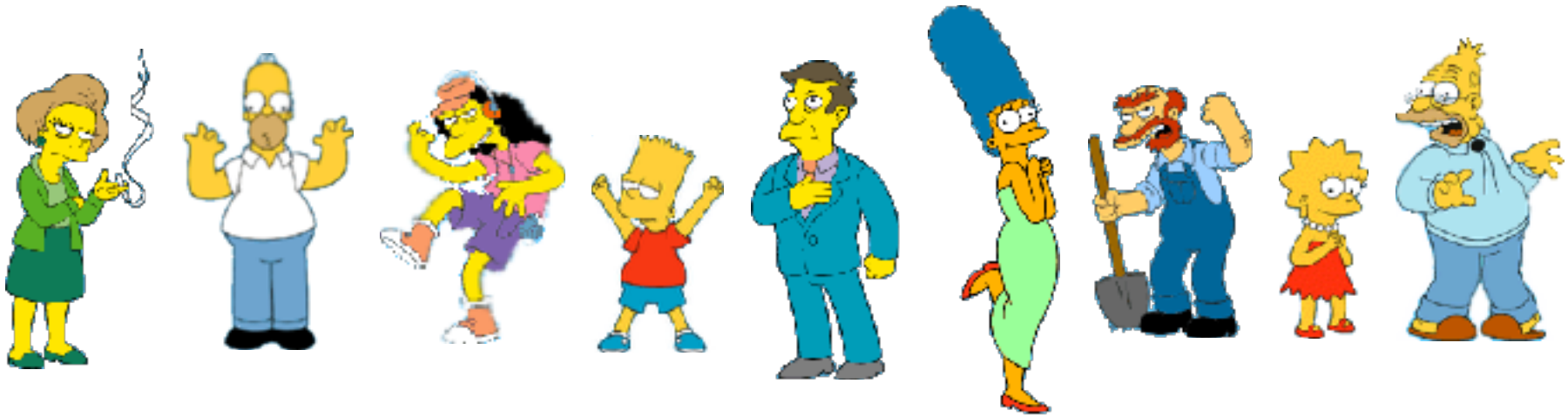
K-means clustering algorithm

What is Clustering?

- Organizing data into classes such that there is
  - high intra-class similarity
  - low inter-class similarity
- Finding the class labels and the number of classes directly from the data (in contrast to classification).
- More informally, finding natural groupings among objects.

What is a natural grouping among these objects?



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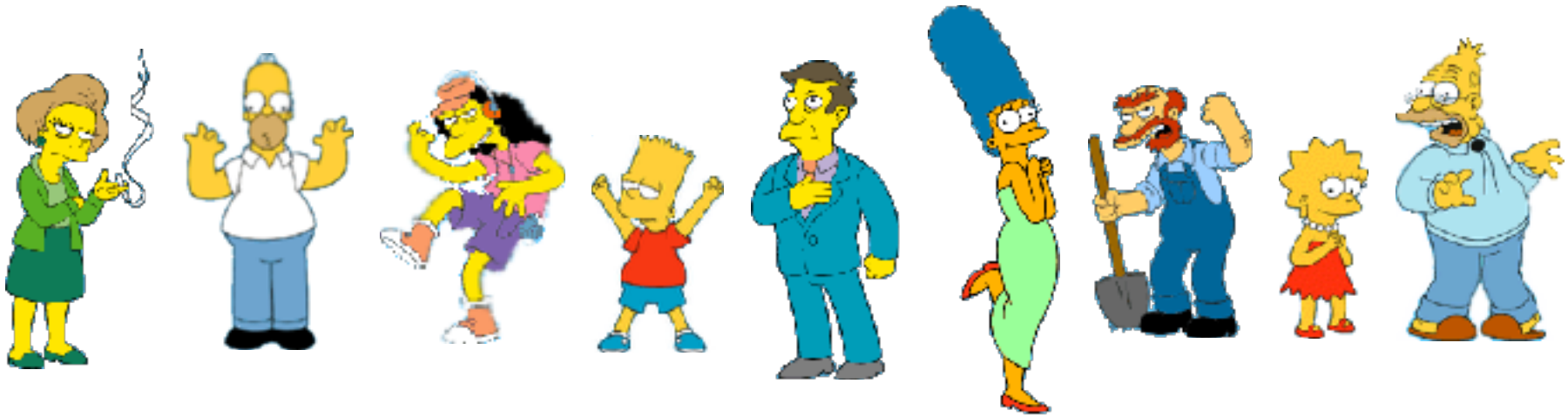
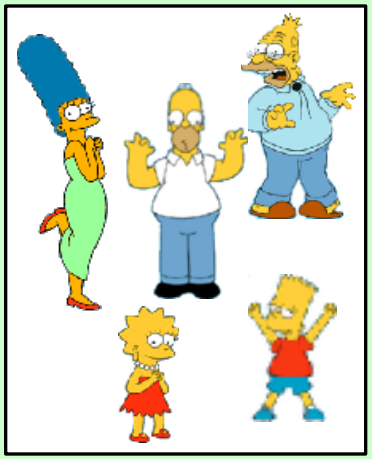
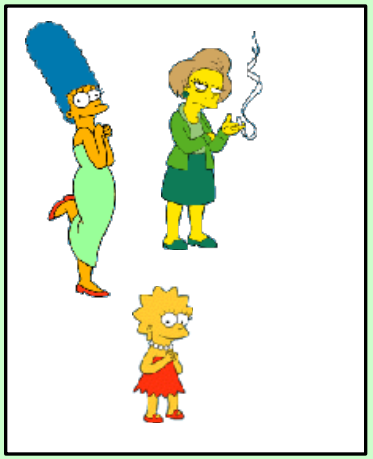


Clustering is subjective



Simpson's Family

School Employees

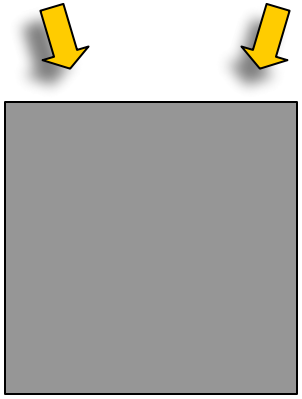


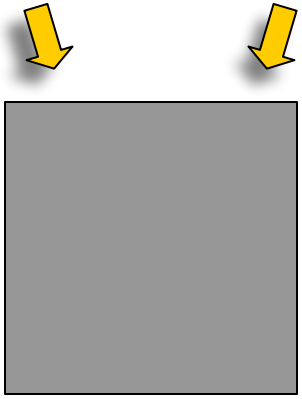
Females

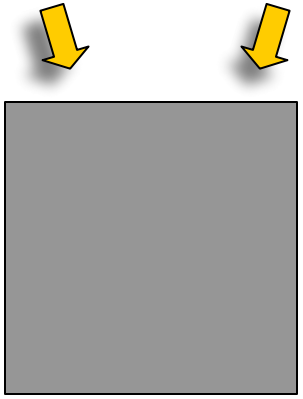
Males

Defining Distance Measures

Definition: Let O_1 and O_2 be two objects from the universe of possible objects. The distance (dissimilarity) between O_1 and O_2 is a real number denoted by $D(O_1,O_2)$







0.23

3

342.7

Consider a Set of Data Points,

$$X = \{x_1, x_2, \ldots, x_n\} \qquad x_i = \begin{pmatrix} x_{i1} \\ x_{i2} \\ . \\ . \\ . \\ x_{id} \end{pmatrix}_{d \times 1}$$

And a Set of Clusters,

$$C = \{c_1, c_2, \ldots, c_K\}$$

The Goal,

$$\mu_k = mean\ of\ the\ cluster\ c_k$$

The squared error,

$$J(c_k) := \sum_{x_i \in c_k} \|x_i - \mu_k\|^2$$

The sum of squared errors,

$$J(C) := \sum_{k=1}^{K} \sum_{x_i \in c_k} \|x_i - \mu_k\|^2$$

Algorithm *k-means*

1. Randomly choose K data items from X as initial centroids.

2. Repeat

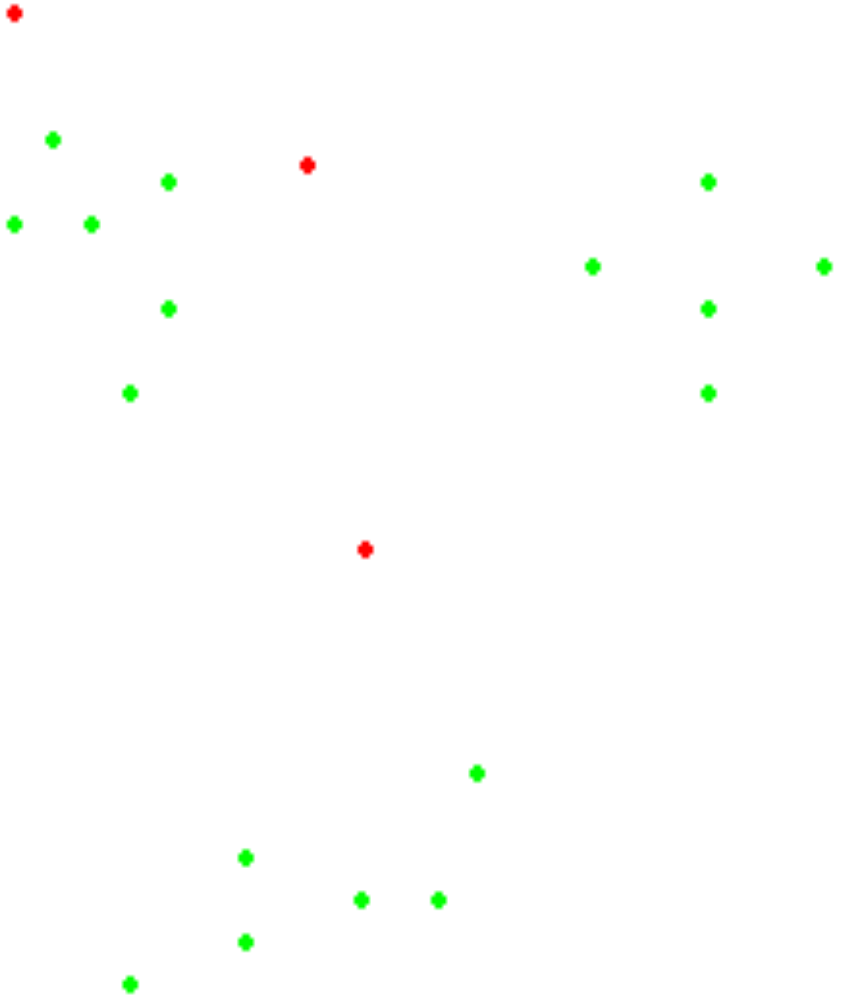
   - Assign each data point to the cluster which has the closest centroid.
   - Calculate new cluster centroids.

   Until the convergence criteria is met.

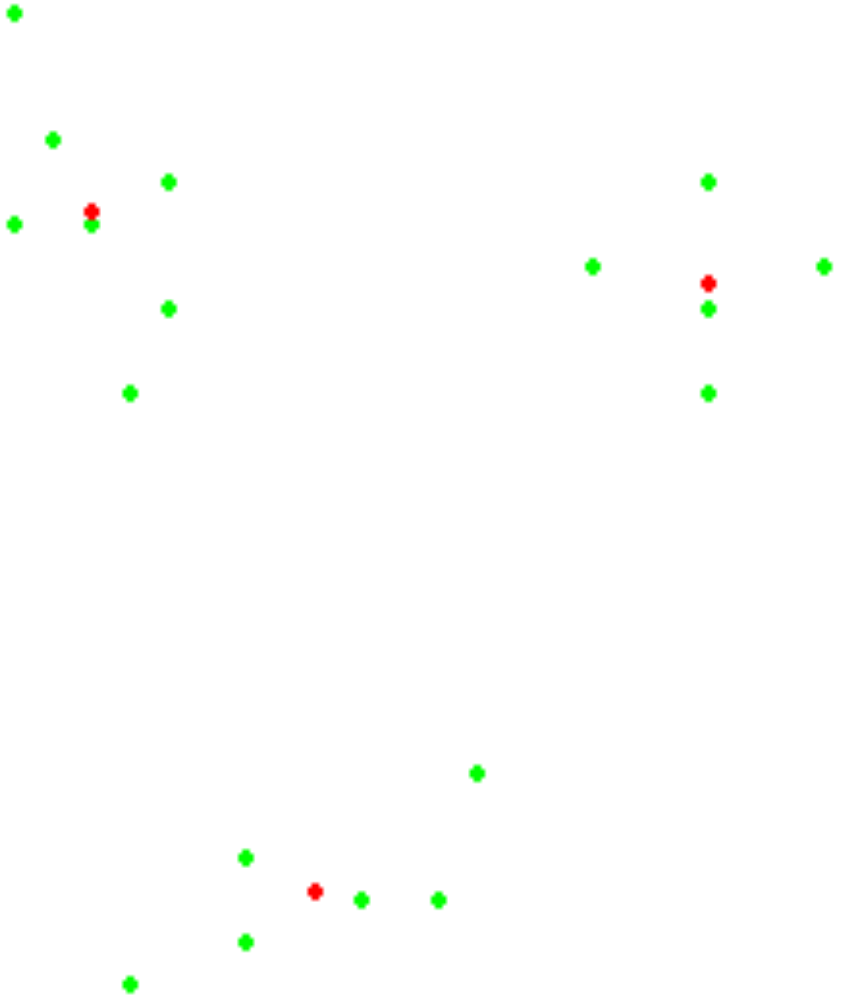
The data points

Initialization

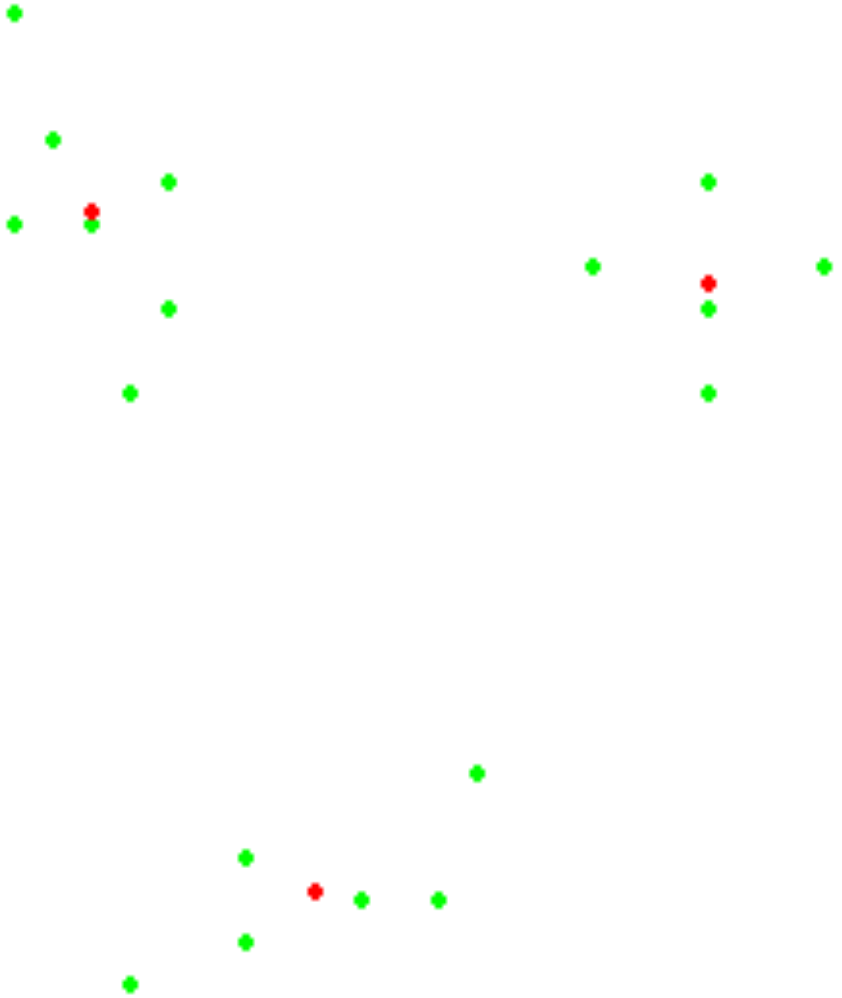
#Runs = 1



#Runs = 2

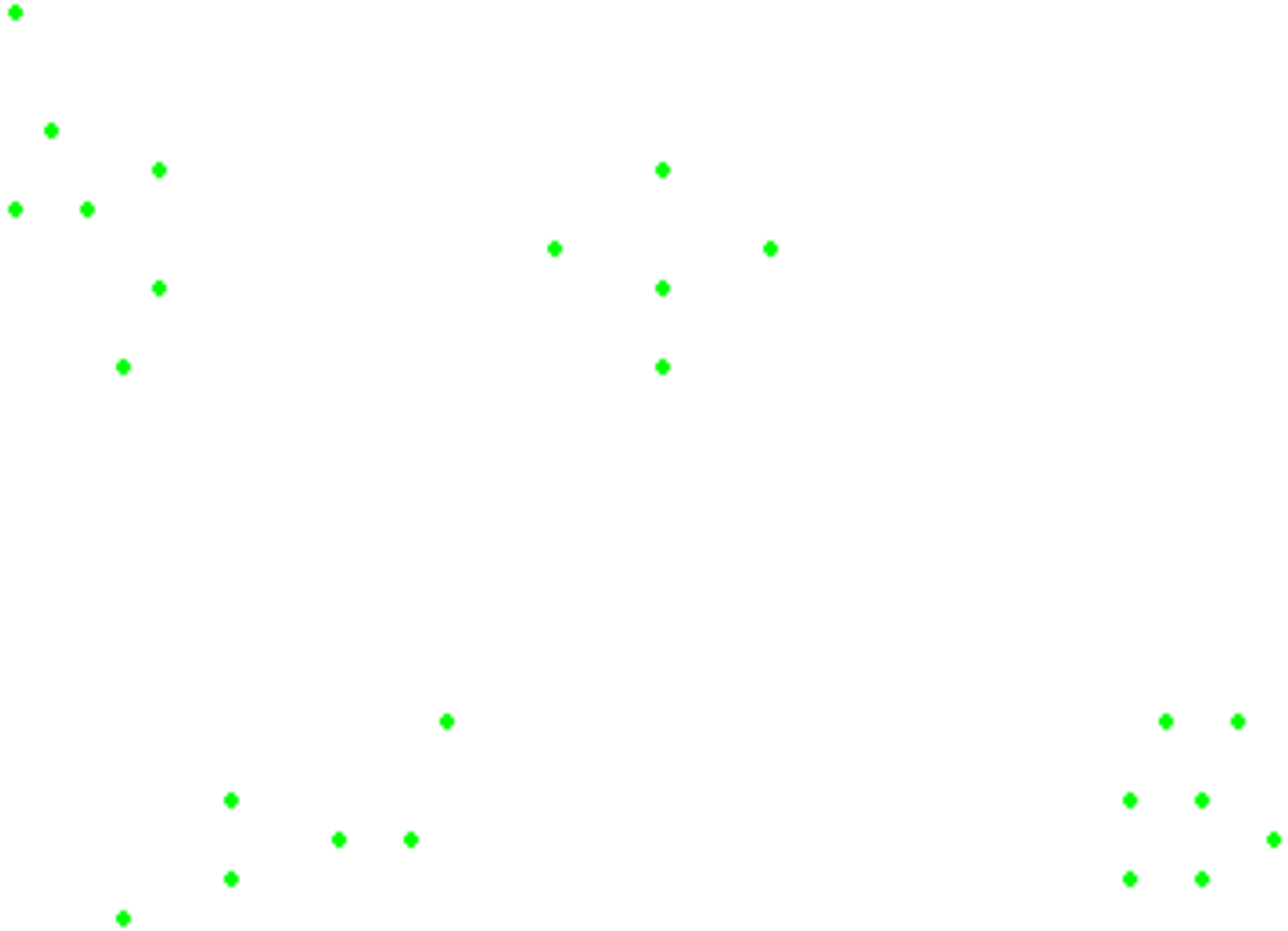


#Runs = 3

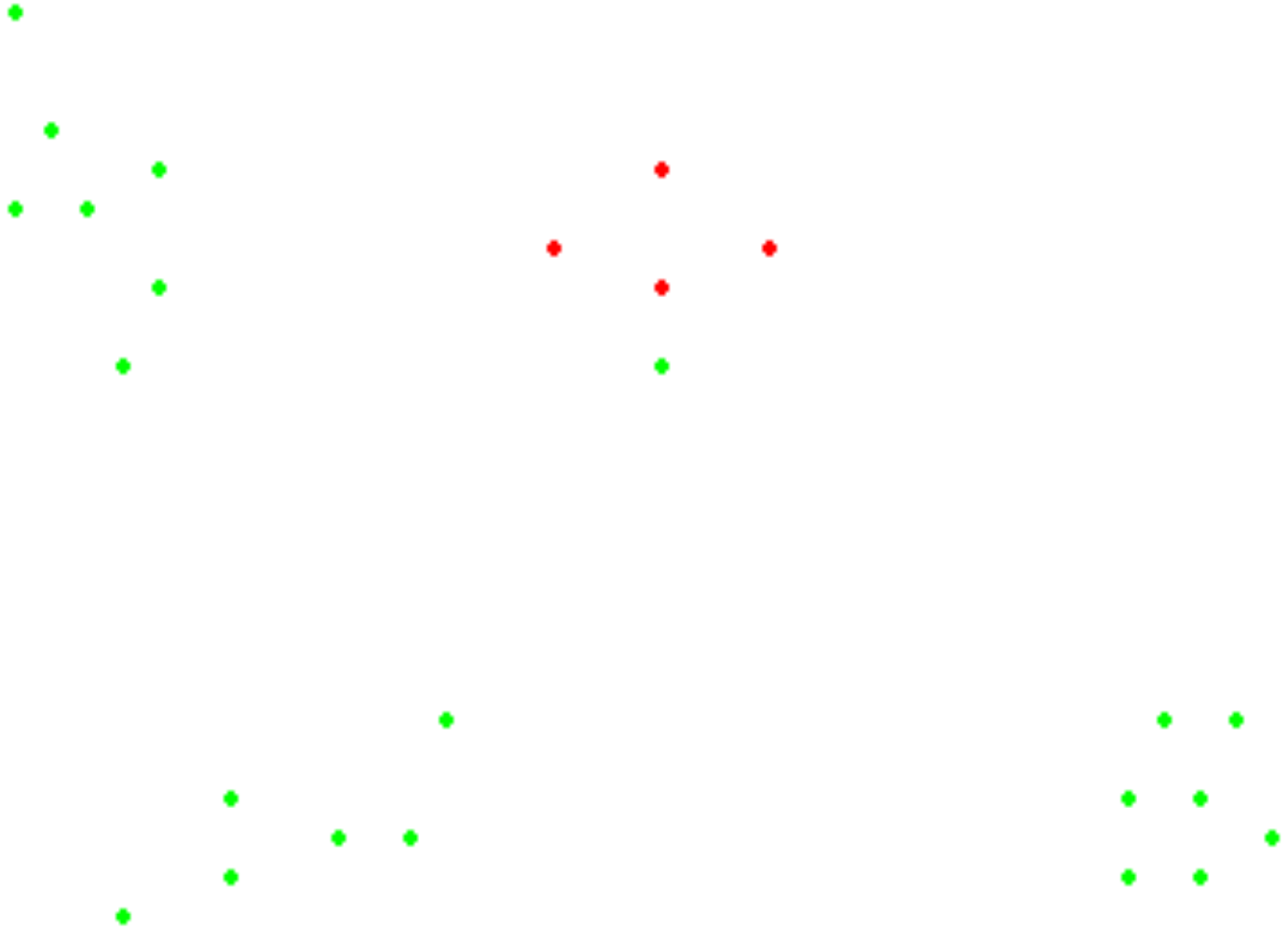


K-means gets stuck in a local optima

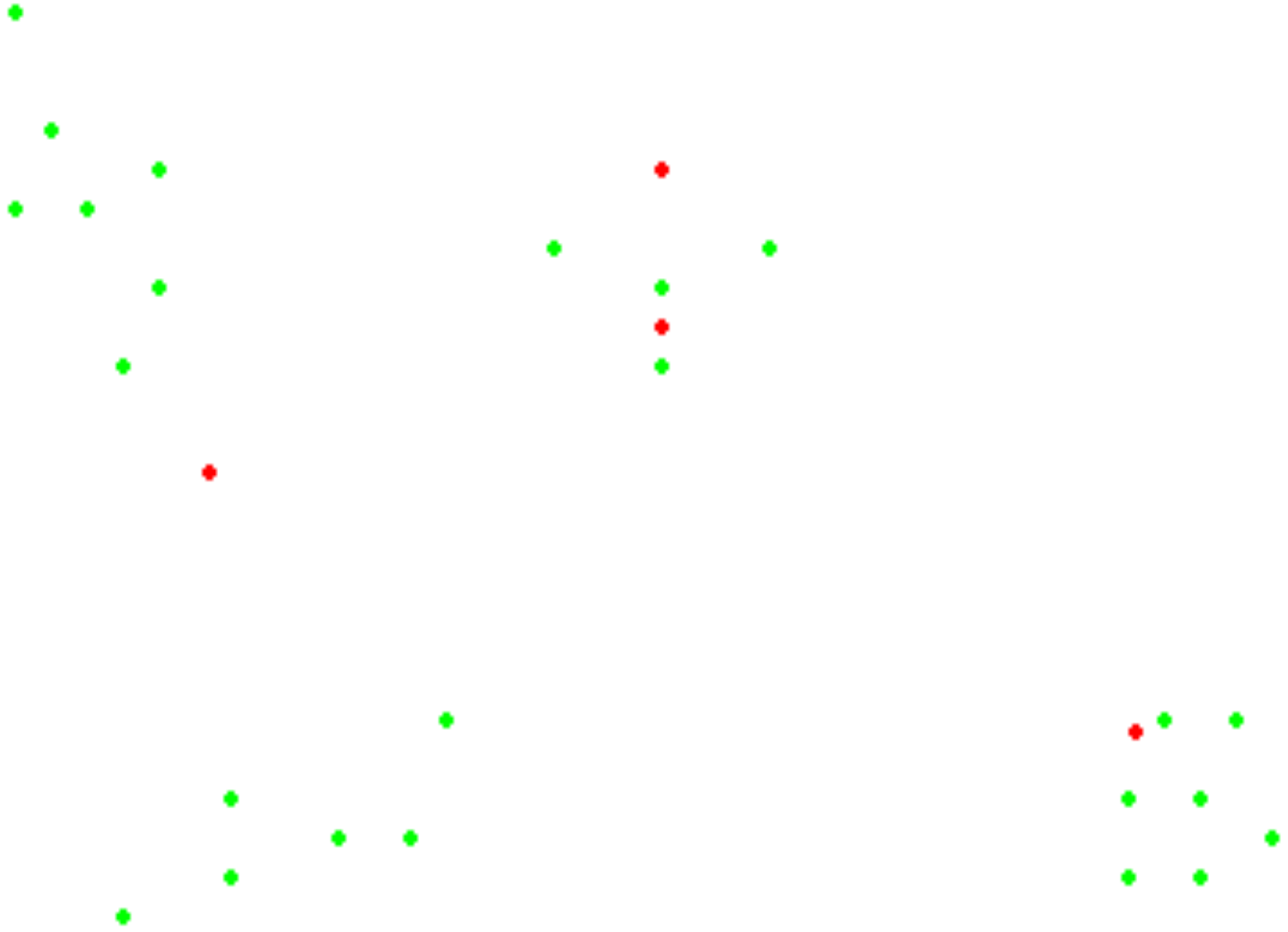
The data points



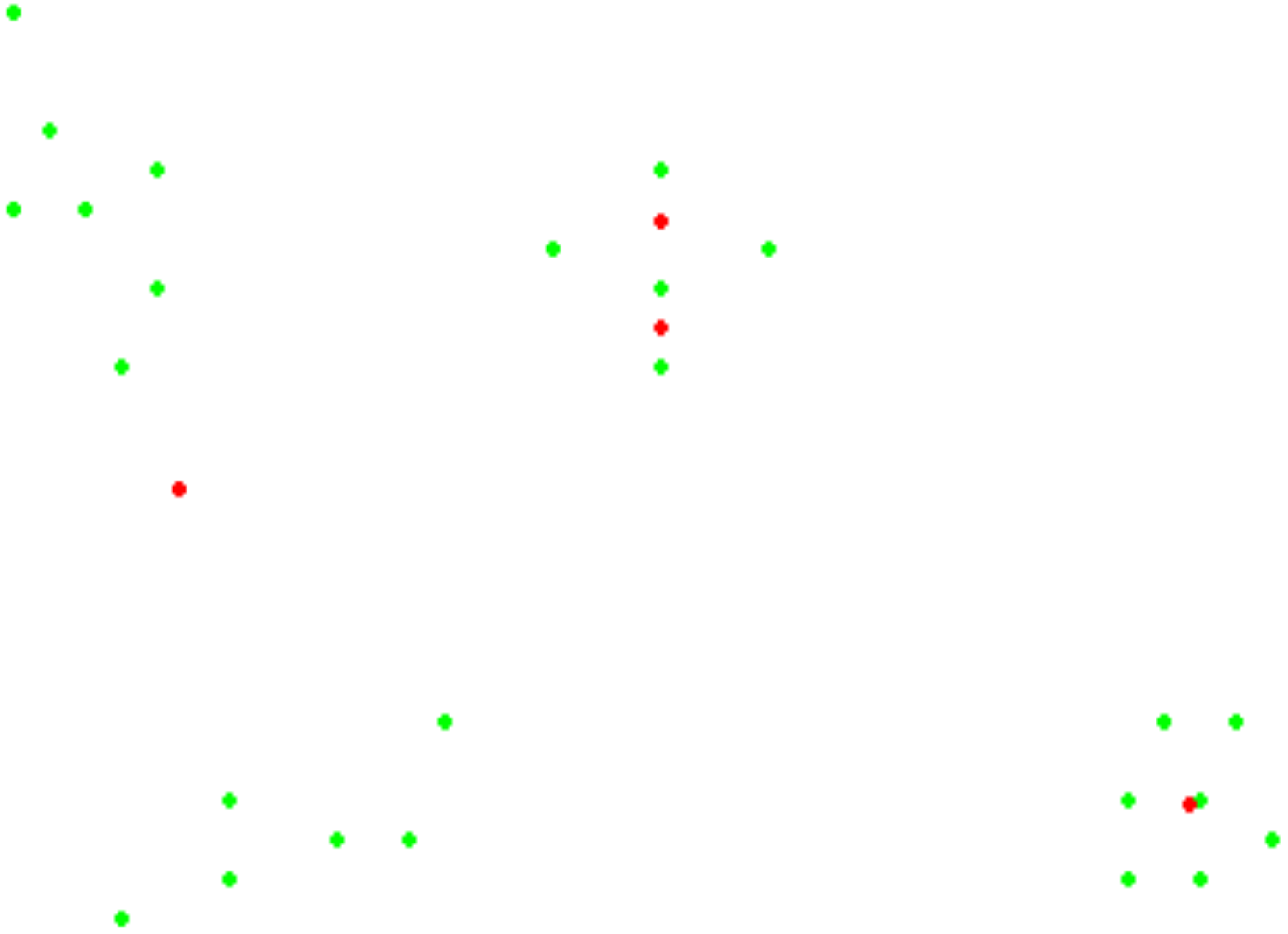
Initialization



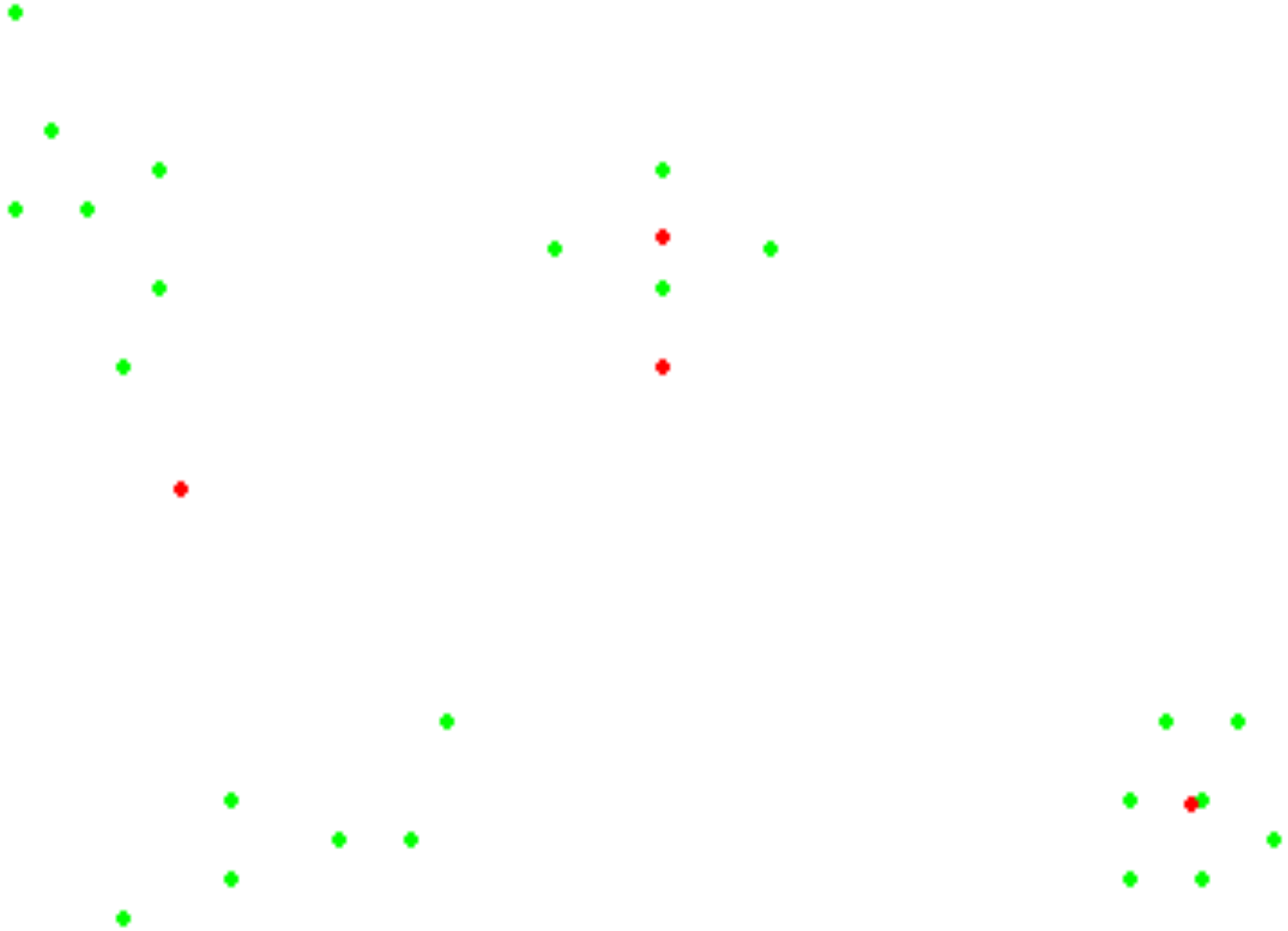
#Runs = 1



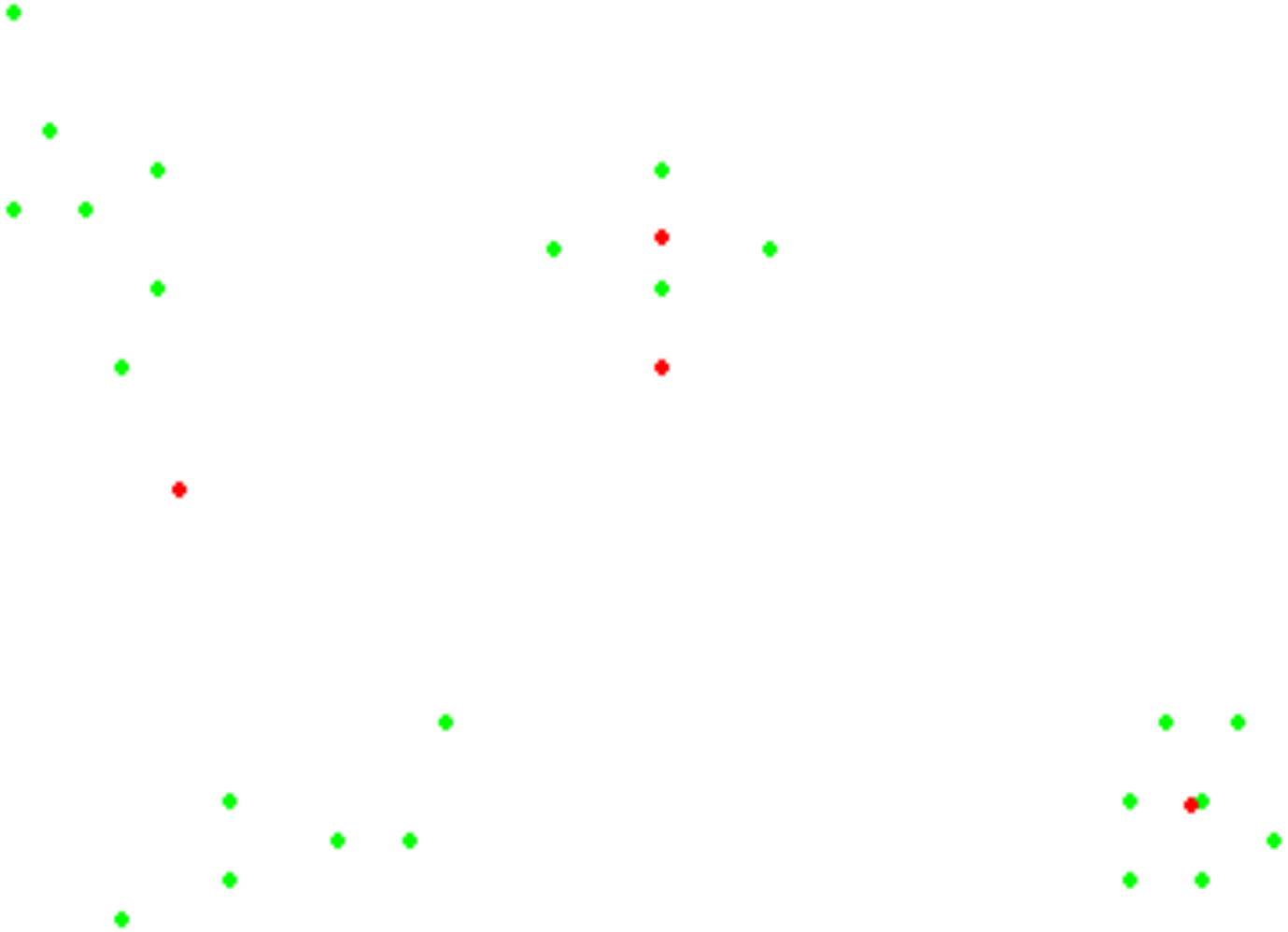
#Runs = 2



#Runs = 3



#Runs = 4



Applications of K-means Method

- Optical Character Recognition
- Biometrics
- Diagnostic Systems
- Military Applications

Comments on the *K-Means* Method

- Strength
  - *Relatively efficient*: $O(tkn)$, where n is # objects, k is # clusters, and t is # iterations. Normally, k, $t << n$.
  - Often terminates at a *local optimum*. The *global optimum* may be found using techniques such as: *deterministic annealing* and *genetic algorithms*
- Weakness
  - Applicable only when *mean* is defined, then what about categorical data?
  - Need to specify *k,* the *number* of clusters, in advance
  - Unable to handle noisy data and *outliers*
  - Not suitable to discover clusters with *non-convex shapes*

Any Questions ?

Thanks for your attention !