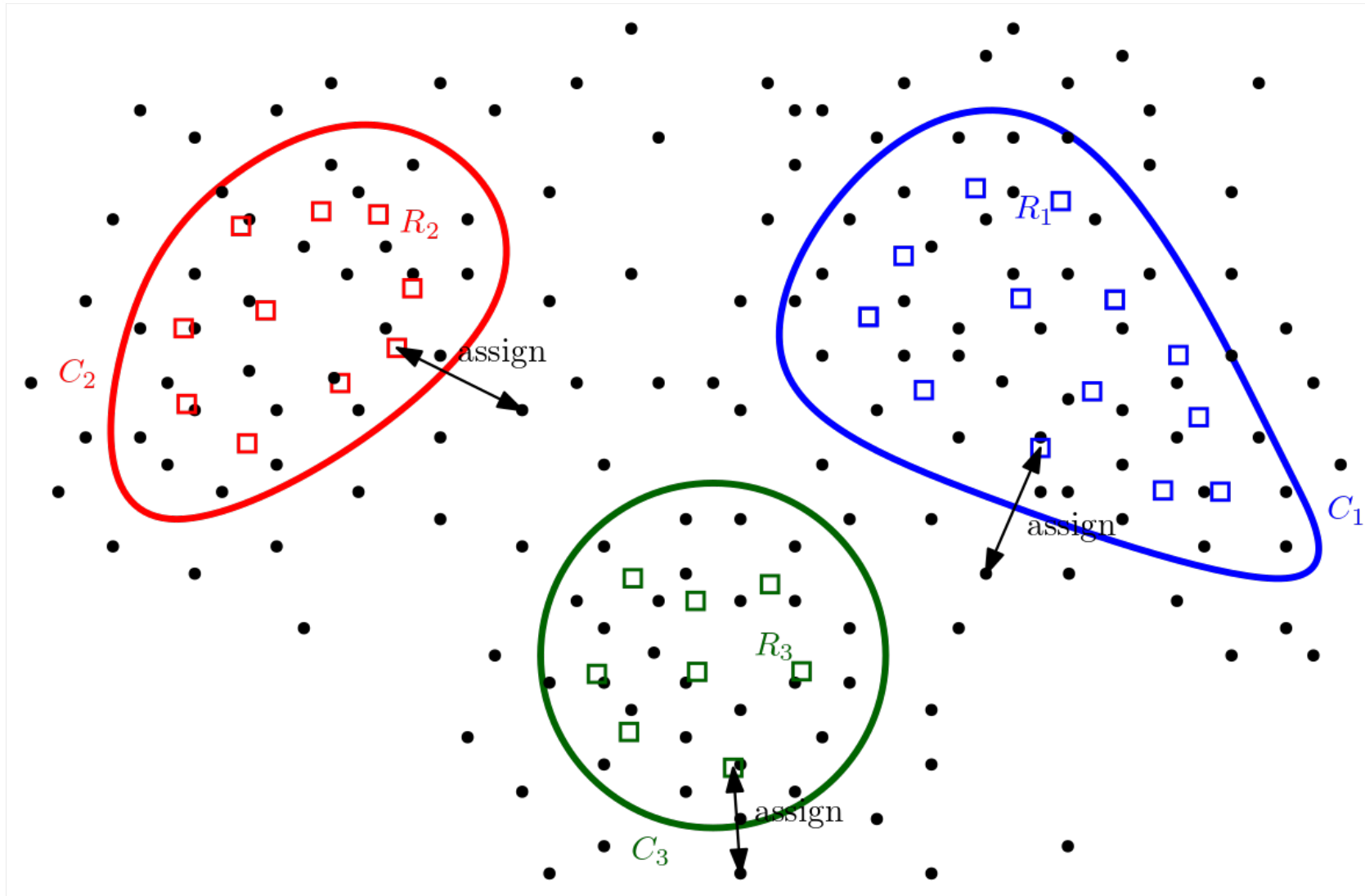
CURE (Clustering Using REpresentatives) algorithm



CURE (Clustering Using REpresentatives) algorithm



CURE (Clustering Using REpresentatives) algorithm



Original CURE algorithm

- Perform hierarchical clustering.
- In each step, (re)compute representatives for each cluster.
- Merge two clusters w.r.t. distance between representatives.
- Stop if desired number of clusters is reached (or other abort condition).
- Running time: $O(n^2 \log(n))$

DBSCAN algorithm

Name: **Density-based spatial clustering of applications with noise**

Parameters: $\varepsilon \in \mathbb{R}, m \in \mathbb{N}$.

Set S of all data points is divided into some different point categories:

- $p \in S$ is a **core point** if $|\{x \in S \mid d(p, x) \leq \varepsilon\}| \geq m$.

DBSCAN algorithm

Name: **Density-based spatial clustering of applications with noise**

Parameters: $\varepsilon \in \mathbb{R}, m \in \mathbb{N}$.

Set S of all data points is divided into some different point categories:

- $p \in S$ is a **core point** if $|\{x \in S \mid d(p, x) \leq \varepsilon\}| \geq m$.
- $x \in S$ is **directly reachable** from $p \in S$ if $d(p, x) \leq \varepsilon$ and p is a core point.

DBSCAN algorithm

Name: **Density-based spatial clustering of applications with noise**

Parameters: $\varepsilon \in \mathbb{R}, m \in \mathbb{N}$.

Set S of all data points is divided into some different point categories:

- $p \in S$ is a **core point** if $|\{x \in S \mid d(p, x) \leq \varepsilon\}| \geq m$.
- $x \in S$ is **directly reachable** from $p \in S$ if $d(p, x) \leq \varepsilon$ and p is a core point.
- $x \in S$ is **reachable** from $p \in S$ if there are points $x_1, \dots, x_k \in S$ such that:
 - $x_1 = p$ and $x_k = x$,
 - x_{i+1} is directly reachable from x_i for all $i \in \{1, \dots, k-1\}$,
 - $x_1, \dots, x_{k-1}$ are core points.

A reachable point that is no core point is called a **rim point**

DBSCAN algorithm

Name: **Density-based spatial clustering of applications with noise**

Parameters: $\varepsilon \in \mathbb{R}, m \in \mathbb{N}$.

Set S of all data points is divided into some different point categories:

- $p \in S$ is a **core point** if $|\{x \in S \mid d(p, x) \leq \varepsilon\}| \geq m$.
- $x \in S$ is **directly reachable** from $p \in S$ if $d(p, x) \leq \varepsilon$ and p is a core point.
- $x \in S$ is **reachable** from $p \in S$ if there are points $x_1, \dots, x_k \in S$ such that:
 - $x_1 = p$ and $x_k = x$,
 - x_{i+1} is directly reachable from x_i for all $i \in \{1, \dots, k-1\}$,
 - $x_1, \dots, x_{k-1}$ are core points.

A reachable point that is no core point is called a **rim point**.

- $x \in S$ is an **outlier (or noise) point** if it is not reachable from any $p \in S$.

DBSCAN algorithm

Initialise: Mark each point as unvisited.

DBSCAN algorithm

Initialise: Mark each point as unvisited.

Check each point p :

- if unvisited:
 - if p is not core, mark as visited (rim point or outlier).

DBSCAN algorithm

Initialise: Mark each point as unvisited.

Check each point p :

- if unvisited:
 - if p is not core, mark as visited (rim point or outlier).
 - if p is core, define cluster:
$$C := \{x \mid x \text{ is reachable from } p \text{ and } x \text{ is not already in a cluster}\}.$$

DBSCAN algorithm

Initialise: Mark each point as unvisited.

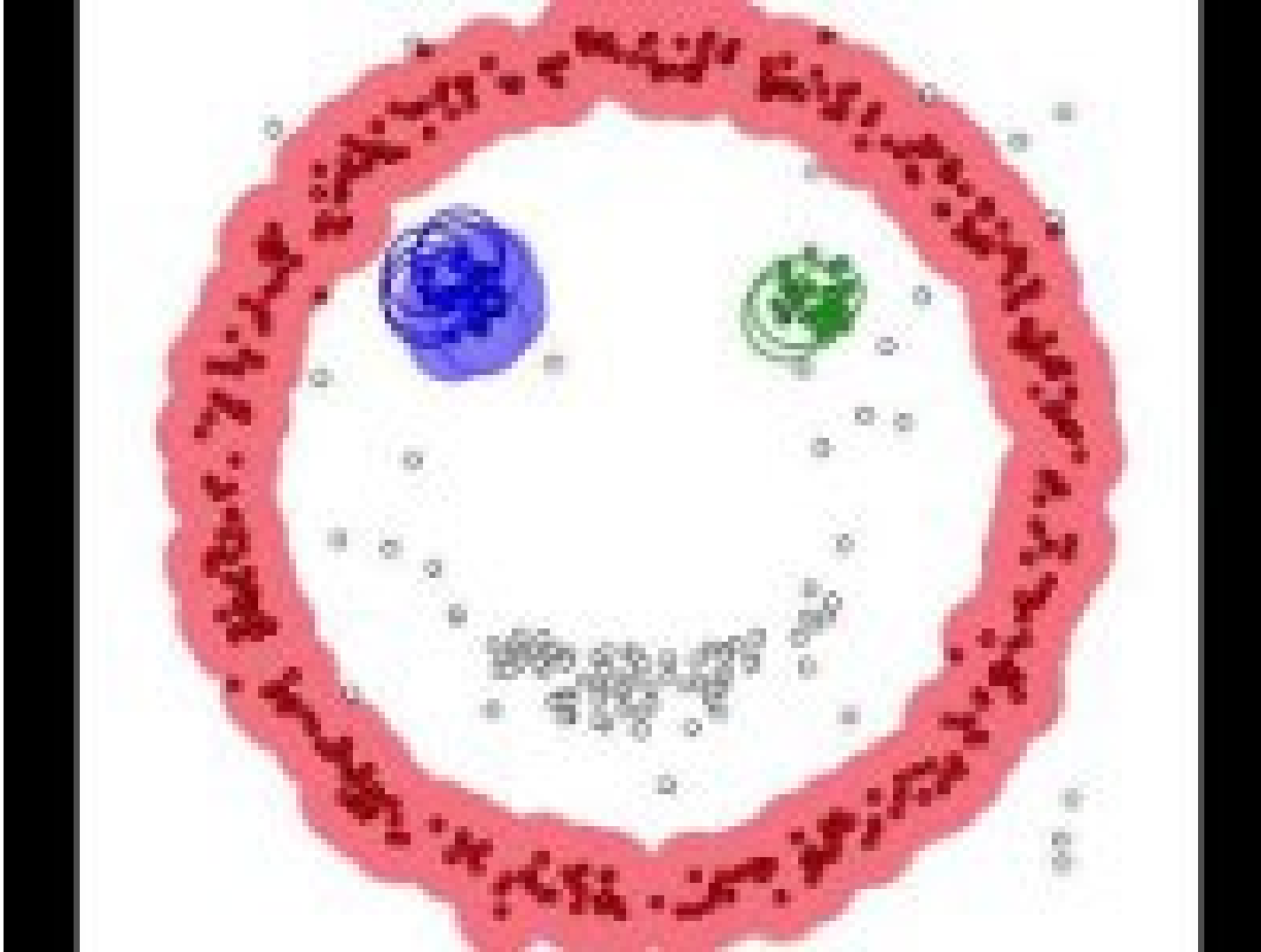
Check each point p :

- if unvisited:
 - if p is not core, mark as visited (rim point or outlier).
 - if p is core, define cluster:
$$C := \{x \mid x \text{ is reachable from } p \text{ and } x \text{ is not already in a cluster}\}.$$

Running time (worst-case): $O(n^2)$

Advantage: Can identify clusters whose shape is more irregular.

DBSCAN algorithm



Published by Karthik Ramasamy
on Youtube. See this [link](#).