Ανάπτυξη Λογισμικού για Δυσεπίλυτα Αλγοριθμικά Προβλήματα

Ενότητα 2: Clustering

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Outline

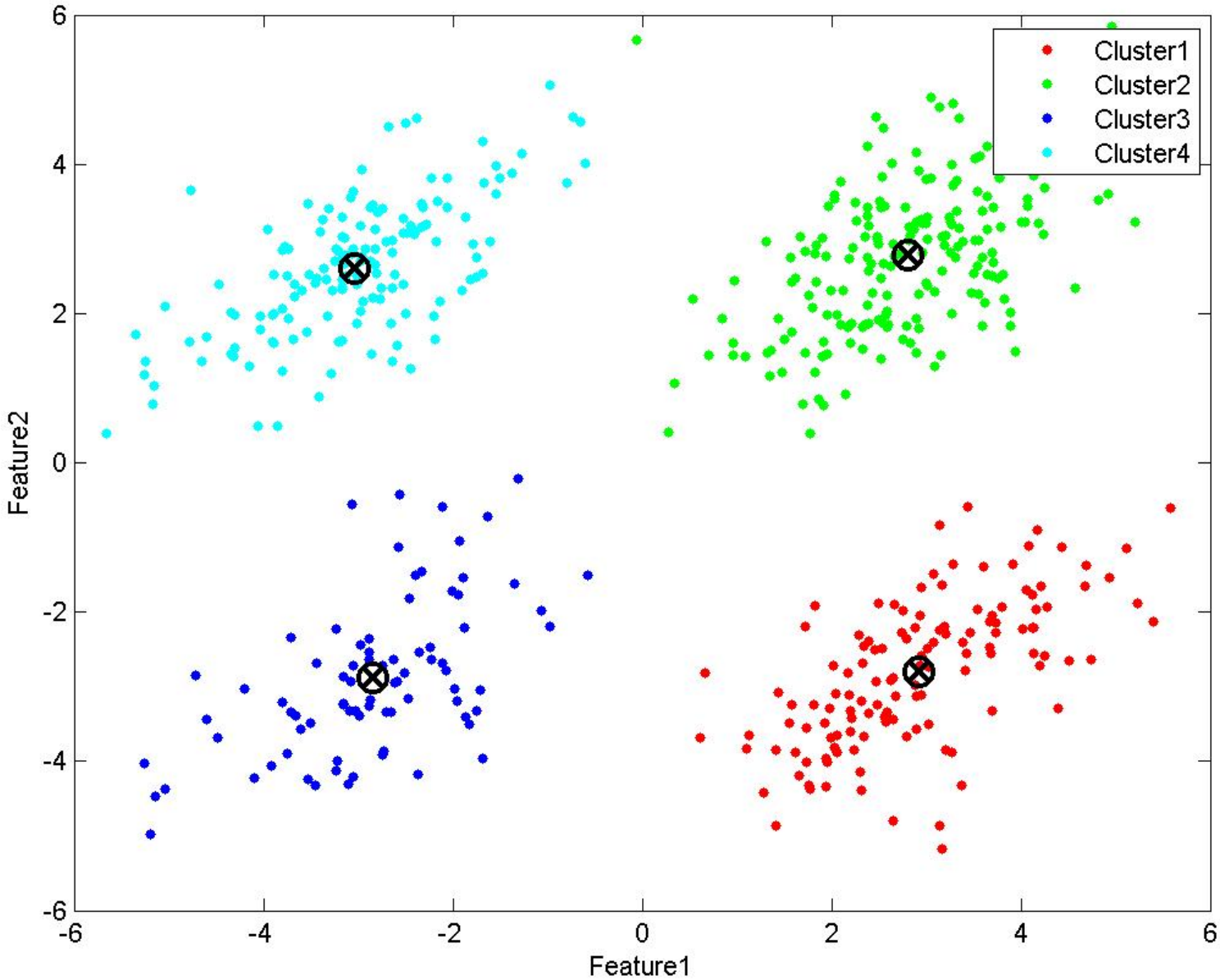
Clustering

Definition (k clusters)

Given n objects, and $k > 1$, partition the objects into k subsets (clusters) so as to optimize some objective function.

- Objects in the same cluster are more "similar" (or closer) to each other than to those in other clusters.
- Possible criteria: minimizing the total distance among all cluster points, minimizing the distance of cluster points to some center, etc.
- Variations: k is unknown and computed, e.g., by the Silhouette method. Capacitated/balanced: k given, clusters of equal cardinality.
- Applications: Classification, Social Network Analysis, Recommender Systems, Market Research, Bioinformatics etc

Good Clustering, with centers



Approaches

- hierarchical (agglomerative): each point initializes a cluster, merge until stopping criterion, e.g., predetermined number of clusters, or if merging creates cluster with points too far apart.
- point-assignment: given some initial clusters, assign points to "best" cluster; might allow combining / splitting clusters, or unassign points. Example: k-means (our focus).

(Ullman et al:Mining Massive datasets)

Outline

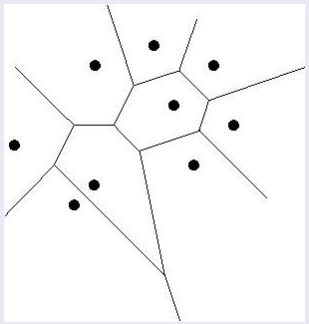
Vector spaces

Problem definition

- Clustering that minimizes objective function.
- k is given.
- Centroids do not have to be part of the dataset

k-means

- k-means is the most common problem: Main algorithms:
  -- Lloyd's algorithm is standard.
  -- Elkan's uses triangular inequality to accelerate updates.
- Also used to construct initial clusters for more sophisticated method.
- In Euclidean space, assignment is point location to the k Voronoi cells.



k-means: Objective function

Typical ambient space is $\mathbb{R}^d$ but can generalize to metric space $\mathcal{Z}$.

Minimization function

In any metric space over points/objects $\mathcal{Z}$ with distance/metric function d, let the dataset be $X = \{x_1, \ldots, x_n\} \subseteq \mathcal{X} \subseteq \mathcal{Z}$, $k > 1$. Given centroids $C \subset \mathcal{Z}$, let

$$\mathrm{d}(x_i, C) = \min_{c \in C} \mathrm{d}(x_i, c).$$

Consider vector $v(C) = (\mathrm{d}(x_1, C), \ldots, \mathrm{d}(x_n, C))$. The k-means objective is:

$$\min_{C \subseteq \mathcal{Z}, |C|=k} \|v(C)\|_2^2 = \sum_{i=1}^{n} \mathrm{d}(x_i, C)^2.$$

The k-means objective is NP-hard, but for the ℓ_2 metric, Lloyd's algorithm converges quickly to a *local* minimum.

Variations

Various minimizations

Recall $X = \{x_i\}$, $v(C) = (\mathrm{d}(x_1, C), \ldots, \mathrm{d}(x_n, C))$, where $C \subset \mathcal{Z}$ are the centroids, and the k-means objective is:

$$\min_{C \subseteq \mathcal{Z}, |C|=k} \|v(C)\|_2^2 = \sum_{i=1}^{n} \mathrm{d}(x_i, C)^2.$$

Similar objectives:

-- k-median: $\min_{C \subseteq \mathcal{Z}, |C|=k} \|v(C)\|_1$,

-- k-medoid: $\min_{C \subseteq X, |C|=k} \|v(C)\|_1$.

-- k-center: $\min_{C \subseteq X, |C|=k} \|v(C)\|_\infty$,

Lloyd's

Algorithm

Initialize k centers randomly (or using some strategy).

1. Assignment: Assign each object to its nearest center.
2. Update: Calculate mean $\frac{1}{T}\sum_{i=1}^{T}\vec{v_i}$ of each cluster, make it new center.

Repeat the two steps until there is no change in the assignments.

Properties

- Each distance calculation $= O(d)$ because vectors in $\mathbb{R}^d$.
- Assignment $= O(nkd)$, Update $= O(nd)$,
- #iterations unknown, in practice $\ll n$.
- Converges to local minimum in Euclidean space (depends on initialization)

Outline

Properties

Lemma

For centers a, b, and point x: $d(x, a) \leq d(a, b)/2 \Rightarrow d(x, a) \leq d(x, b)$.

Proof. $x \in$ Ball centered at a with radius $d(a, b)/2$.

Corollary: x shall not be assigned to b.

Lemma (Triangular)

If center c is updated to c' then:

$|d(x, c) - d(c, c')| \leq d(x, c') \leq d(x, c) + d(c, c')$.

Maintain bounds

Initialisation

- Pick initial centers c and assign each x to closest center $c(x)$.
- Set $u(x) \leftarrow d(x, c(x))$, $l(x, c) \leftarrow d(x, c)$, $\forall c \neq c(x)$.
- Compute $d(c, c')$ for all centers $c \neq c'$.

Update bounds

Compute $d(c, c')$ for all centers $c \neq c'$.

- Upper bound $u(x)$ on distance of x to its center c;
  for new center c' of x's cluster: update $u(x) \leftarrow u(x) + d(c, c')$.
- Lower bound $l(x, c)$ to any other center $c \neq c(x)$;
  update when c changes to c': $l(x, c') \leftarrow |l(x, c) - d(c, c')|$.

These bounds follow from the triangular inequalities.

Elkan's Assignment

for each point x **do**
  if $u(x) \leq d(c(x), c')/2$, for all centers $c' \neq c(x)$ **then** Skip x; **continue**
  end if
  for each c' to which x is not assigned **do**
    if $u(x)$ not opt, compute $u(x) \leftarrow d(x, c(x))$; mark $u(x)$ as opt;
    if $u(x) \leq d(c, c')/2$, or $u(x) \leq l(x, c')$ **then** Skip c'; **continue**
    end if
    compute $d(x, c')$;
    if $d(x, c') < u(x)$ **then** assign x to c'; set $u(x) \leftarrow d(x, c')$
    end if
    update $l(x, c') \leftarrow d(x, c')$;
  end for
end for

Elkan's algorithm

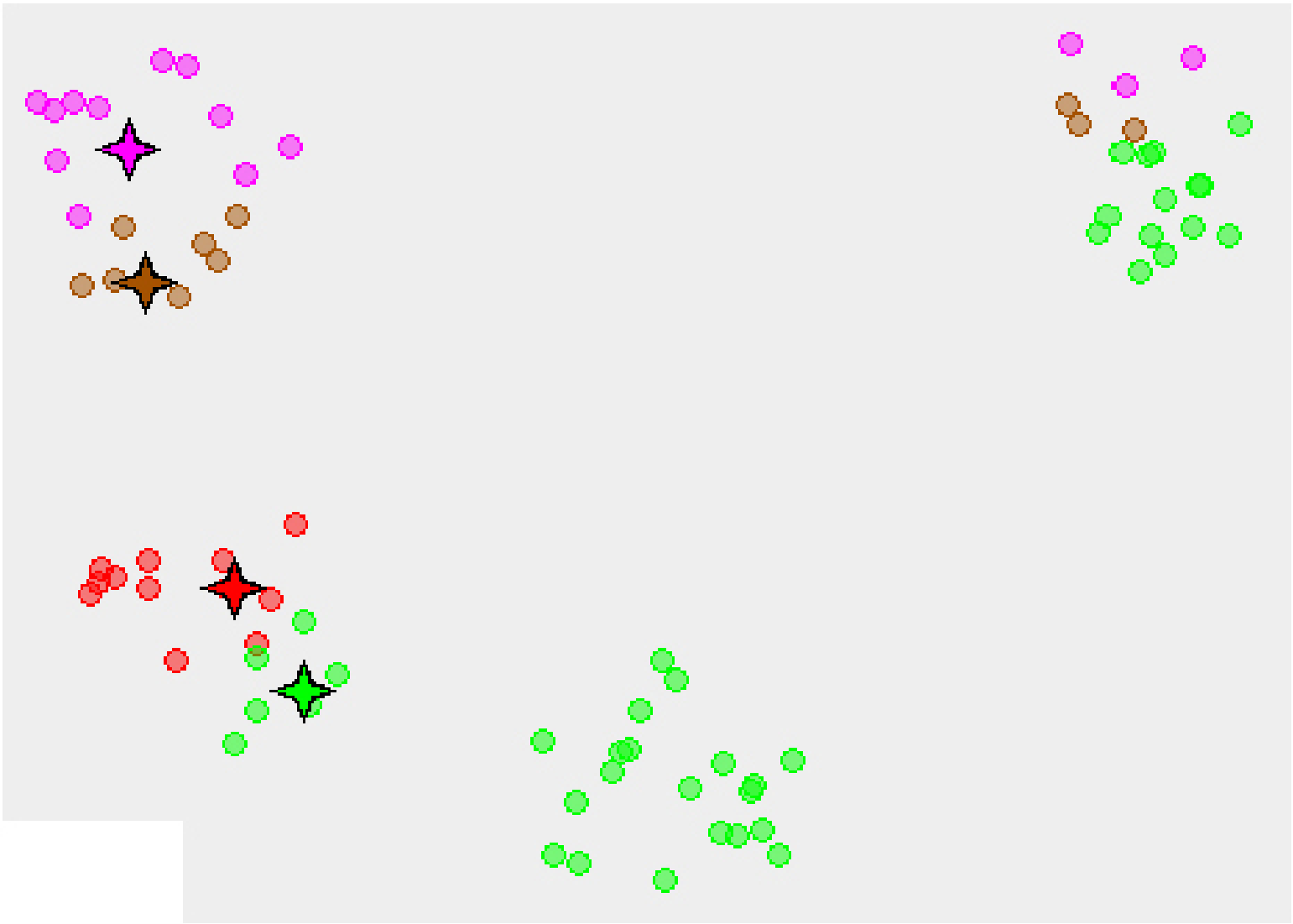
Elkan's algorithm offers, compared to Lloyd's,

-- large experimental speedup,

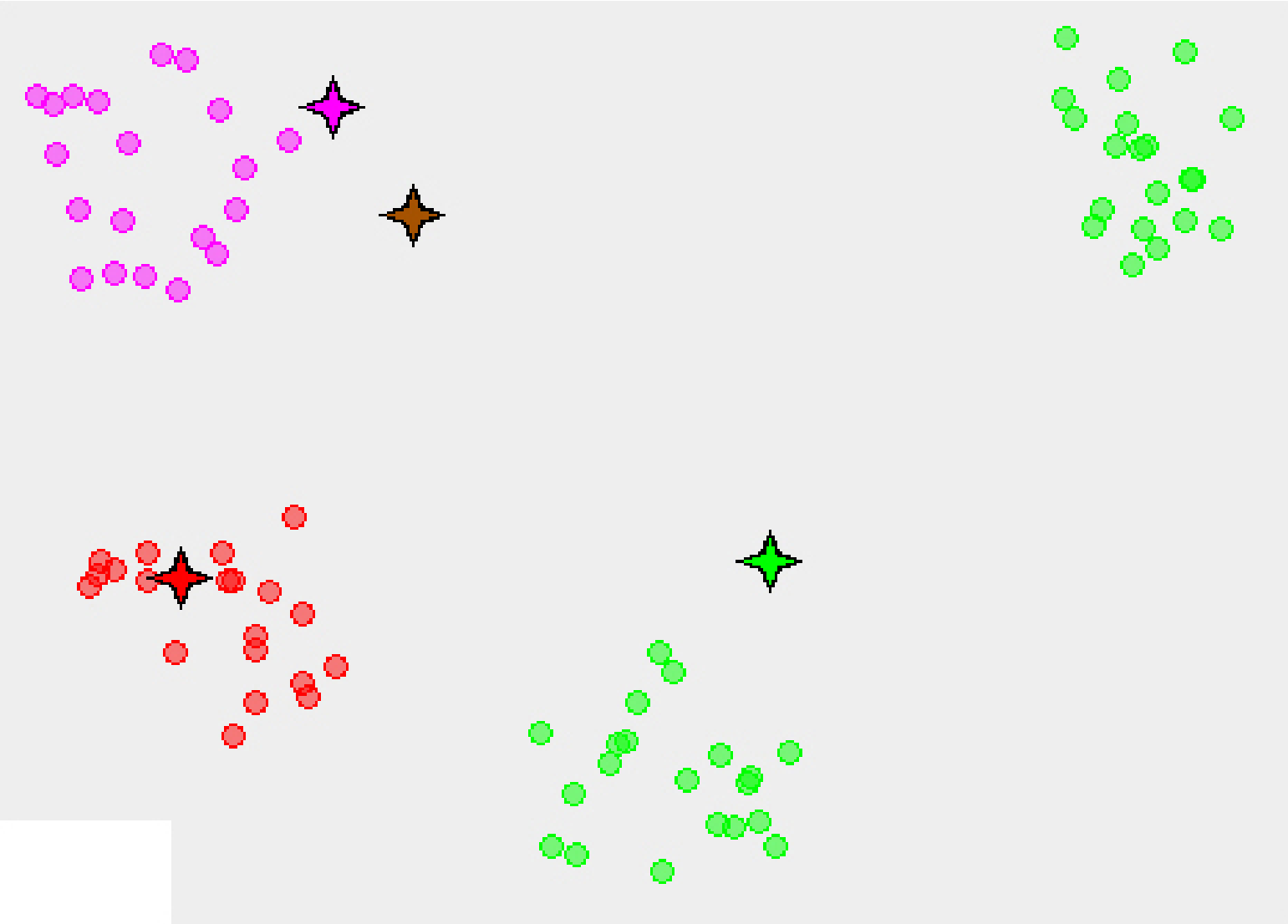
-- same output, same convergence,

-- requires much higher storage.

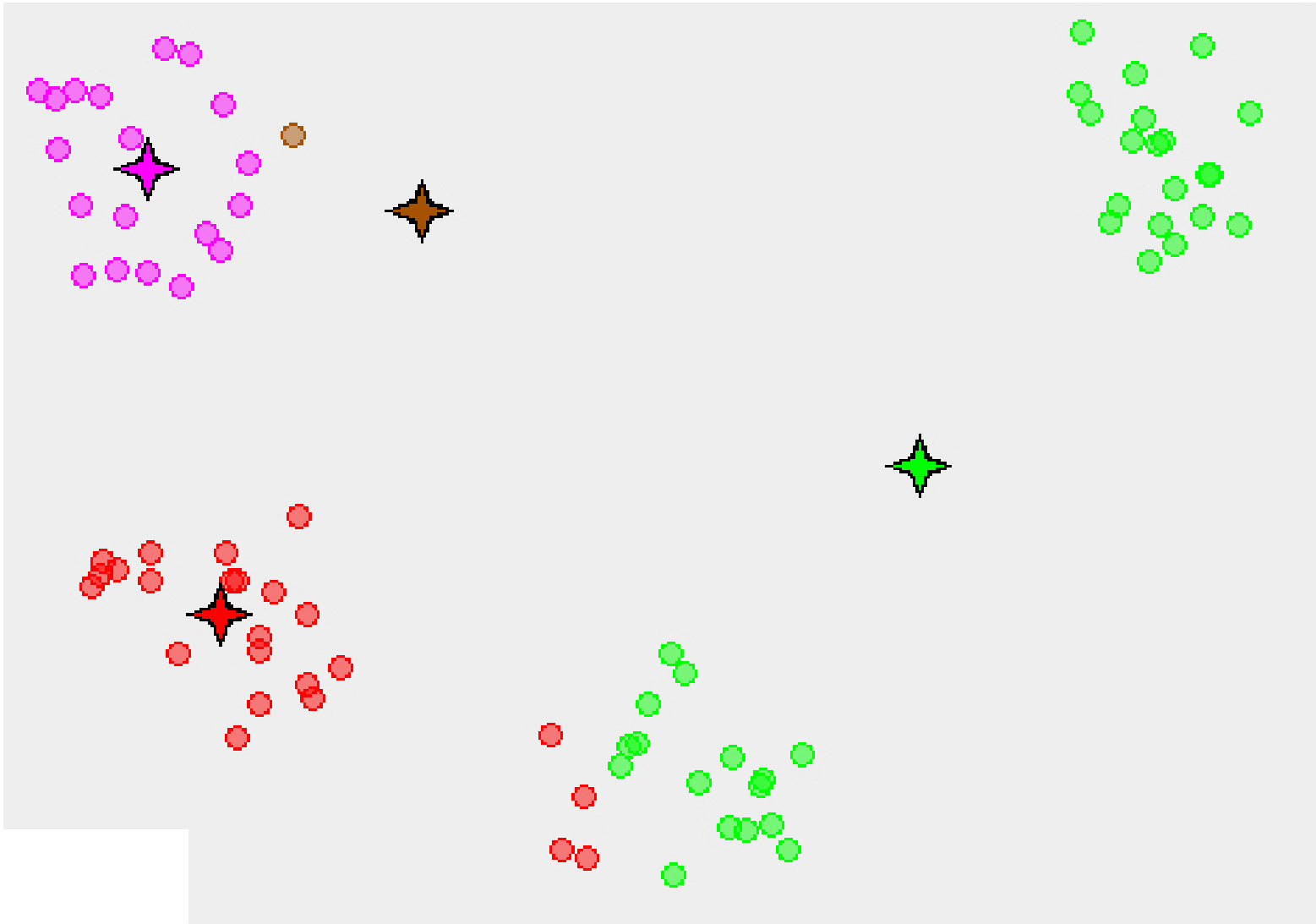
Initialization



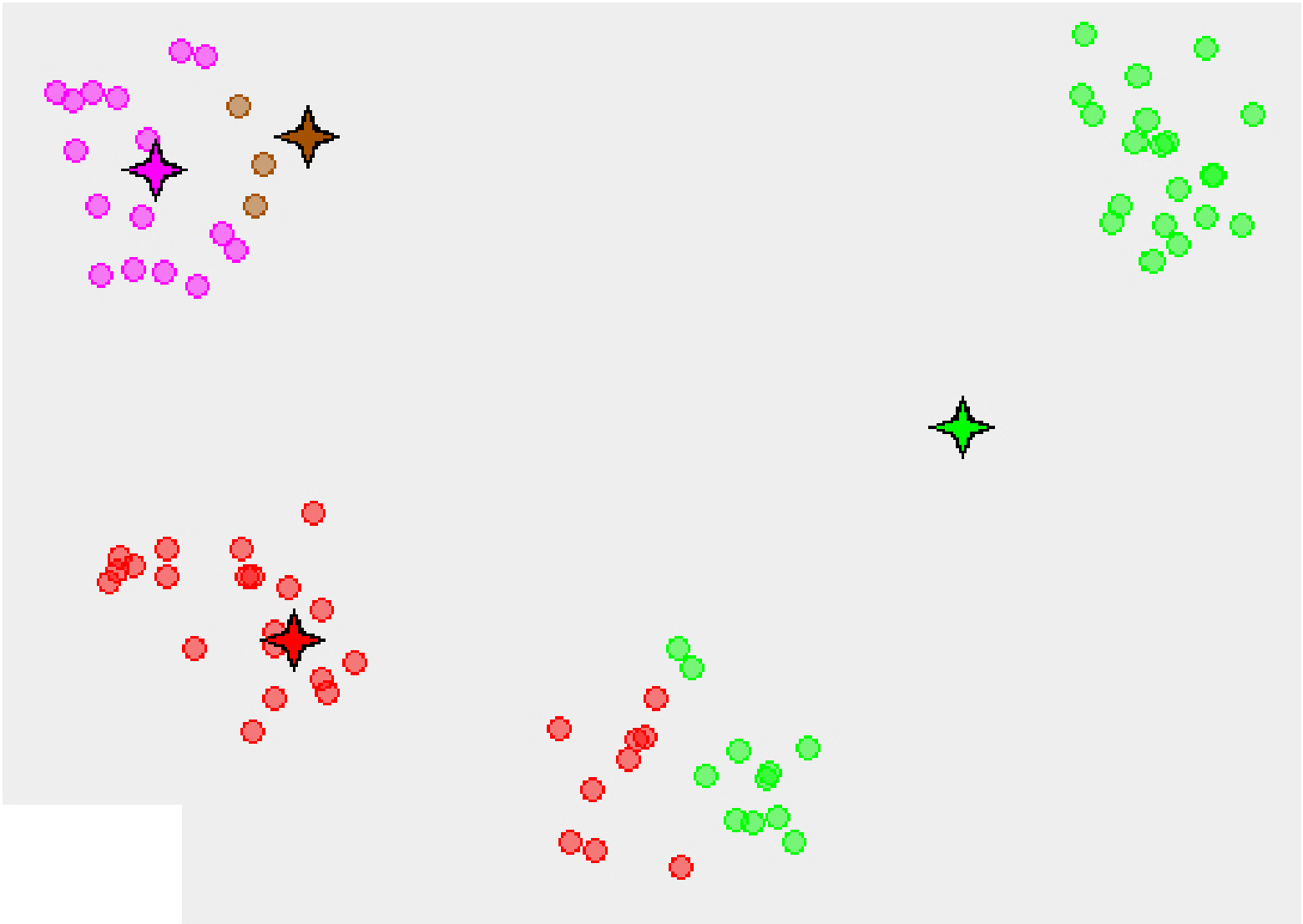
Lloyd's 1



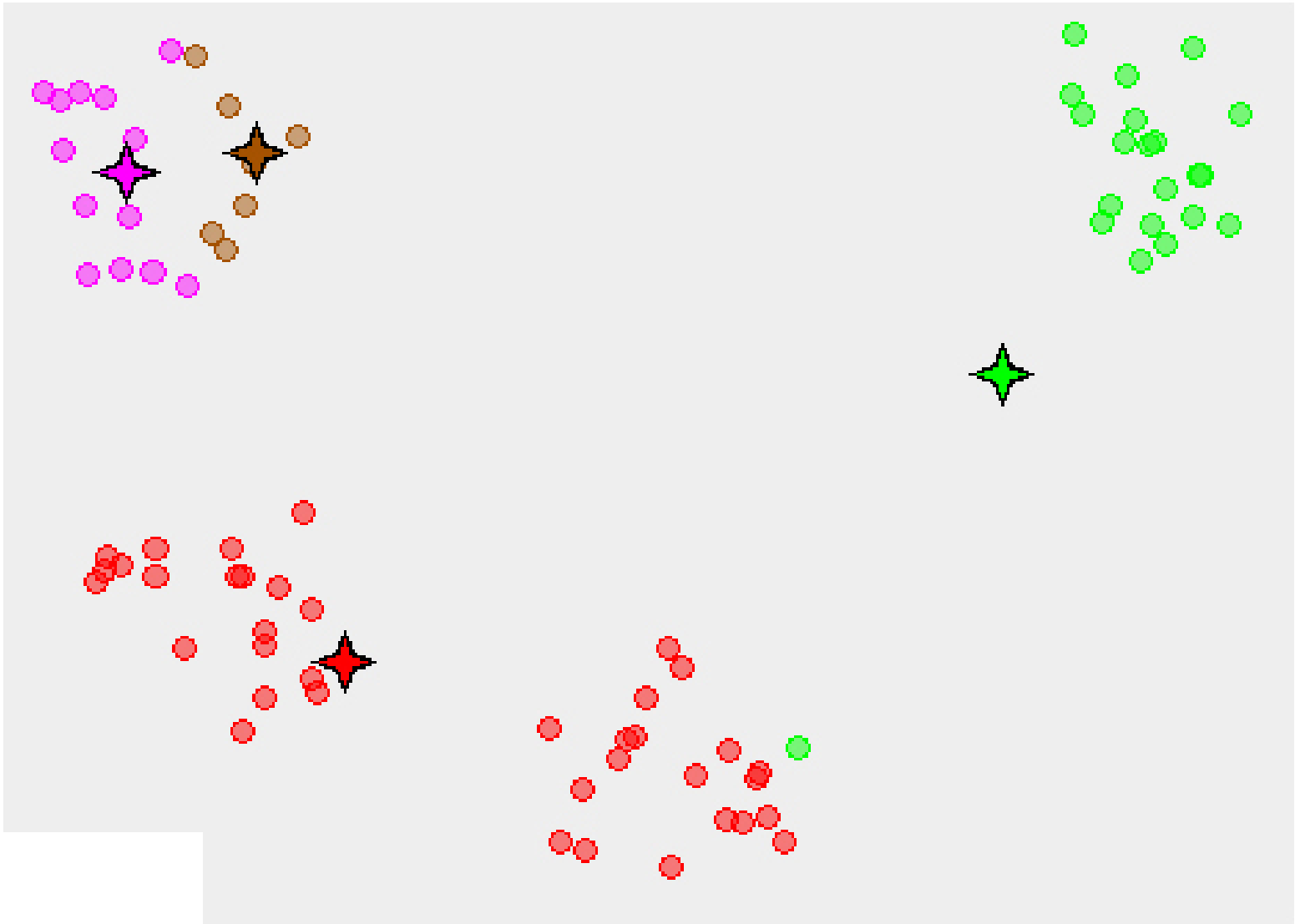
Lloyd's 2



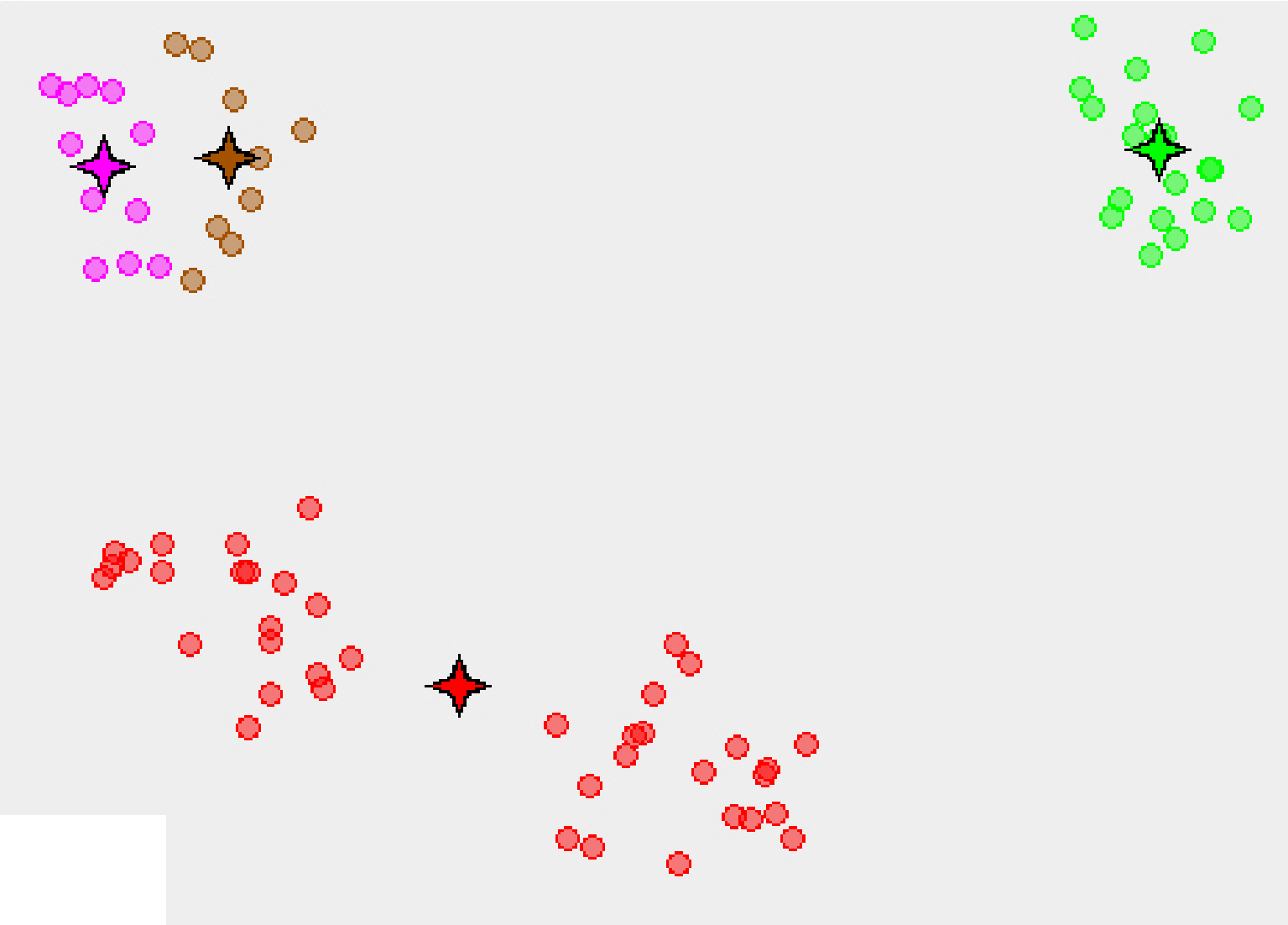
Lloyd's 3



Lloyd's 4



Final



Outline

k-medoids

Goal: Handle any distance metric; k-means only if consistent with mean.

k-medoids (PAM is simplest algorithm) use centroids that **belong** to the dataset:

Definition (Medoid)

The medoid of a set is the object of the set that minimizes total dissimilarity (distance) to all other objects in the set.

Objective function (cf. above): Minimize sum of distances to point's centroid.

vs k-means

-- k-means tends to select convex spherical clusters; k-medoids less so.

-- k-means is more sensitive to noisy data and outliers.

-- k-means is faster and easier to implement.

(Kaufman-Rousseeuw'87)

Partitioning Around Medoids (PAM)

Initialize k centroids randomly.

1. Assignment: Assign each object to nearest centroid; compute objective
2. Update:

for each centroid m **do**
for each non-centroid t **do**
Swap m and t, compute new objective function value.
end for
end for
Keep configuration (centroids) with min objective value.

Repeat steps 1 and 2 until there is no change of configuration (centroids).

Let distance calculation $= O(d')$. Update of Objective $= O((n-k)d')$, if 2nd best centroid known. Hence, update $= O((n-k)^2 kd') \sim n^2$.

Update of Objective cost function

Objective function: $J = \sum_{i=1}^{n-k} \text{dist}(i, c(i)),\ c(i) =$ centroid of i's cluster.

For each i store 2nd best centroid c'. Centroid m replaced by non-centroid t:

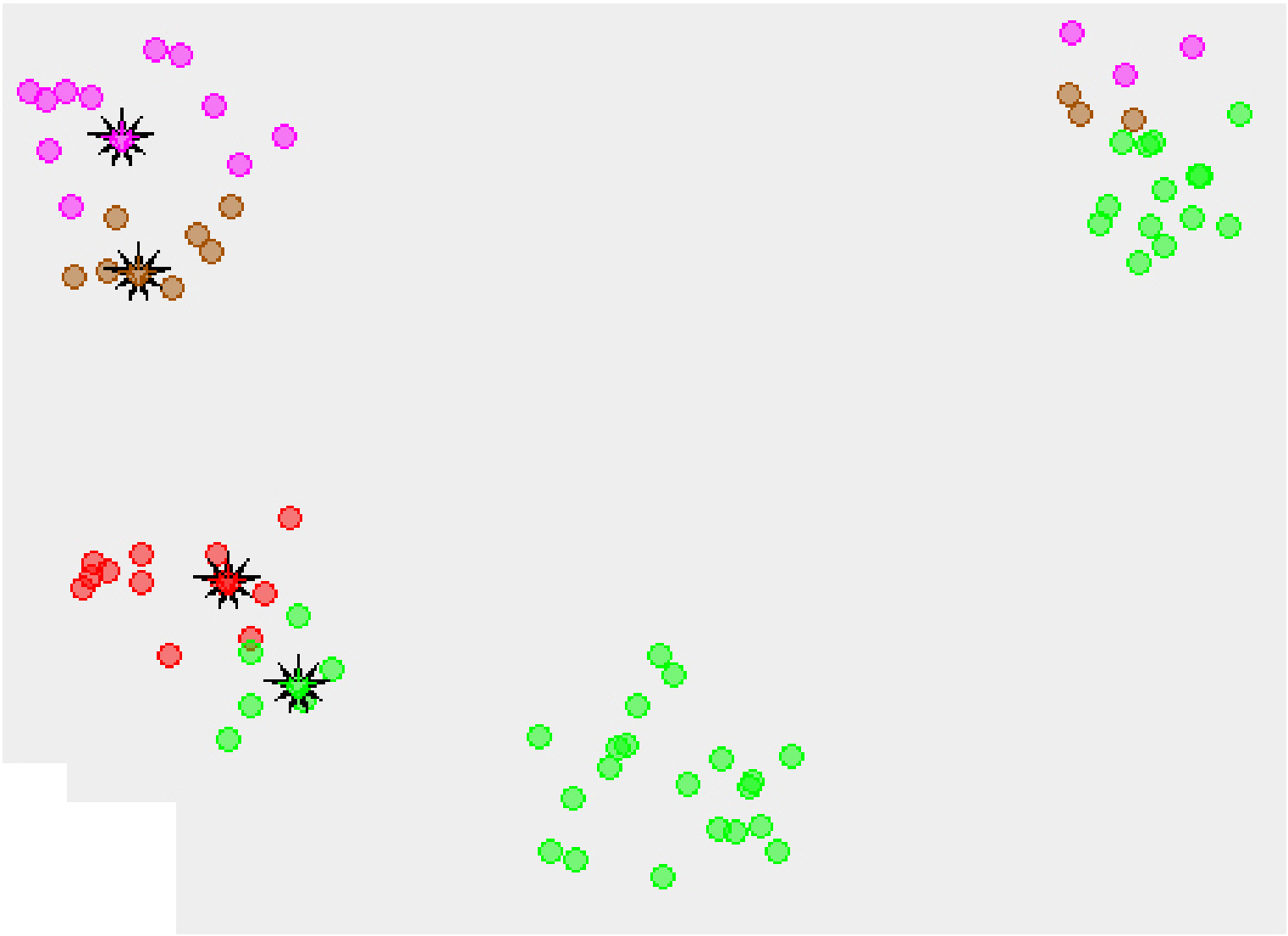
- For $i : c(i) = m$,

$$\Delta J = \begin{cases} \text{dist}(i,t) - \text{dist}(i,m), & \text{if } \text{dist}(i,t) \leq \text{dist}(i,c') : \text{ do nothing} \\ \text{dist}(i,c') - \text{dist}(i,m), & \text{if } \text{dist}(i,t) > \text{dist}(i,c') : \text{ assign } i \text{ to } c', \\ & \text{update } i\text{'s 2nd best centroid} \end{cases}$$

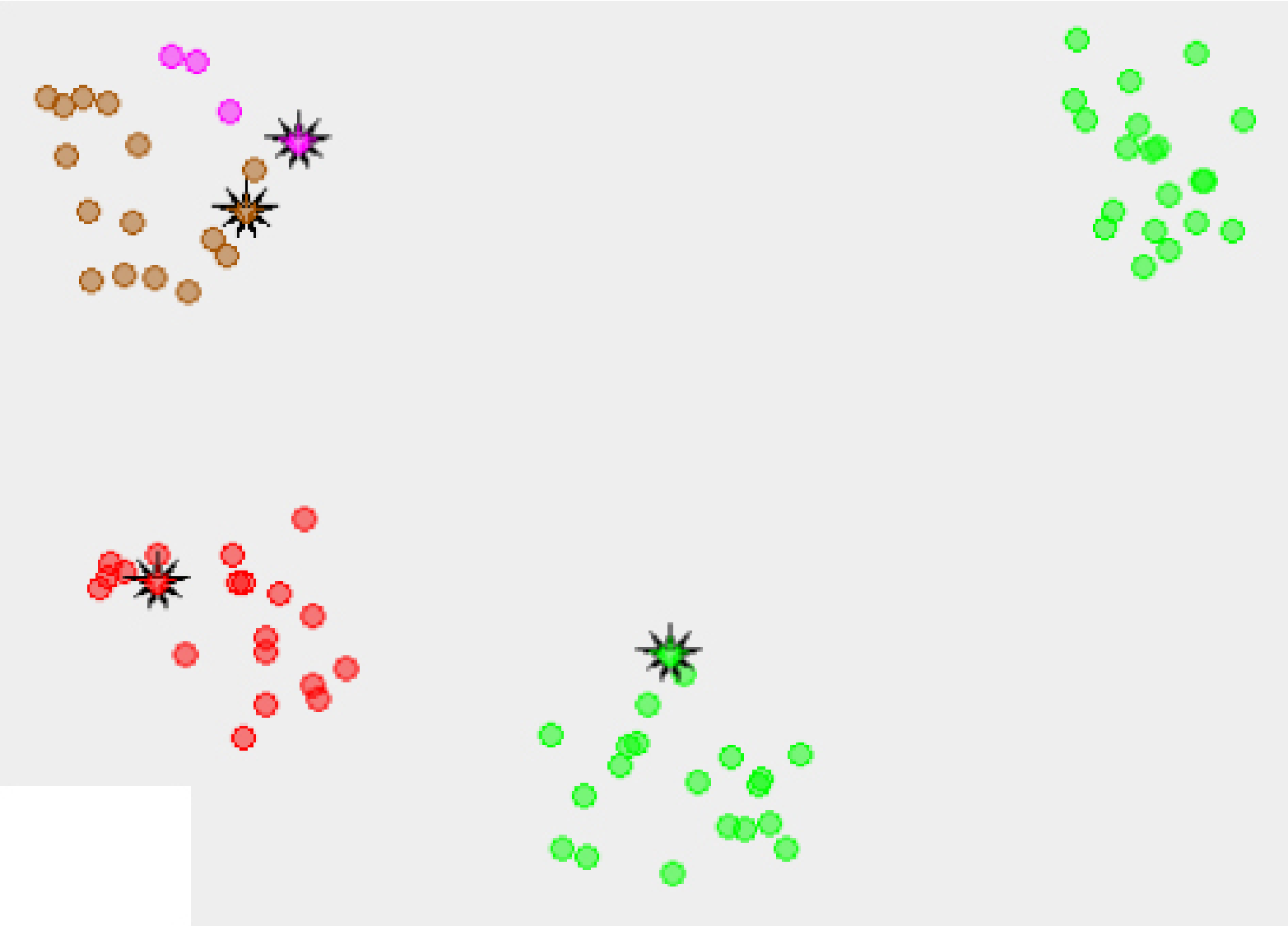
- For $i : c(i) \neq m$,

$$\Delta J = \begin{cases} 0, & \text{if } \text{dist}(i,t) \geq \text{dist}(i,c(i)) : \text{ do nothing} \\ \text{dist}(i,t) - \text{dist}(i,c(i)), & \text{if } \text{dist}(i,t) < \text{dist}(i,c(i)) : \text{ assign } i \text{ to } t \end{cases}$$

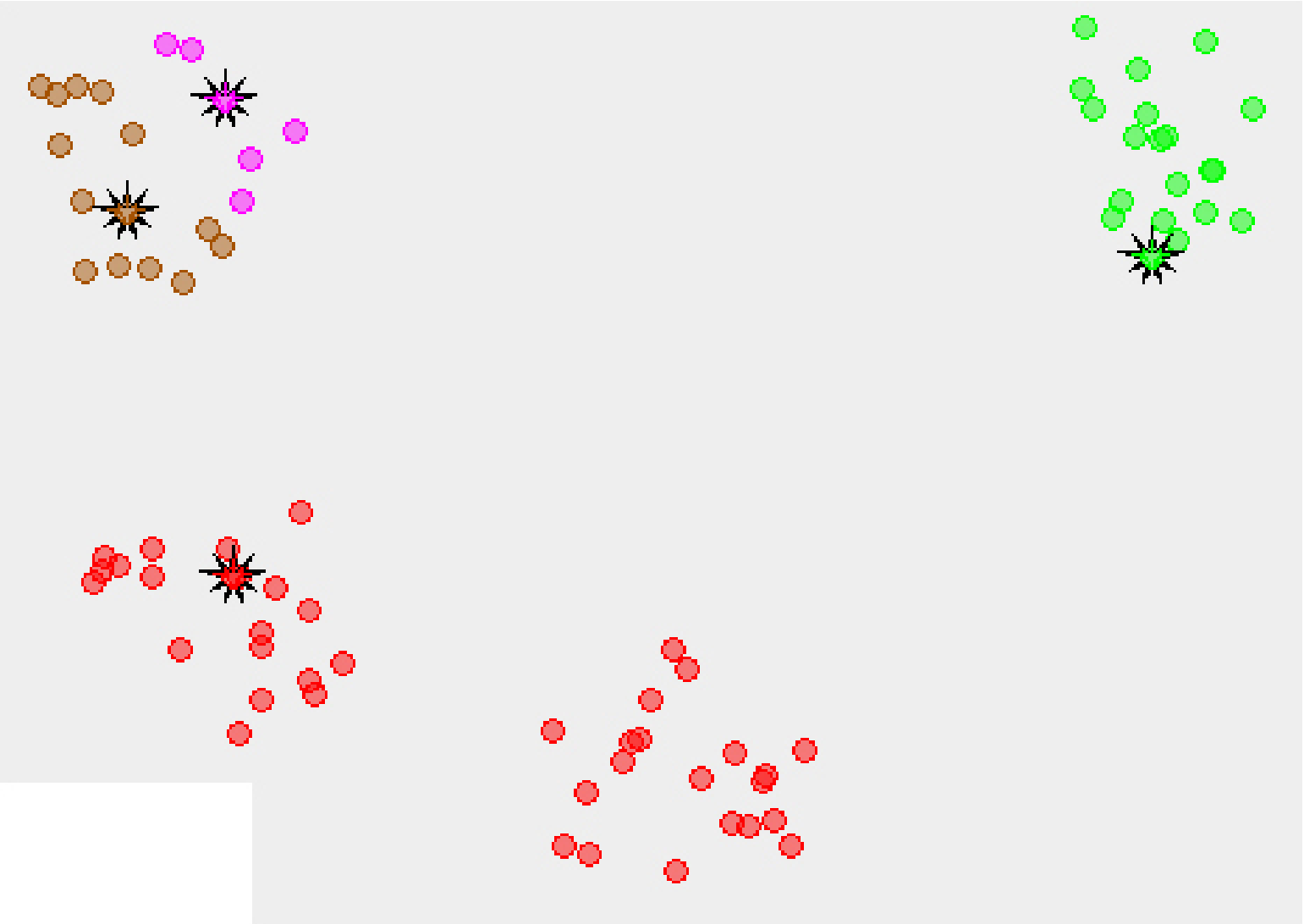
Initial



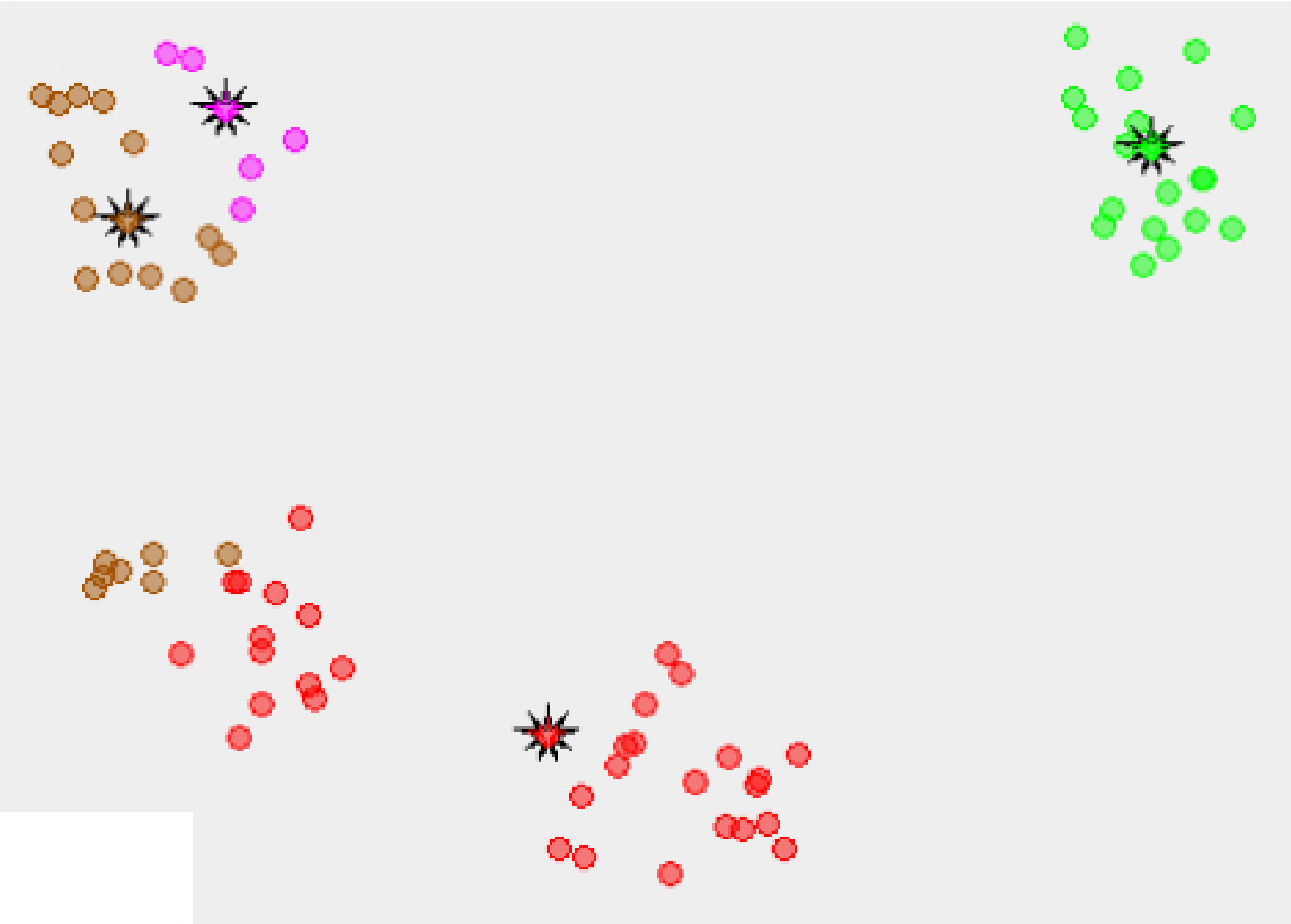
PAM 1



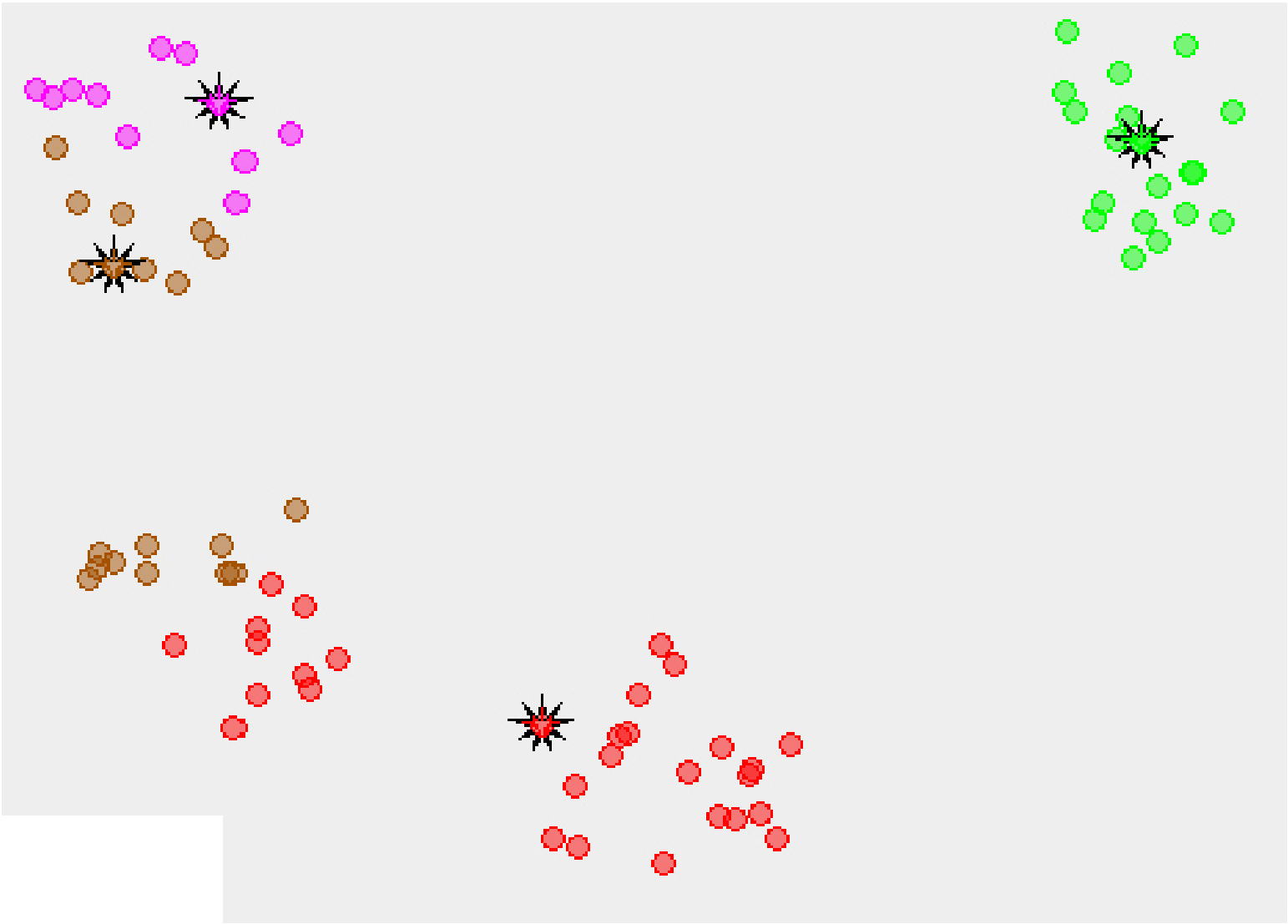
PAM 2



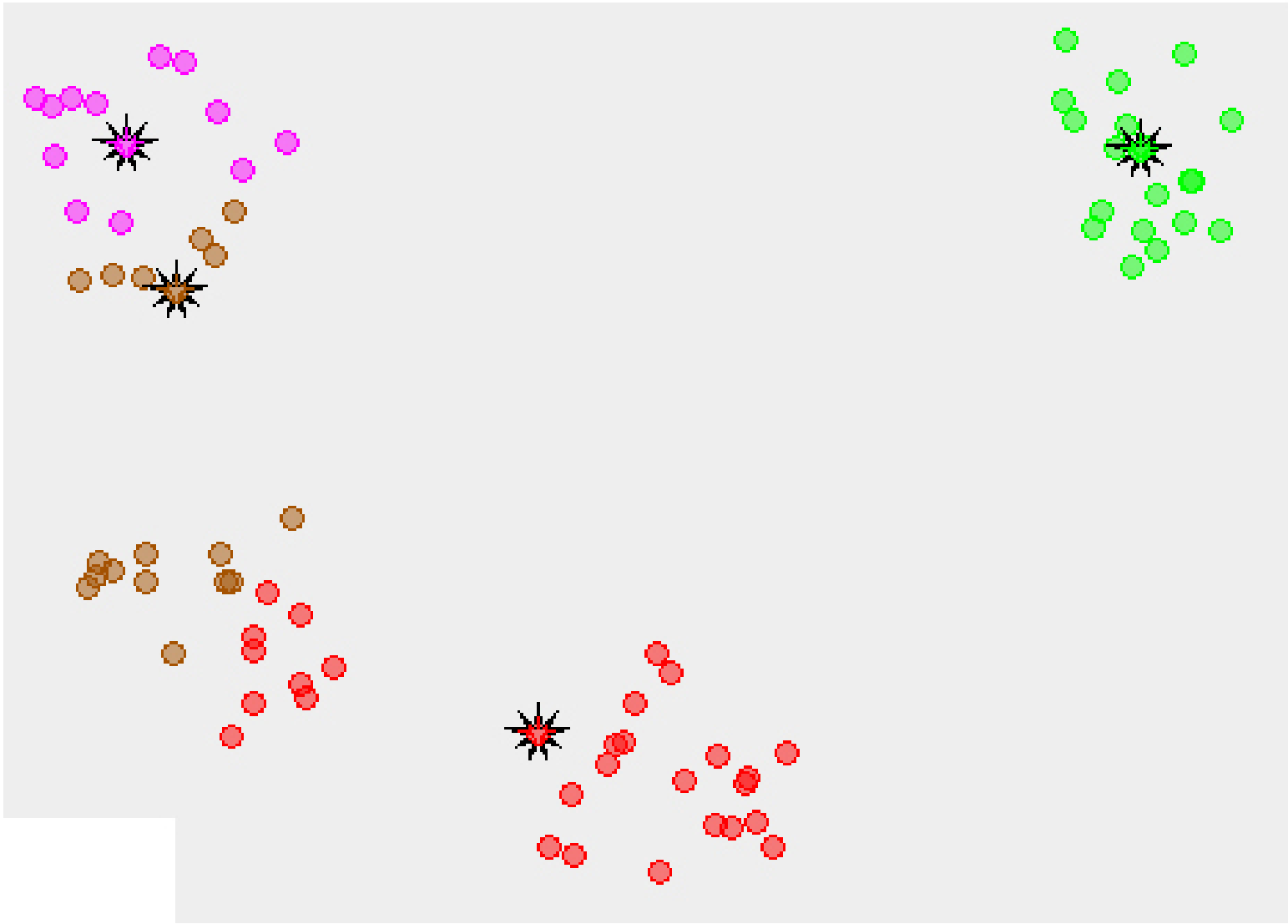
PAM 3



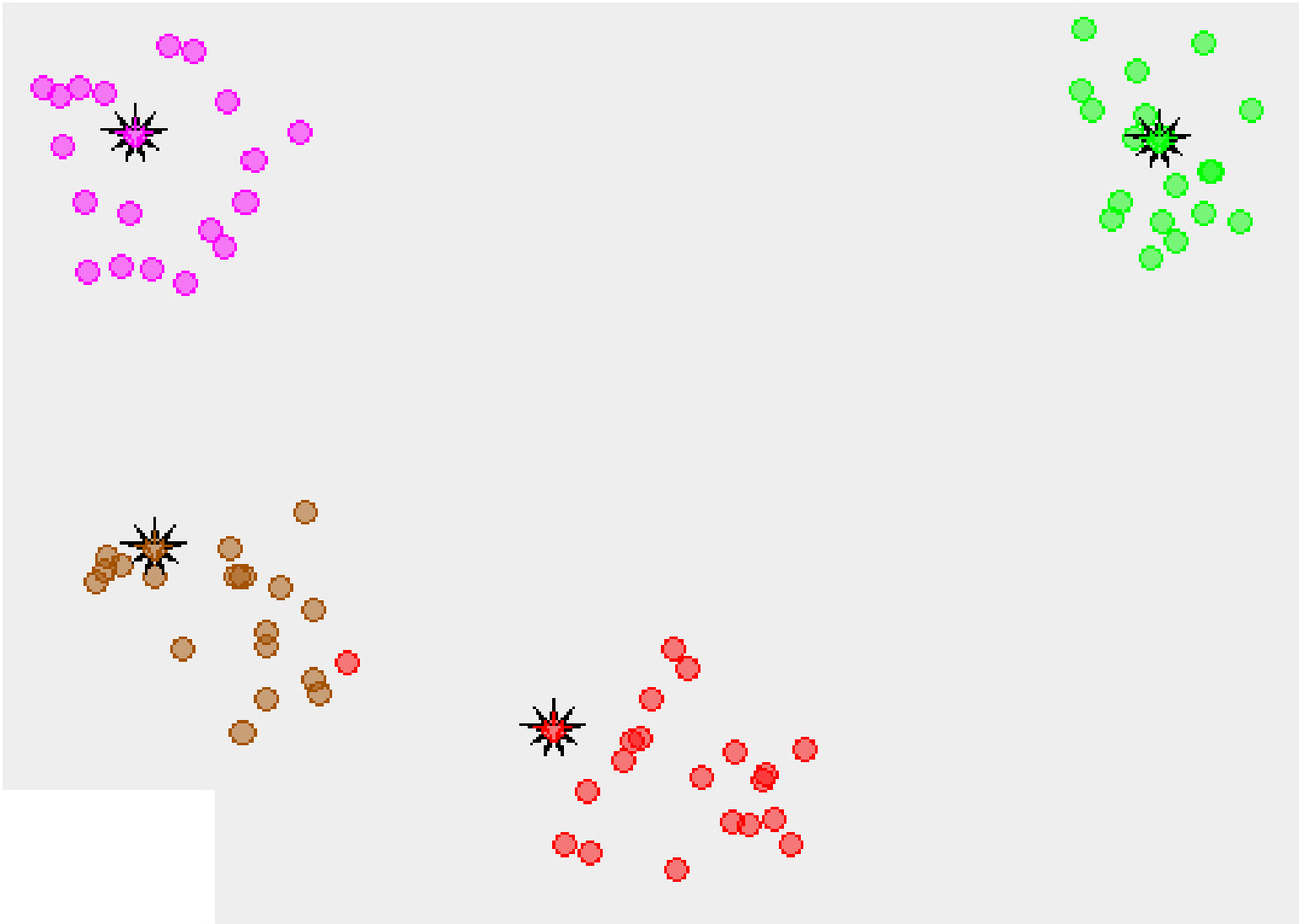
PAM 4



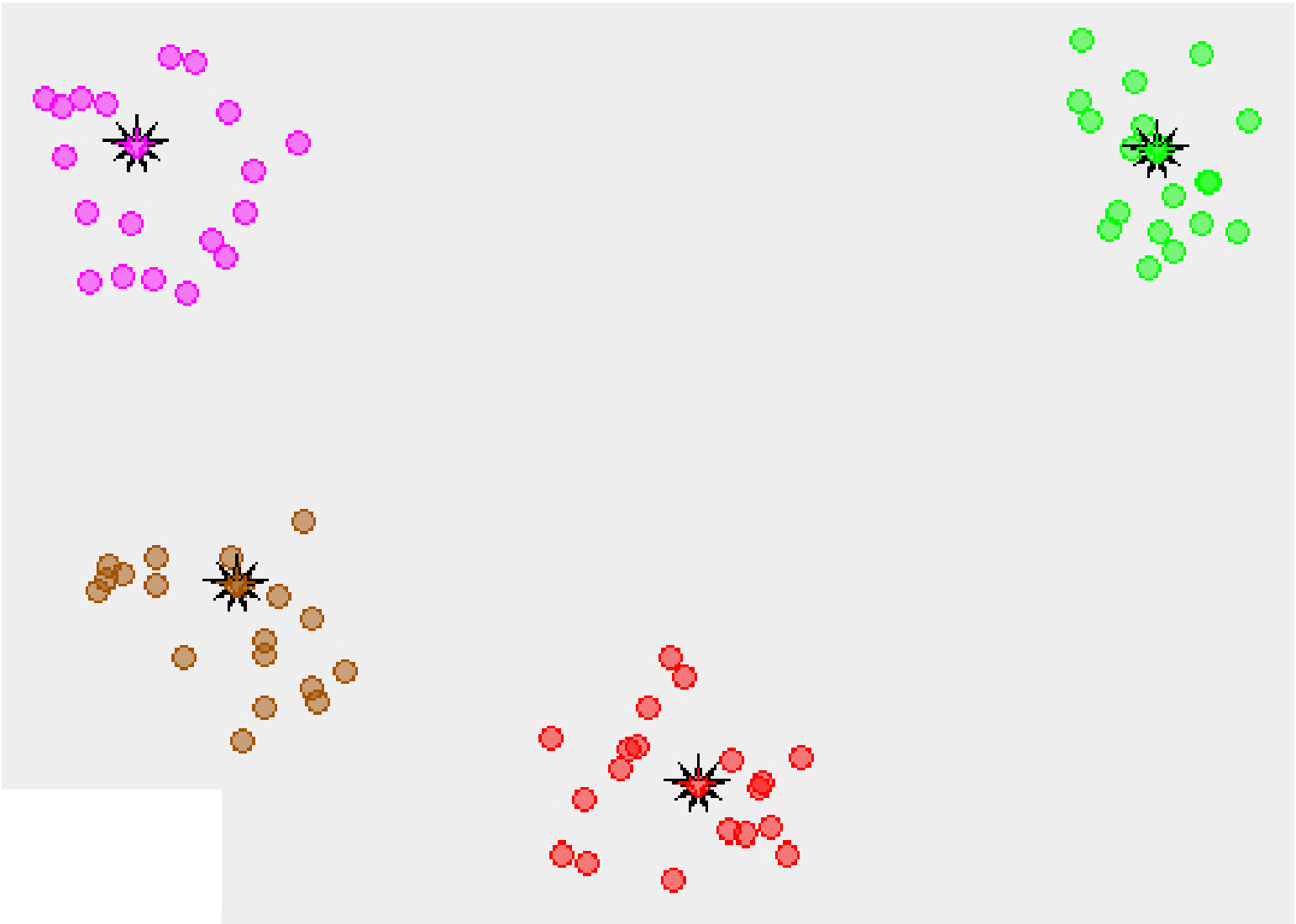
PAM 5



PAM 6



Final



Outline

Outline

Accelerating updates

Two faster updates, which may however lose accuracy compared to PAM.
Recall that after every swap we compute J in $O((n-k)d')$.

1. Improved Update

Instead of swapping centroid m with every point t, swap m only with every non-centroid in same cluster as m.

Complexity: $n-k$ iterations instead of $k(n-k)$, hence update $= O((n-k)^2 d')$

2. Update à la Lloyd's

For every cluster: (i) compute its medoid t, (ii) swap its current centroid m with t.

The medoid t minimizes $\sum_{i \in C} d(i,t)$ over all possible objects t in cluster C.
Computed in $O(a^2 d')$, assuming clusters have $a \simeq n/k$ items.

Total Complexity $= O((ka^2 + k(n-k))d') = O((n^2/k + nk)d') = O(n^2 d')$
(Park-Jun'09).

Outline

Clustering Large Applications (CLARA)

General Idea: run entire algorithm with sample of size $n' \ll n$. Use s samples drawn independently, return best clustering.

Overall algorithm:

for $i = 1, \ldots, s$ **do**
    apply PAM on a random (uniform) sample of size n'
    assign n points to k computed centroids
    calculate the total cost of the partitioning
end for
return best partitioning

Experimental results recommend: $s = 5$, $n' = 40 + 2k$.

CLARA based on RANdomised Search (CLARANS)

- Update: swap m's with t's, for some randomly selected (m, t)'s only.
- Picking random $Q \subset \{1, \ldots, k\} \times \{1, \ldots, n-k\}$, s times.

Select k centroids by some initialization method.
for $i = 1, \ldots, s$ **do**
    Cluster $n - k$ points to k centroids by some assignment method.
    Randomly select set Q of $|Q|$ pairs (m, t), $|Q| < k(n-k)$.
    for $(m, t) \in Q$ **do**
        Swap m with t; compute new objective value.
    end for
    Keep centroids with minimum objective value over $|Q|$ choices.
end for
Output centroids yielding minimum objective value over s candidates.

Experimentals recommend: $s = 2$, $|Q| = \max\{0.12 \cdot k(n-k), 250\}$.
(Ng-Han:IEEE Tran.Know.Data Eng'02) (Theodoridis et al.:Patt.Recognition,ch.14)

Implement CLARANS

Consider a dataset of n points/objects with k clusters.
How to choose one uniformly distributed pair from

$$\{(m, t) : \ m = 0, \ldots, k-1, \ t = 0, \ldots, n-1\}.$$

Pick a uniformly distributed integer $x \in [0, kn-1]$ and return

$$(x \bmod k, \ \left\lfloor \frac{x}{k} \right\rfloor).$$

PAM vs CLARA / CLARANS

CLARA / CLARANS are approximations of PAM, but: CLARA applies to the overall algorithm, while CLARANS is an approximation of the update.

CLARANS is in $O(n^2)$, CLARA is significantly faster.

CLARANS leads to a better clustering, especially if CLARA's random sample is biased.

Both methods rely heavily on their random choices/parameters.

Outline

Improve Initialisation 1: Spread-out

initialization++ : k-means++ / k-medoids++:

(1) Choose a centroid uniformly at random; $t \leftarrow 1$.

(2) $\forall$ non-centroid point $i = 1, \ldots, n - t$, let $D(i) \leftarrow$ min distance to some centroid, among t chosen centroids.

(3) Choose new centroid: r chosen with probability proportional to $D(r)^2$:

$$\text{prob}[\text{choose } r] = D(r)^2 / \sum_{i=1}^{n-t} D(i)^2.$$

Let $t \leftarrow t + 1$.

(4) Go to (2) until $t = k =$ given #centroids.

Expected approximation ratio $= O(\log k)$ (Arthur-Vassilvitskii:SODA'07)

Implement initialization++

Given $D(i) > 0$, $i = 1, \ldots, n - t$, compute $n - t$ (`float`) partial sums

$$P(r) = \sum_{i=1}^{r} D(i)^2, \quad r = 1, \ldots, n - t,$$

and store them in an array (or binary tree) P. To avoid the $P(r)$'s being very large, we may normalize all $D(i)$'s by dividing them by $\max_i D(i)$.

Pick a uniformly distributed `float` $x \in [0, P(n - t)]$ and return

$$r \in \{1, 2, \ldots, n - t\} \ : \ P(r - 1) < x \leq P(r),$$

where $P(0) = 0$: r chosen with probability proportional to $P(r) - P(r - 1) \sim D(i)^2$. Can find r by binary search in array P.

Improve Initialisation 2: Concentrate

Select centroids close to dataset's center of mass (and to each other) as follows.

(1) Calculate symmetric $n \times n$ distance matrix of all objects, i.e. all distances d_{ij} from every object $i = 1, \ldots, n$ to every other object $j = 1, \ldots, n$, $i \neq j$.
(2) For object i compute

$$v_i = \sum_{j=1}^{n} \frac{d_{ij}}{\sum_{t=1}^{n} d_{jt}}, \qquad i = 1, \ldots, n.$$

(3) Return the k objects with k smallest v_i values.

Algorithm proposed in (Park-Jun'09).

Outline

Assignment by direct method

Exact approach for small data

At each iteration:

1. For every point, compute distance to every centroid.
2. Return (exact) nearest centroid.

Approximate approach for big data

At each iteration:

1. Index k centroids into data-structure, e.g. LSH hashtables.
2. For every non-centroid point, run ANN to find nearest centroid.
3. Return (approximate) nearest centroid.

This is the standard approach in almost all big data implementations today.

Assignment by Range search

Reverse approach (LSH/DBH)

- Index n points into L hashtables: once for entire algorithm.
- LSH/DBH TableSize $\leq n/8$: avoid buckets with very few items.
- At each iteration, for each centroid c, range/ball queries centered at c.
- Mark assigned points: either move them at end of LSH buckets (and insert "barrier", or mark them using "flag" field).
- Increase radii by $\times 2$, start with min(dist between centers)/2, until all points assigned, or most ranges/balls do not assign a new point.
- For a given radius, if a point lies in ≥ 2 balls, compare its distances to the respective centroids, assign to closest centroid.
- At end: for every unassigned point, compare its distances to all centroids

Outline

Internal evaluation

Evaluate clustering without reference to objective function. Try to capture meaning of clustering.

- Let k be the number of computed clusters.
- Internal evaluation considers the given pointset and the clusters, produces quality coefficient for each partition; k may be a parameter.
- External evaluation: use known class labels and benchmarks; often created by humans.

In the sequel we present internal evaluation methods, mainly Silhouette.

Silhouette

-- For $1 \leq i \leq n$, $a(i) =$ average distance of i to other objects in same cluster.
-- Let $b(i) =$ average distance of i to objects in *next best* (neighbor) cluster, i.e. cluster of 2nd closest centroid.

Silhouette of Object i

$$s(i) = \frac{b(i) - a(i)}{\max\{a(i), b(i)\}} = \left\{ \begin{array}{ll} 1 - a(i)/b(i), & \text{if } a(i) < b(i) \\ 0, & \text{if } a(i) = b(i) \\ b(i)/a(i) - 1, & \text{if } a(i) > b(i) \end{array} \right\} \in [-1, 1].$$

Interpret silhouette

$s(i) \to 1$: i seems correctly assigned to its cluster;
$s(i) \simeq 0$: borderline assignment (but not worth to change);
$s(i) \to -1$: i would be better if assigned to next best cluster.

Silhouette: Cluster and clustering

Specific clusters

-- Evaluate a cluster: Compute average $s(i)$ over all i in some cluster.

-- If k is too large or too small, some clusters shall display much smaller silhouettes than the rest.

-- Silhouette plots are used to improve k: try different k's and see if clusters have roughly equal silhouettes.

Overall Clustering

Overall Silhouette coefficient = average $s(i)$ over $i = 1, \ldots, n$.

High if well clustered, low may indicate bad k (or existance of outlier points).