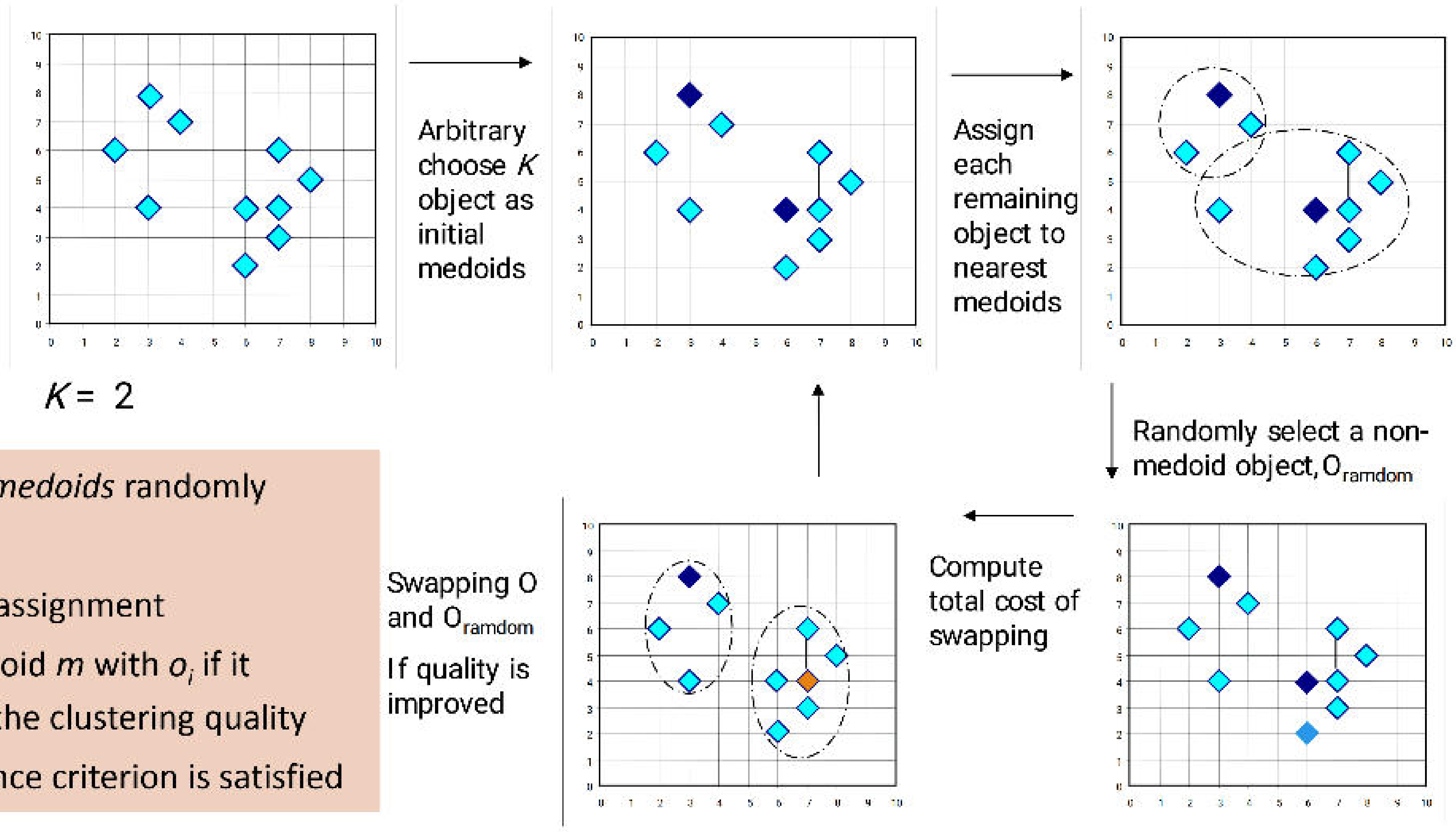
The *K-Medoids* Clustering Method

Handling Outliers: From *K-Means* to *K-Medoids*

- The *K-Means* algorithm is sensitive to outliers!—since an object with an extremely large value may substantially distort the distribution of the data
- *K-Medoids*: Instead of taking the **mean** value of the object in a cluster as a reference point, **medoids** can be used, which is the **most centrally located** object in a cluster
- The *K-Medoids* clustering algorithm:
  - Select K points as the initial representative objects (i.e., as initial K *medoids*)
  - **Repeat**
    - Assigning each point to the cluster with the closest medoid
    - Randomly select a non-representative object o_i
    - Compute the total cost S of swapping the medoid m with o_i
    - If $S < 0$, then swap m with o_i to form the new set of medoids
  - **Until** convergence criterion is satisfied

PAM: A Typical *K-Medoids* Algorithm



Select initial *K medoids* randomly

Repeat

Object re-assignment

Swap medoid *m* with o_i if it improves the clustering quality

Until convergence criterion is satisfied

Discussion on *K-Medoids* Clustering

- *K-Medoids* Clustering: Find *representative* objects (medoids) in clusters
- *PAM* (Partitioning Around Medoids: Kaufmann & Rousseeuw 1987)
  - Starts from an initial set of medoids, and
  - Iteratively replaces one of the medoids by one of the non-medoids if it improves the total sum of the squared errors (SSE) of the resulting clustering
  - *PAM* works effectively for small data sets but does not scale well for large data sets (due to the computational complexity)
  - Computational complexity: PAM: $O(K(n - K)^2)$ (quite expensive!)
- Efficiency improvements on PAM
  - *CLARA* (Kaufmann & Rousseeuw, 1990):
    - PAM on samples; $O(Ks^2 + K(n - K))$, s is the sample size
  - *CLARANS* (Ng & Han, 1994): Randomized re-sampling, ensuring efficiency + quality