Machine Learning

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Unsupervised Learning : Clustering

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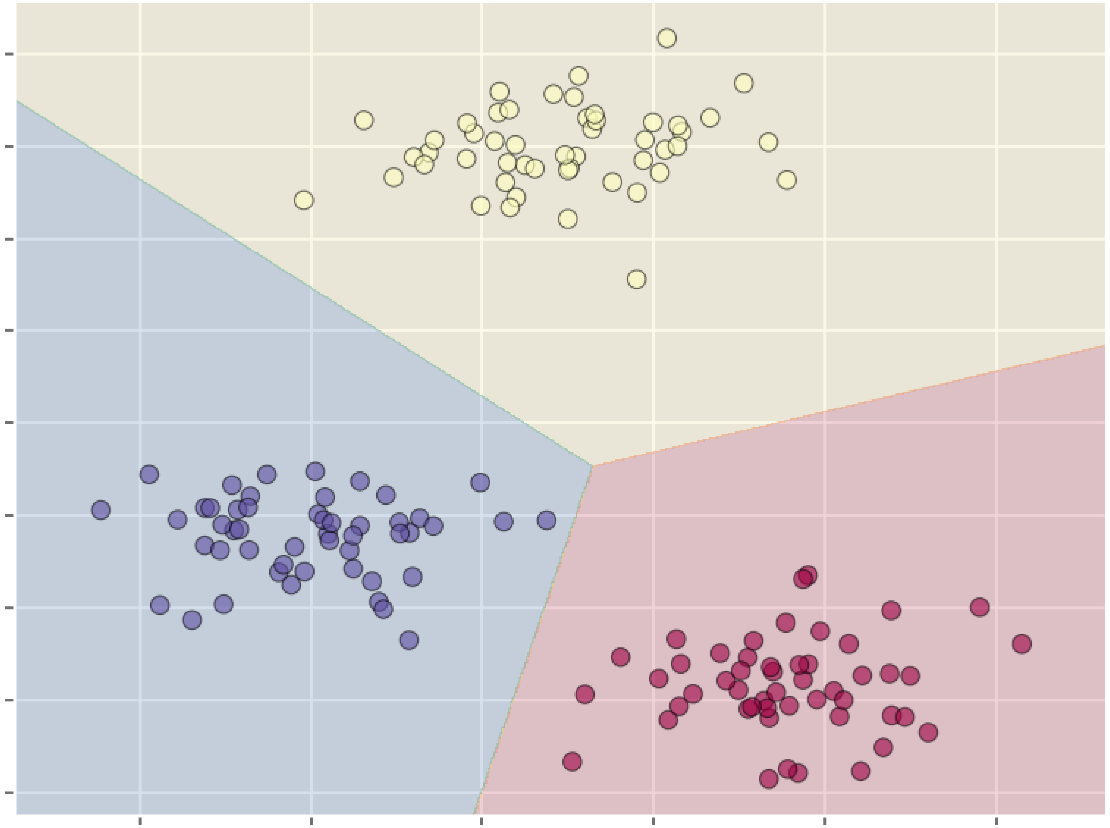
Reminder: Supervised learning

- Supervised Learning. For each example, the correct answer is given.

$$\boxed{\{(x^{(1)},y^{(1)}),(x^{(2)},y^{(2)}),\cdots,(x^{(m)},y^{(m)})\}}$$

Training set



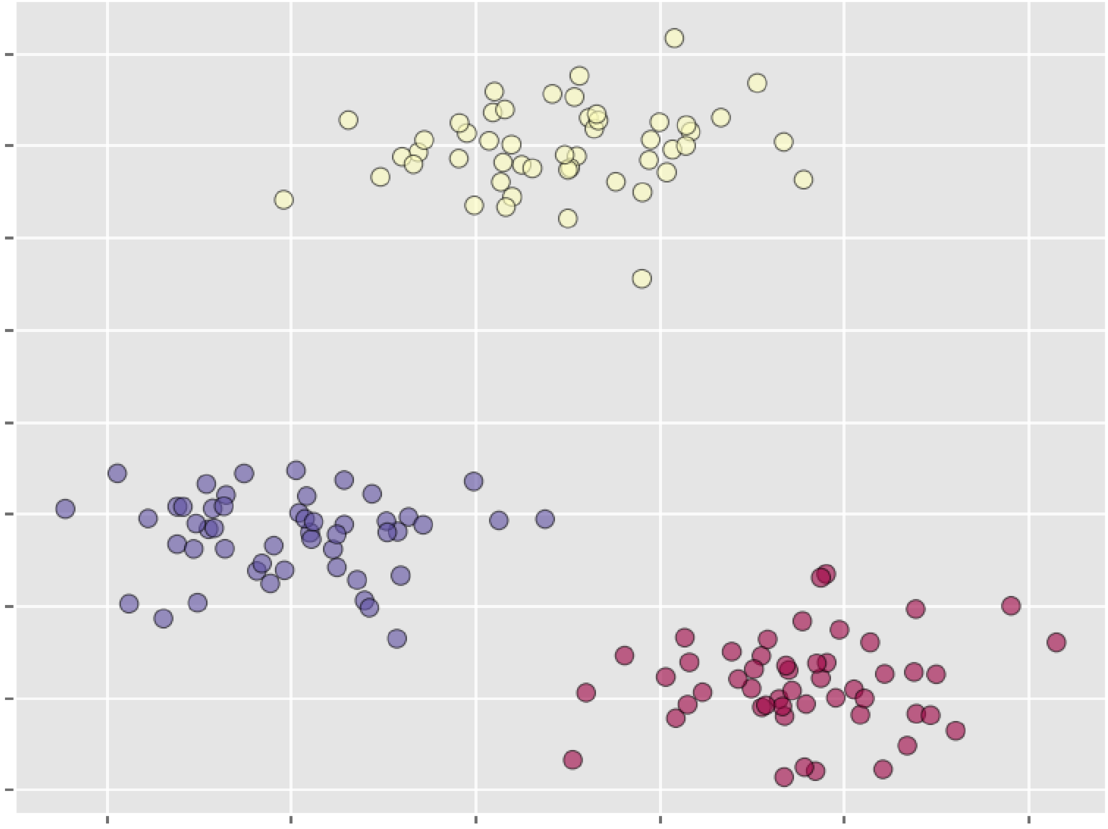
- Types Of Supervised Learning.
  - Regression: Estimation of a continuous quantity.
  - Classification: Estimation of a discrete quantity.

Unsupervised Learning

- Unsupervised Learning. Not knowing the correct answers.

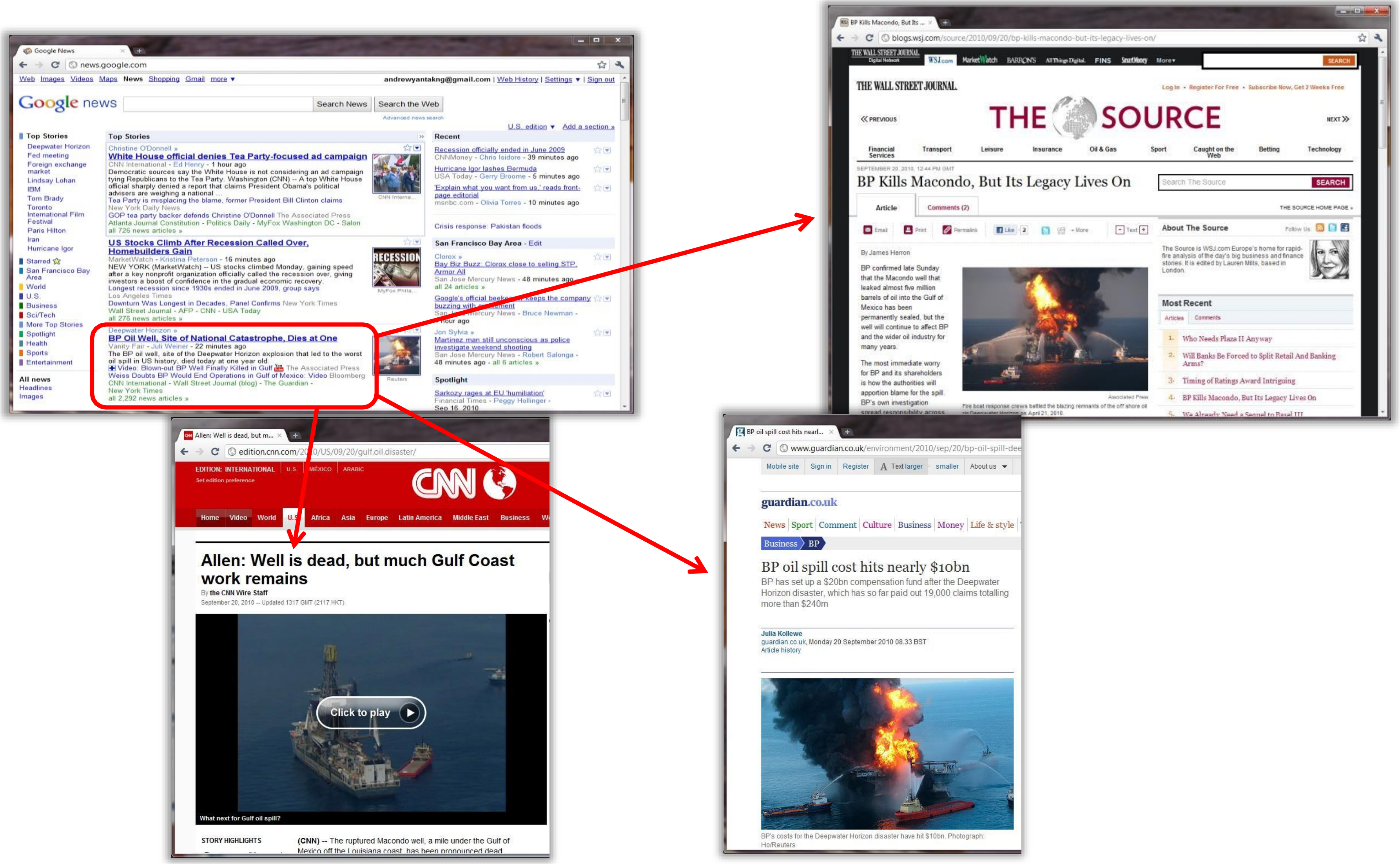
$$\boxed{\{x^{(1)}, x^{(2)}, x^{(3)}, \dots, x^{(m)}\}}$$

Training set



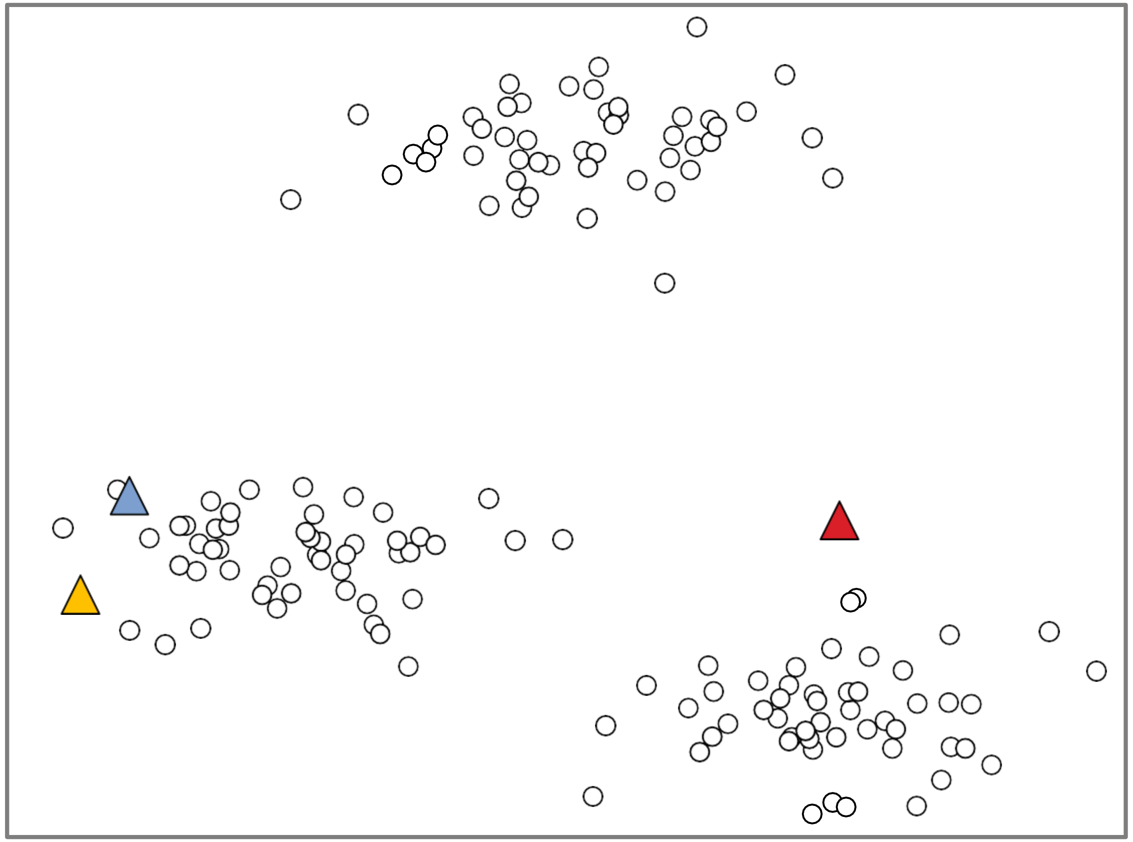
- Goal. Structure detection in input data

Applications of clustering: grouping related news



K-means Clustering Algorithm

- Its an iterative clustering algorithm
  - It choosing K points randomly as the center of the clusters.
  - Repeat the following steps:
    - Assign each data to a cluster with the closest center.
    - Update the centroid of each cluster by averaging the data assigned to that cluster
  - Stop time : When no data changes its cluster in an iteration.



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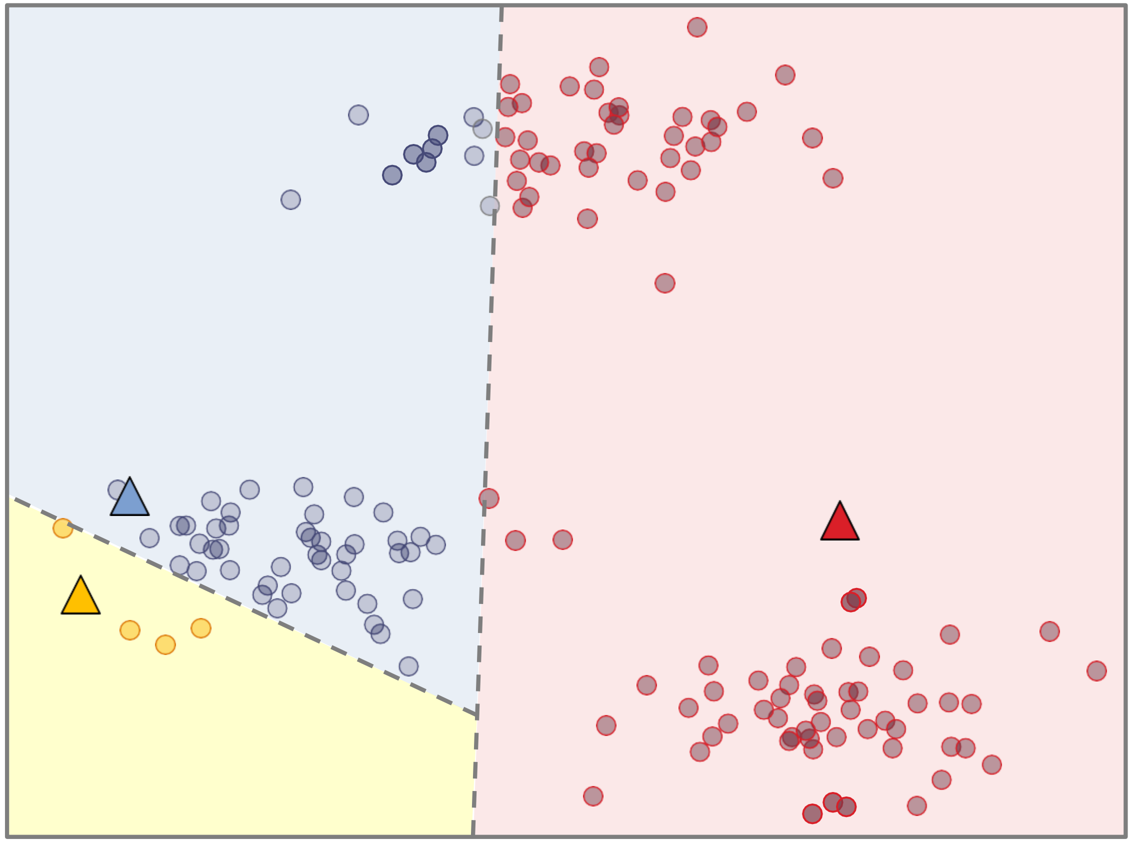

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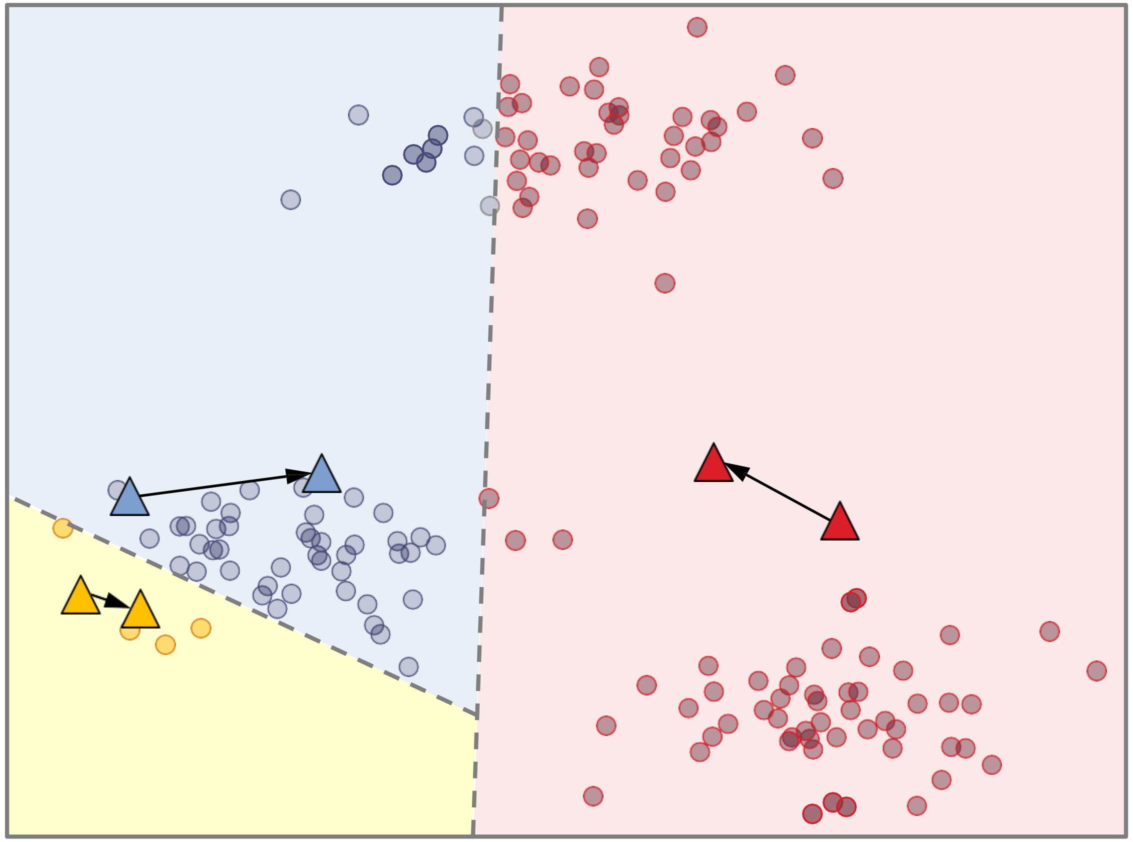
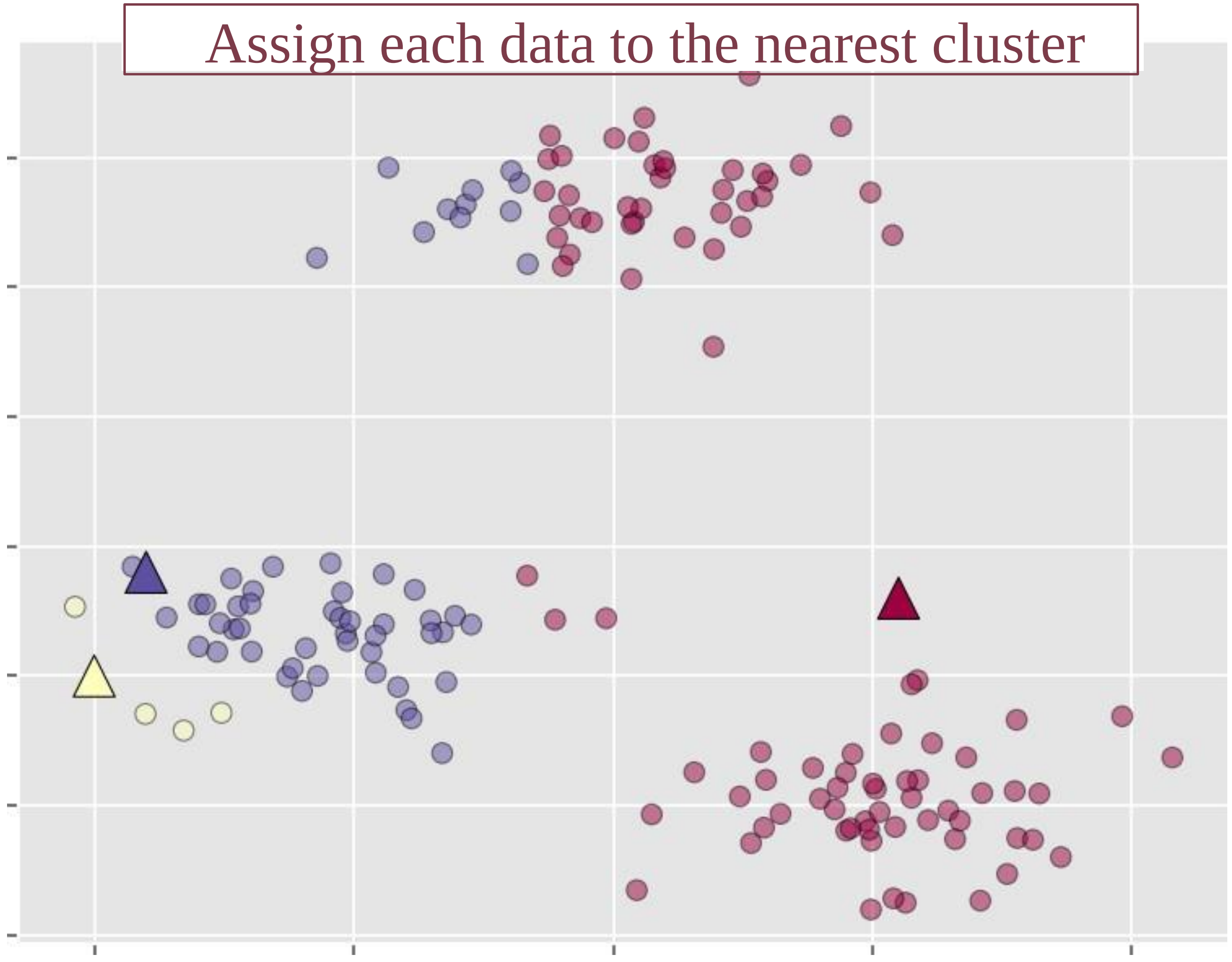


Illustrations of algorithm process



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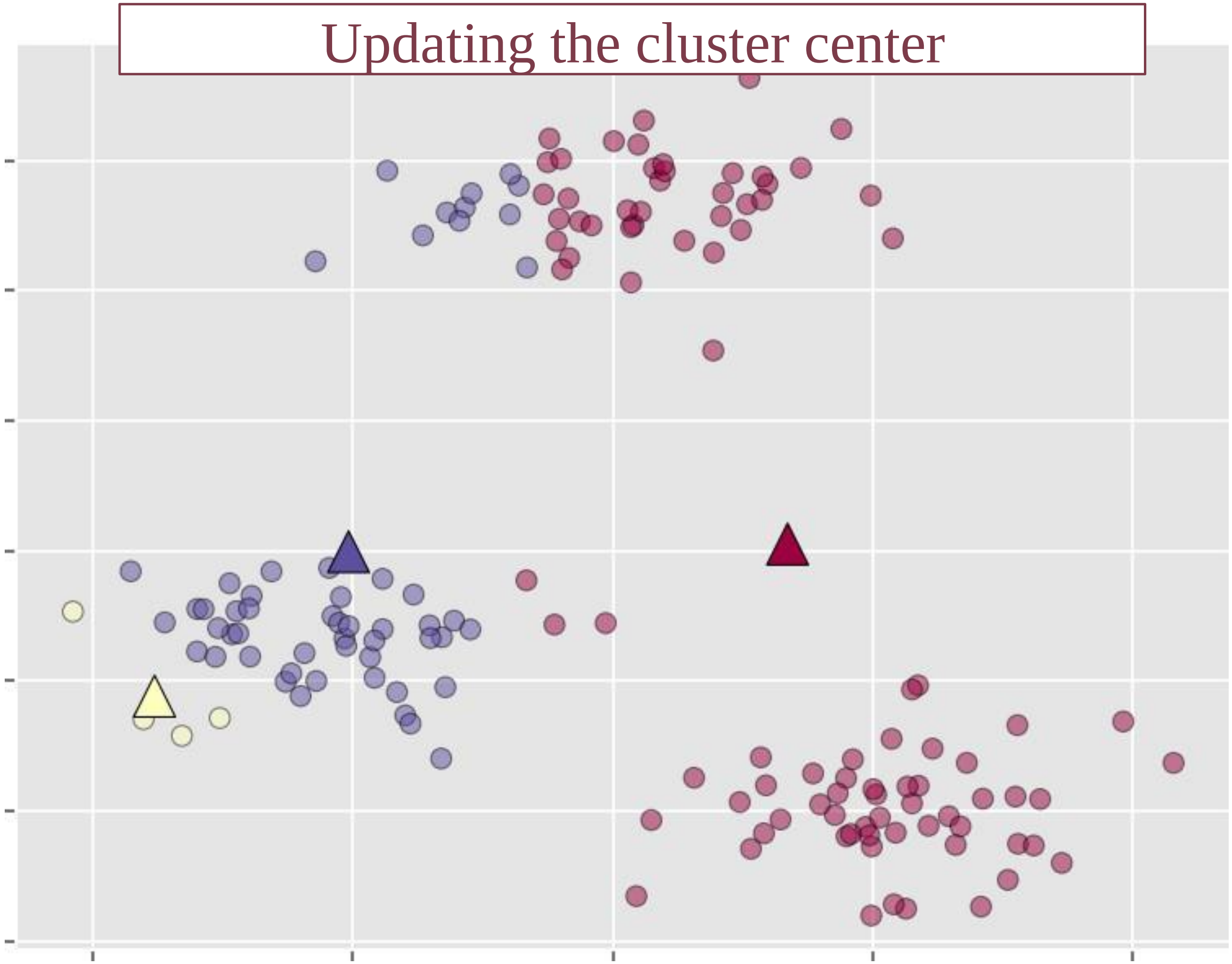
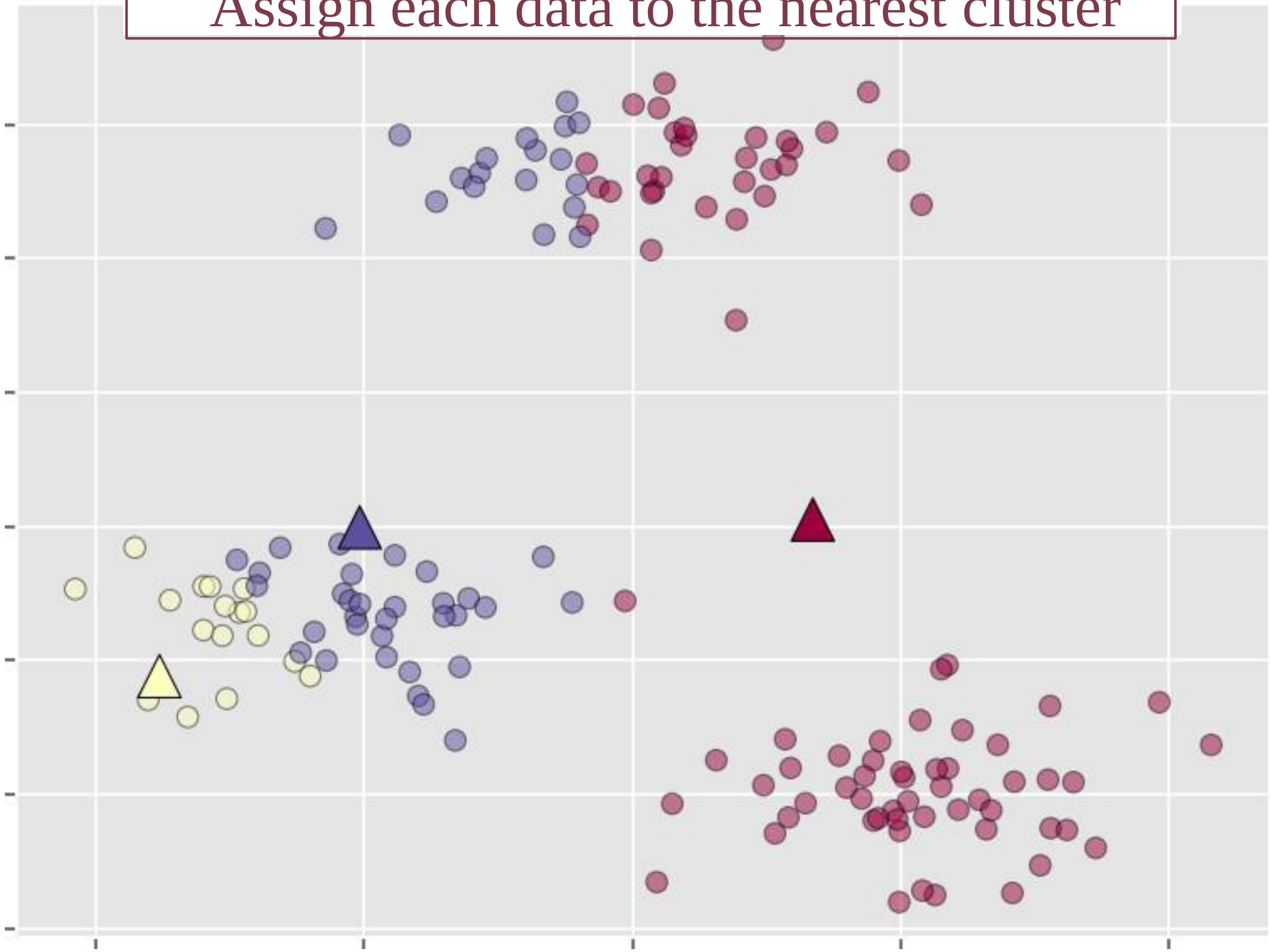


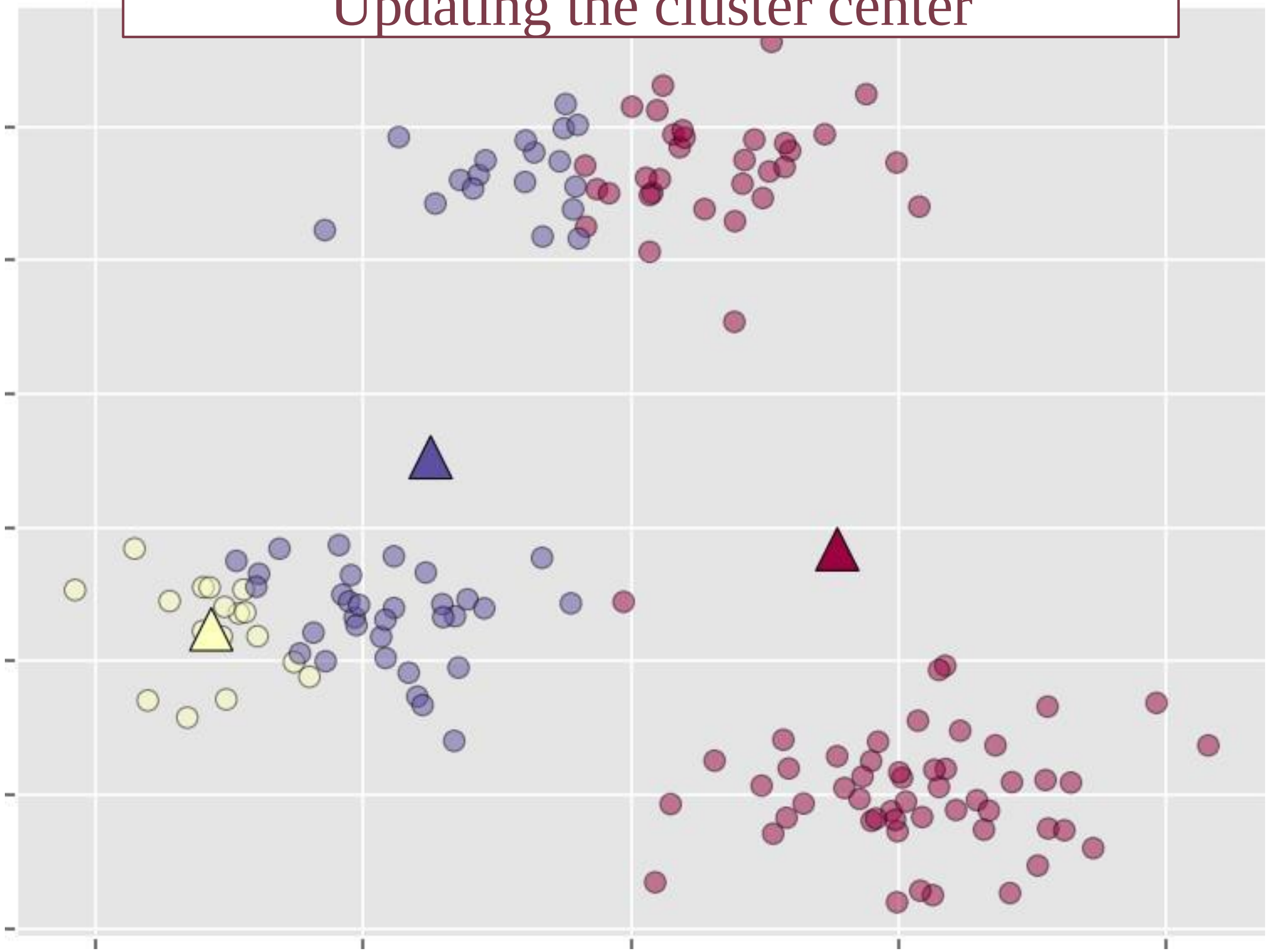
Illustrations of algorithm process

Assign each data to the nearest cluster



Illustrations of algorithm process

Updating the cluster center



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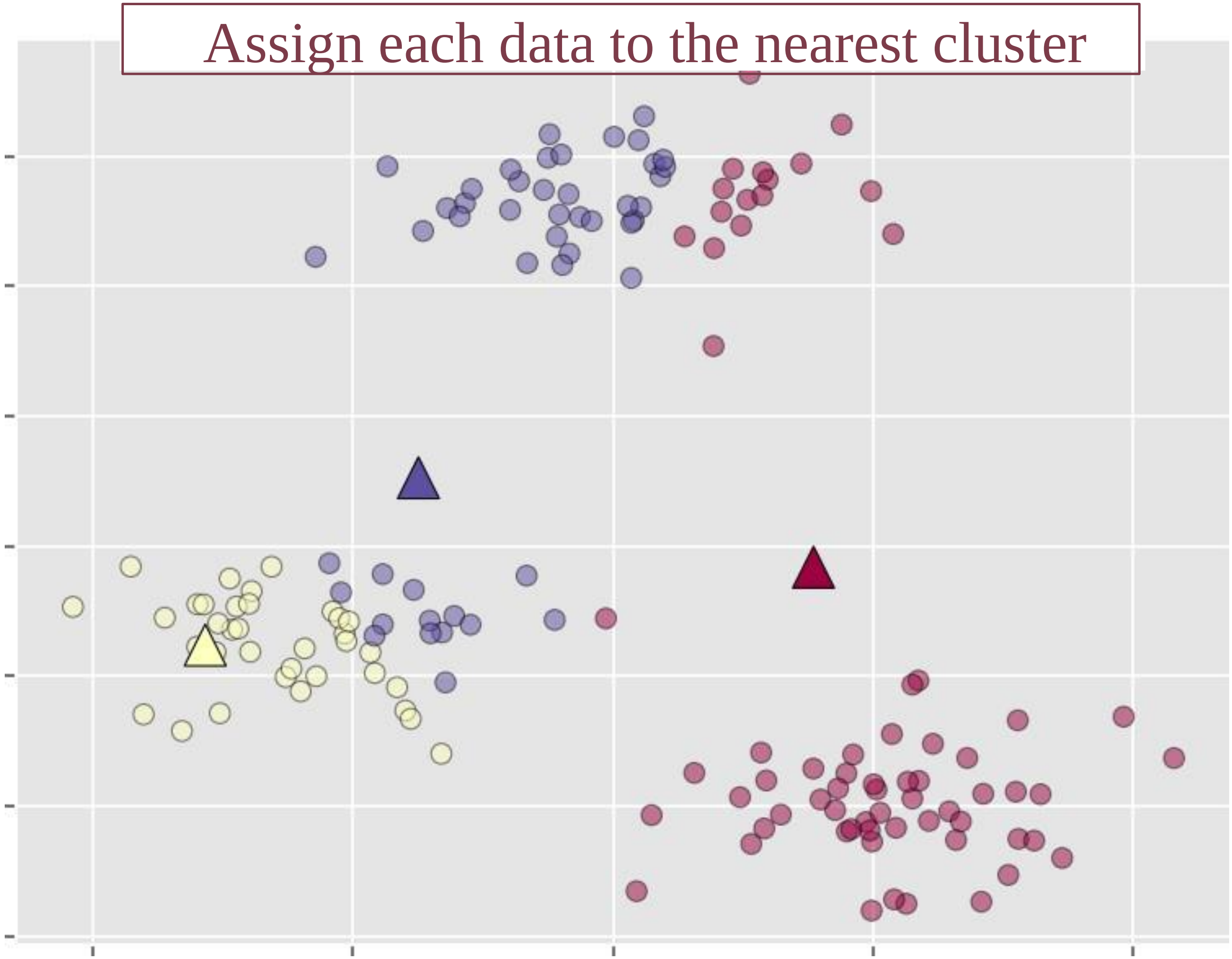

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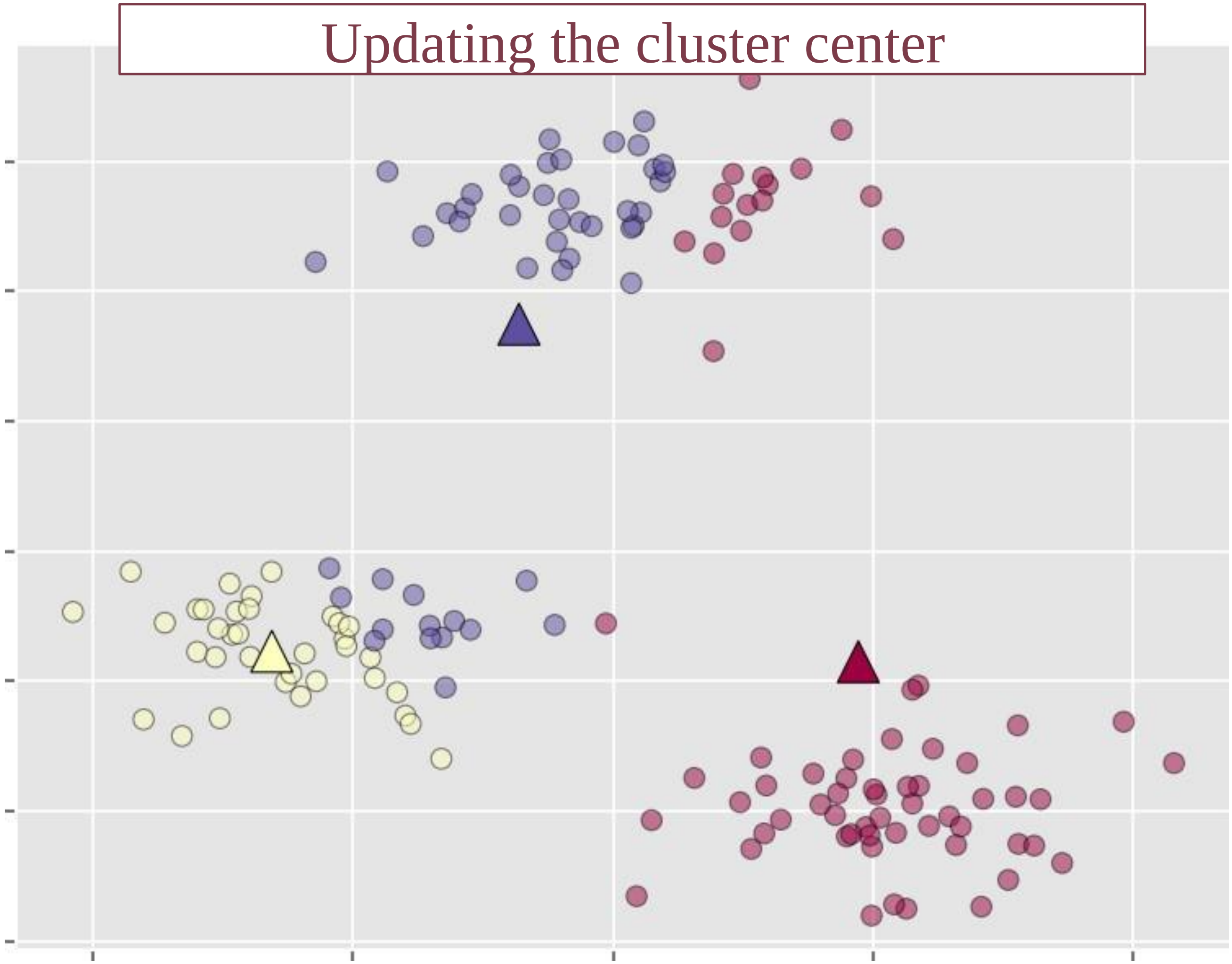

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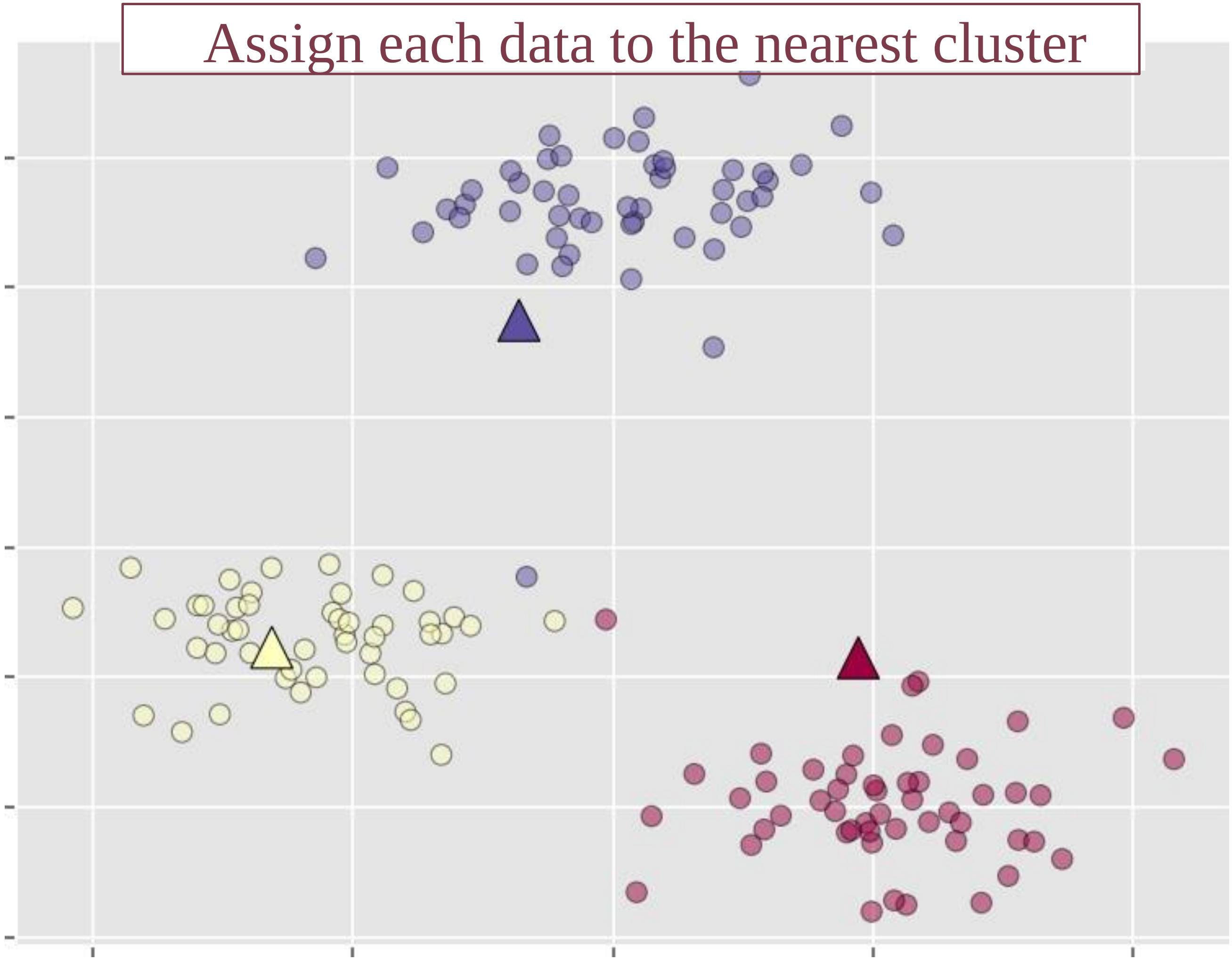
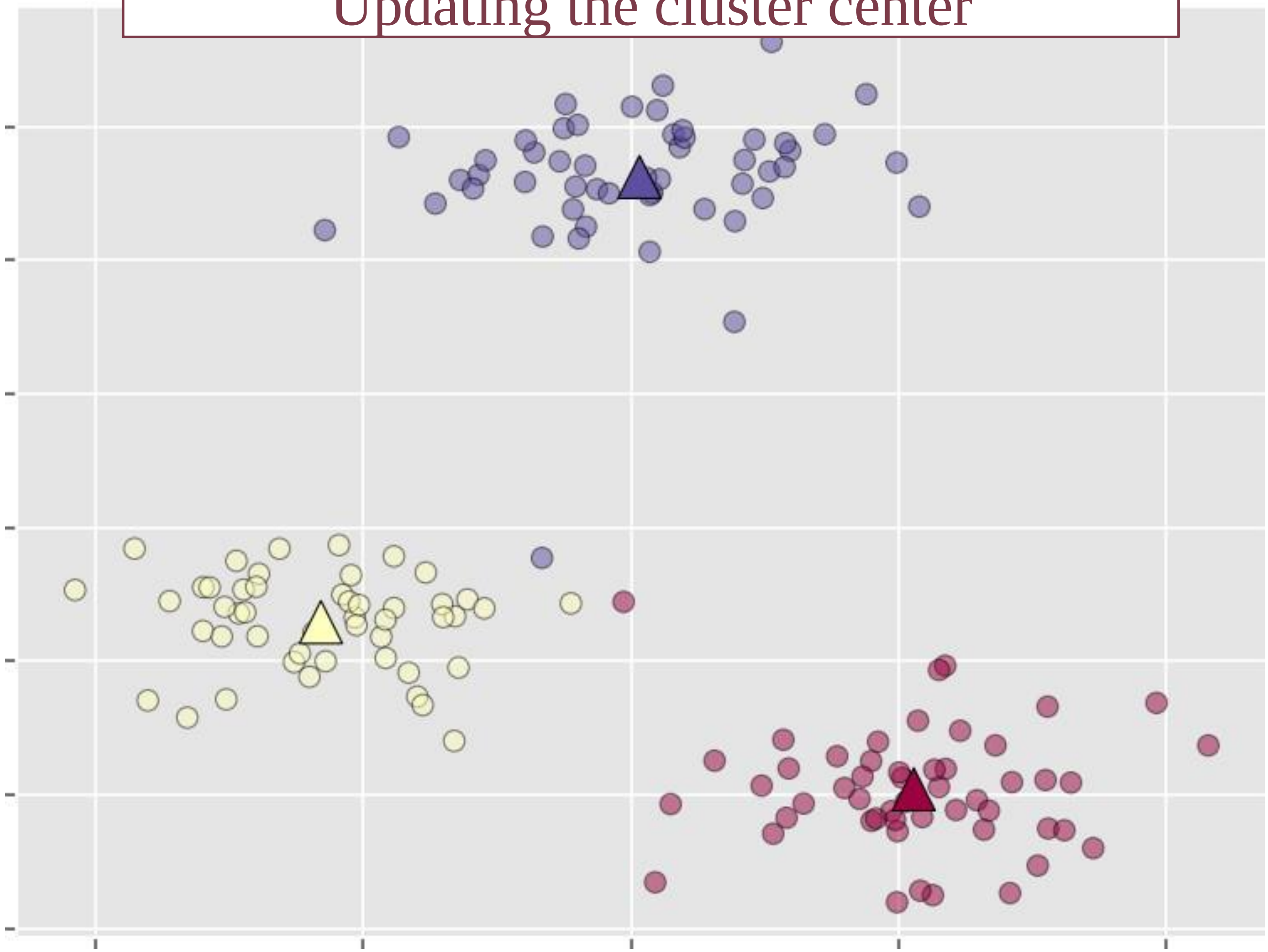


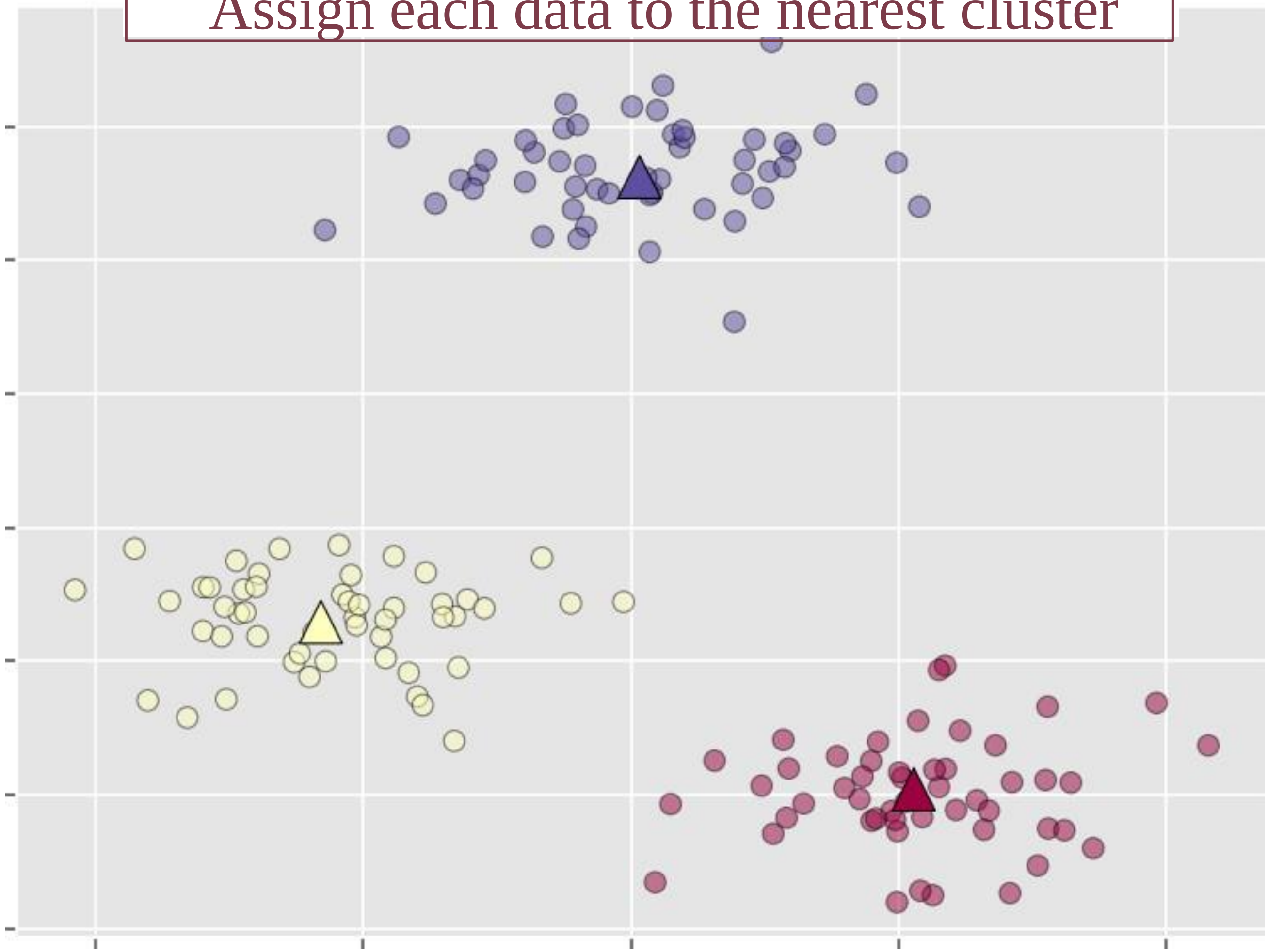
Illustrations of algorithm process

Updating the cluster center



Illustrations of algorithm process

Assign each data to the nearest cluster



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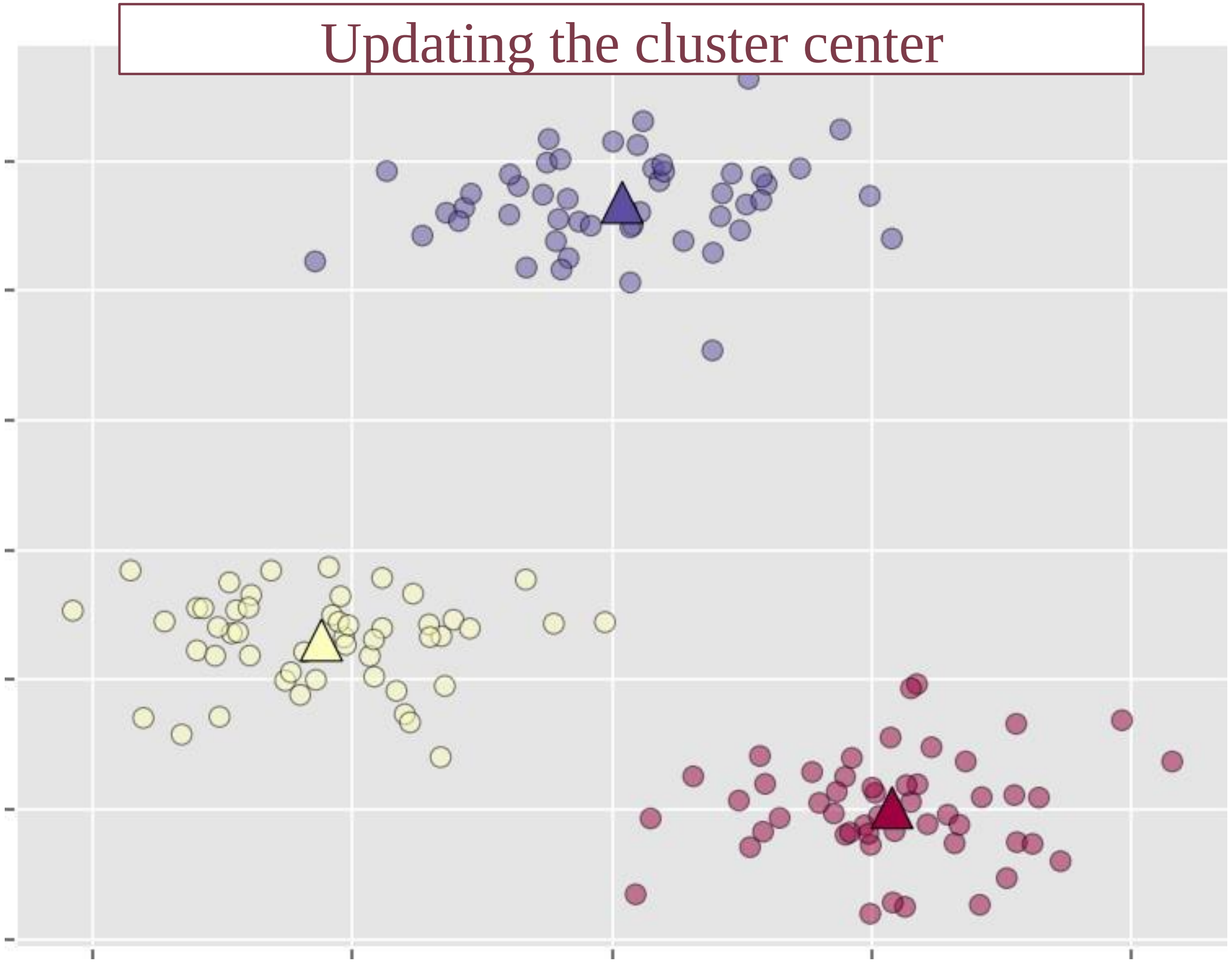

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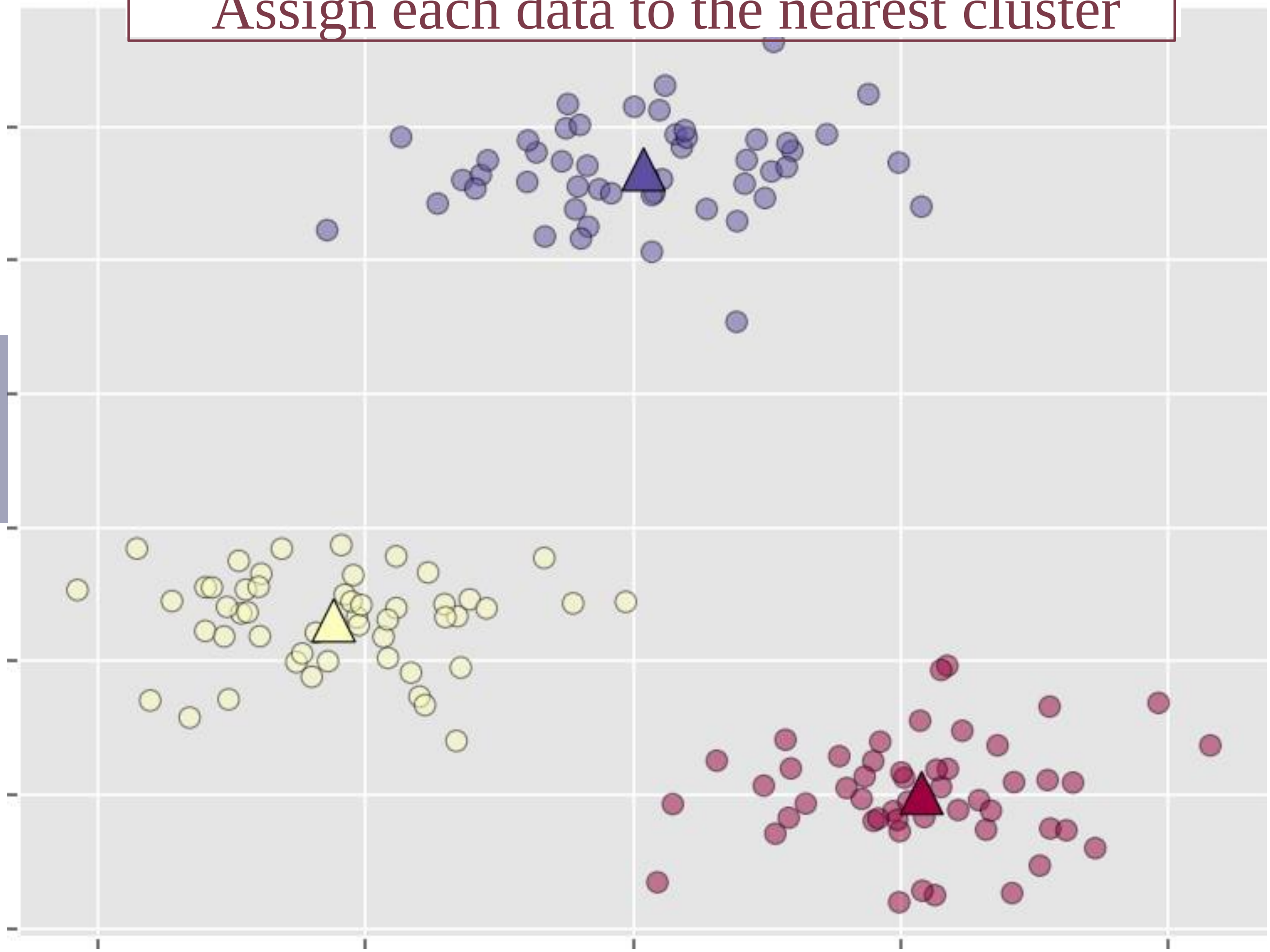
Assign each data to the nearest cluster



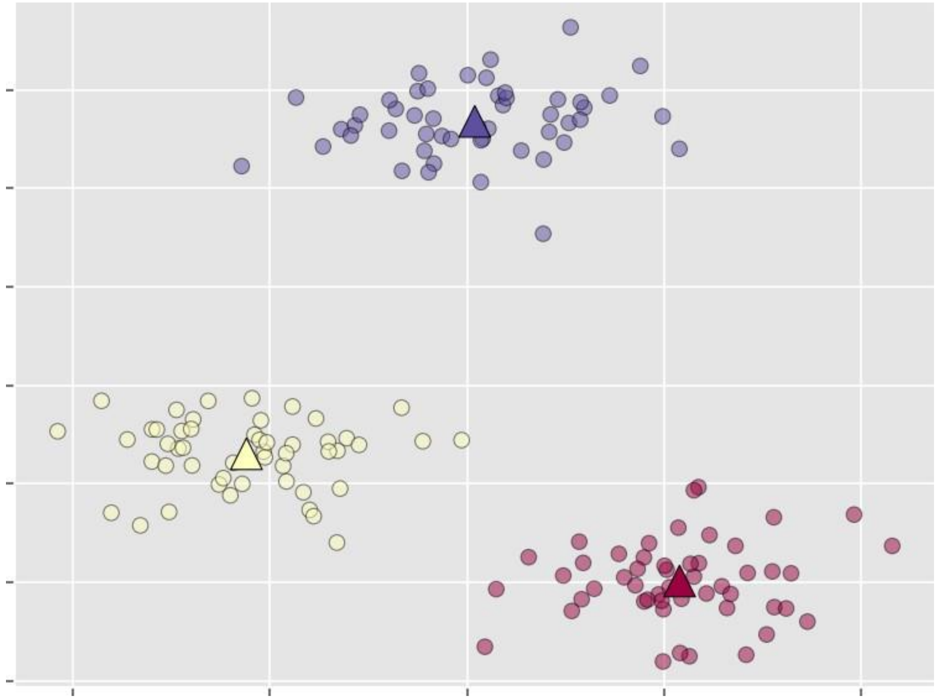
Convergence :

None of the data clusters were changed .

K-mean Algorithm

- Inputs.
  - Number Of Clusters : K
  - Training set

$$\{x^{(1)}, x^{(2)}, x^{(3)}, \dots, x^{(m)}\}$$



- Note : In the training set, no label is assigned to the data.
- Note: There is no need to add the feature $x_0 = 1$ in the clustering.

K-mean Algorithm

randomly initialize K cluster centroids $\mu_1, \mu_2, \dots, \mu_k \in \mathbb{R}^n$

repeat

{

for $i = 1$ **to** m

$$c^{(i)} = \arg\min_k \|x^{(i)} - \mu_k\|$$

Assigning data to clusters

for $k = 1$ **to** K

$\mu_k =$ average of points assigned to cluster k

Updating the cluster center

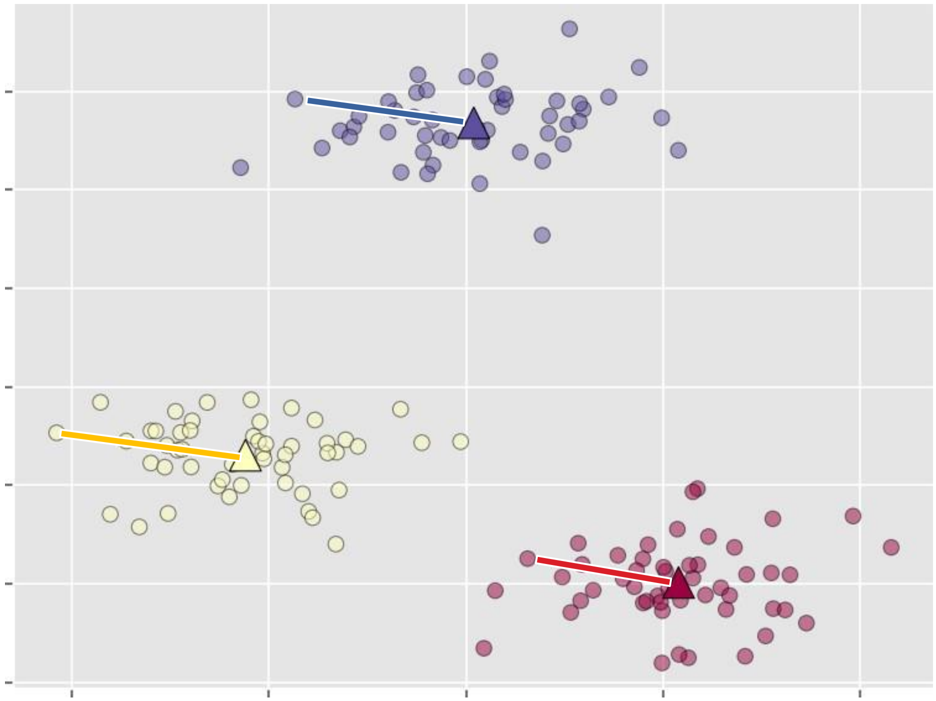
}

K-mean Algorithm


```
centroids = np.random.random((K, n))

while True:

    for i in range(m):
        c[i] = np.argmin(np.linalg.norm(X[i] - centroids, axis=1))

    for k in range(K):
        centroids[k] = np.mean(X[c == k], axis=0)
```

Clustering: Objective function

Objective function



- Symbols.
  - μ_k : center of the cluster k
  - $c^{(i)}$: Cluster number assigned to data $x^{(i)}$
  - $\mu_c(i)$: Cluster center assigned to data $x^{(i)}$

- Objective function

$$J(c^{(1)}, c^{(2)}, \ldots, c^{(m)}, \mu_1, \mu_2, \ldots, \mu_k) = \frac{1}{m}\sum_{i=1}^{m}\left\|x^{(i)} - \mu_{c^{(i)}}\right\|^2$$

K-mean Algorithm

randomly initialize K cluster centroids $\mu_1, \mu_2, \dots, \mu_k \in \mathbb{R}^n$

repeat

{

for $i = 1$ **to** m

$$c^{(i)} = \arg\min_k \left\| x^{(i)} - \mu_k \right\|$$

Minimization of the objective with respect to $c^{(i)}$ parameters

for $k = 1$ **to** K

μ_k= average of points assigned to cluster k

Minimization of the objective with respect to μ parameters

}

Setting initial value for cluster centers

K-mean Algorithm

randomly initialize K cluster centroids $\mu_1, \mu_2, \ldots, \mu_k \in \mathbb{R}^n$

repeat

{

for $i = 1$ **to** m

$$c^{(i)} = \arg\min_k \left\| x^{(i)} - \mu_k \right\|$$

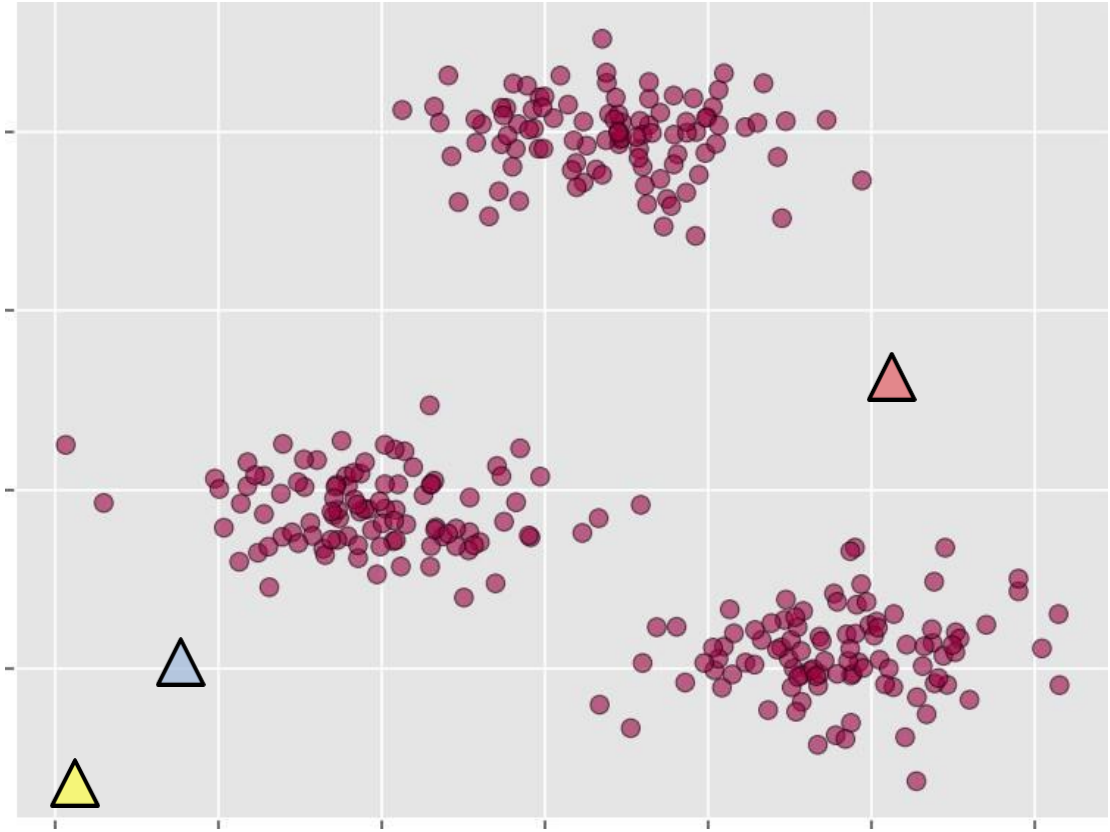
for $k = 1$ **to** K

μ_k= average of points assigned to cluster k

}

Setting initial value for cluster centers

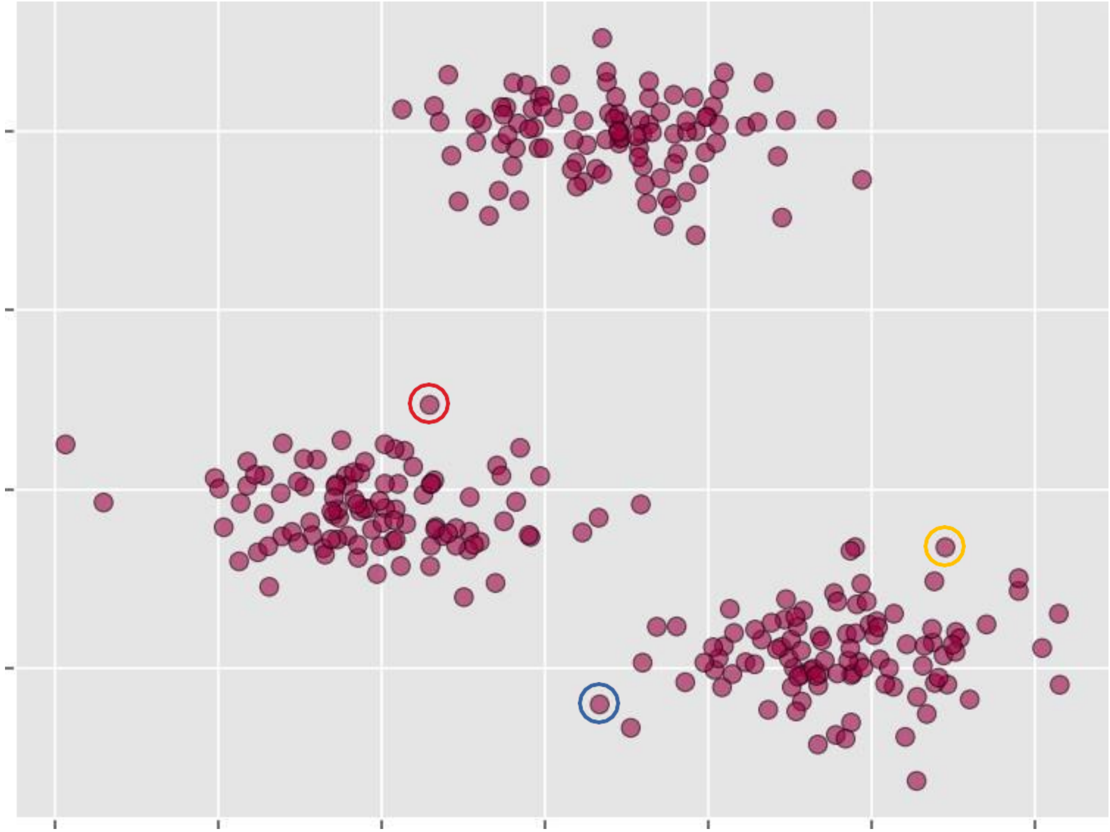
- Setting initial value. $[K \leq m]$
  - Selection of K training samples randomly
  - Assigning center of each cluster to K selected samples



A center may be selected in such a way that no data is assigned to it.

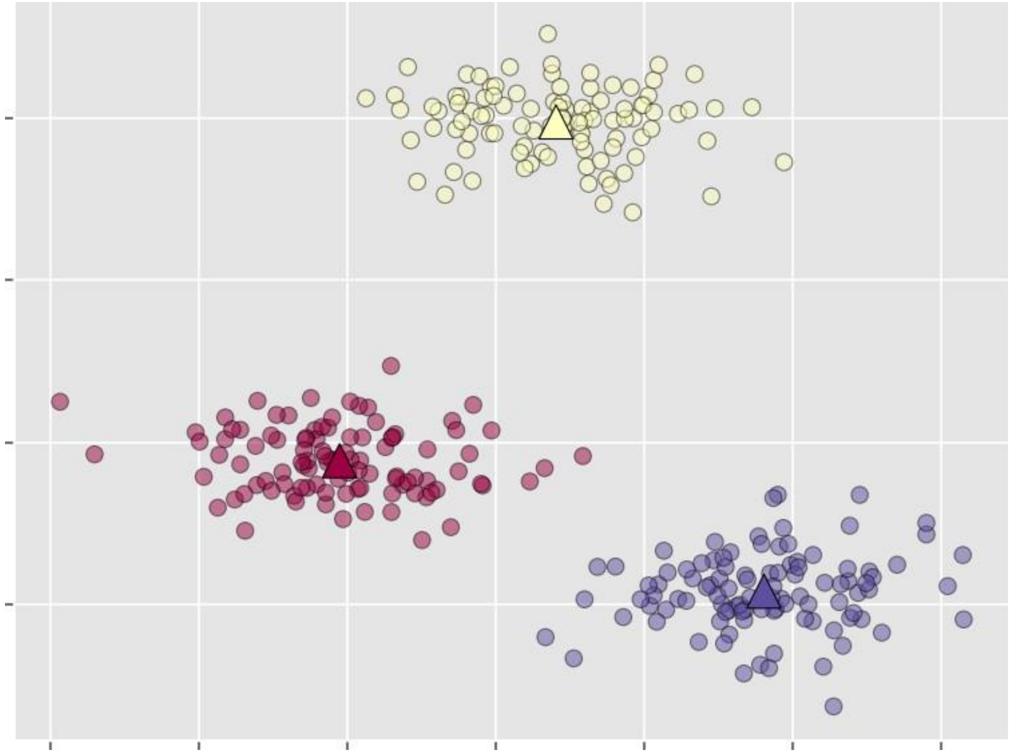
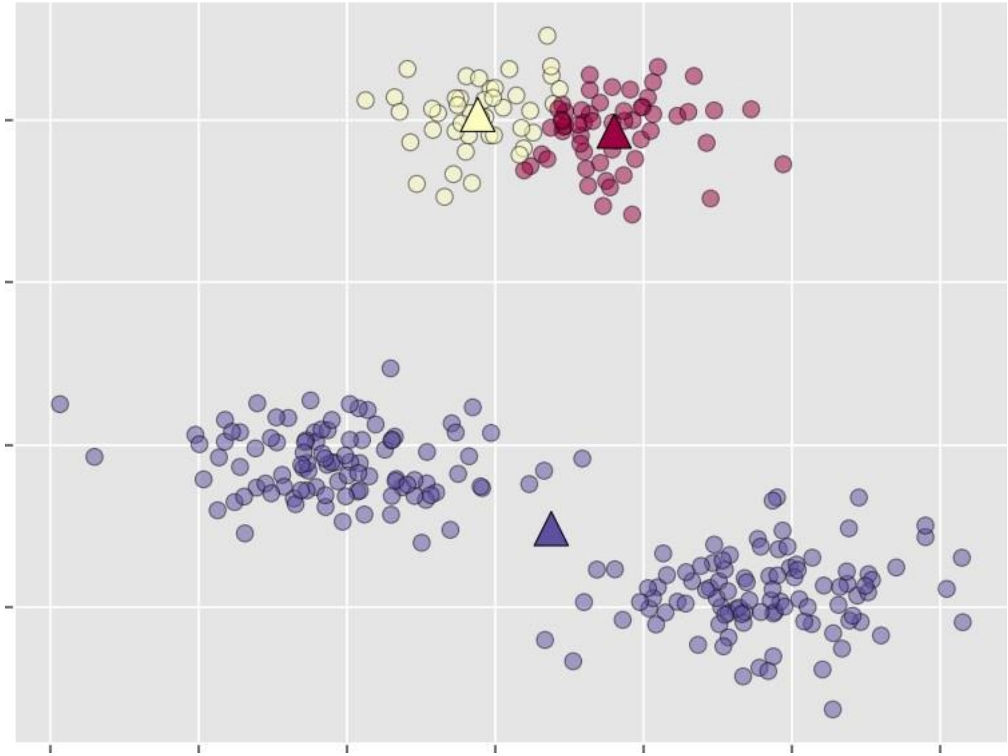
Setting initial value for cluster centers : Better way

- Setting initial value. $[K \leq m]$
  - Choosing k amount of training samples randomly
  - Assigning center of each cluster to K selected samples



```
C = np.random.permutation(X)[:K]
```

Global optimization and Local optimization

Local optimization	Global optimization
	

Avoid local optima

for $t = 1$ **to** MAX

{

randomly initialize cluster centroids $\mu_1, \mu_2, \dots, \mu_k$

run K-means to get $c^{(1)}, c^{(2)}, \dots c^{(m)}, \mu_1, \mu_2, \dots, \mu_k$

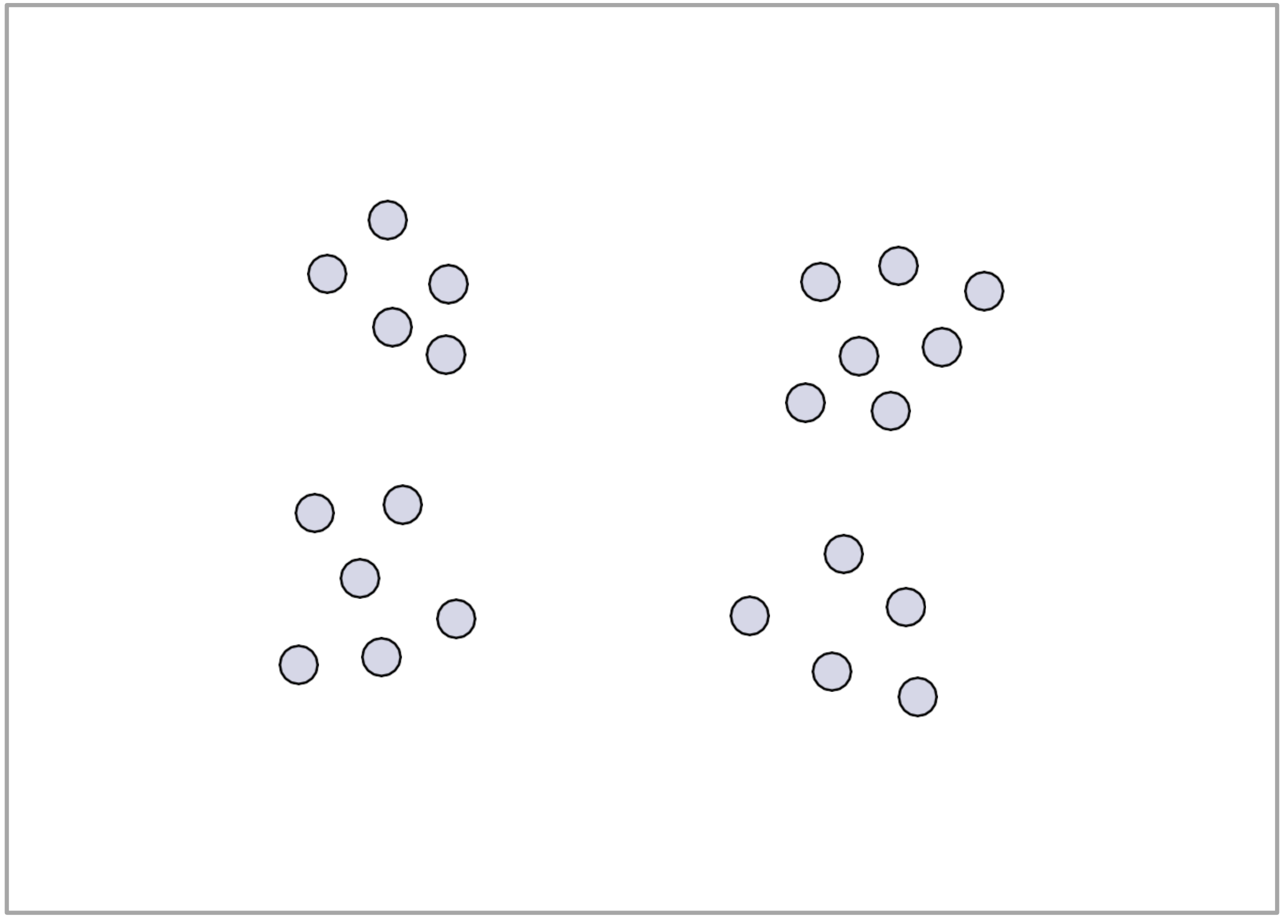
compute cost function $J(c^{(1)}, c^{(2)}, \dots c^{(m)}, \mu_1, \mu_2, \dots, \mu_k)$

}

pick clustering with minimum cost

Determine the number of clusters

What is the right value for K?



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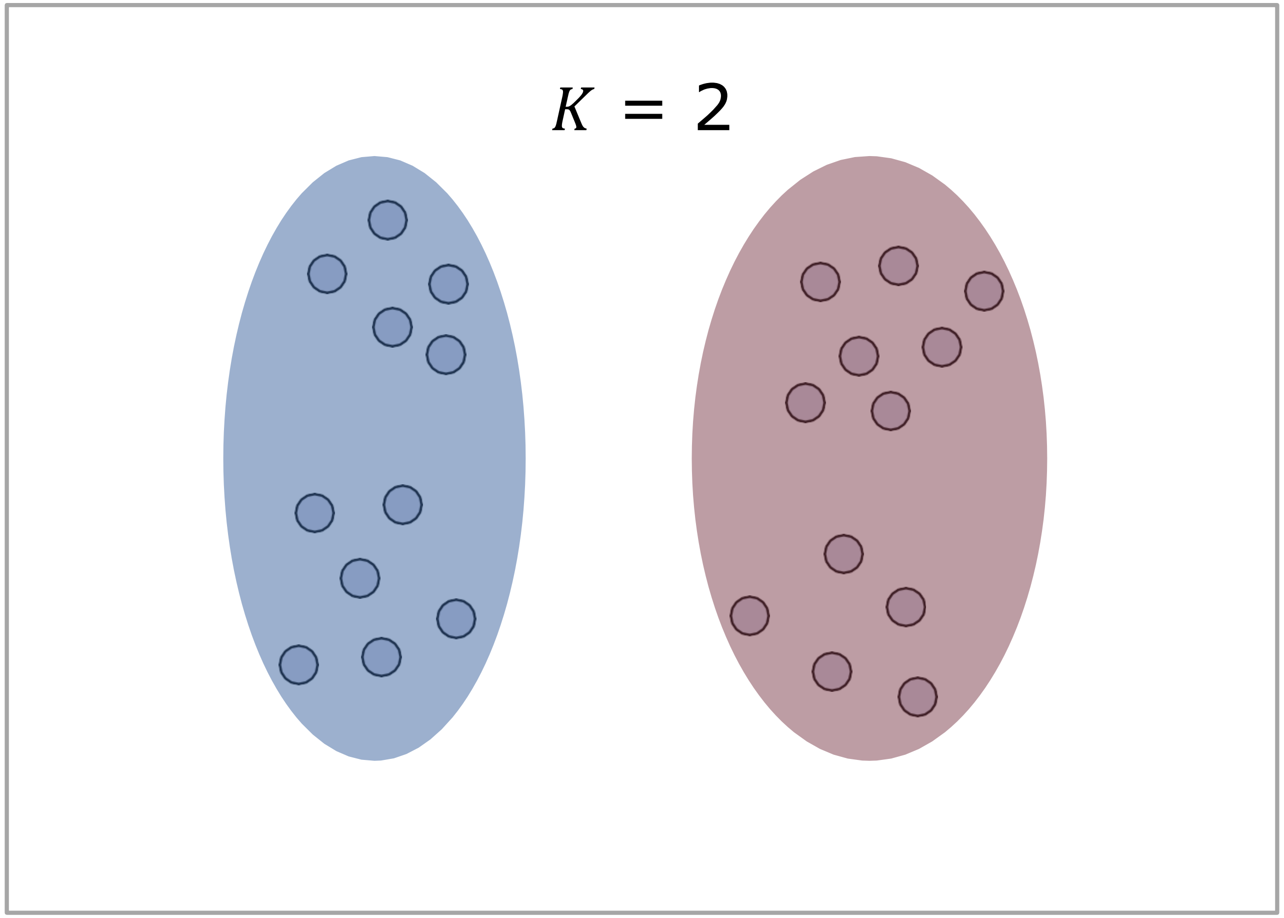

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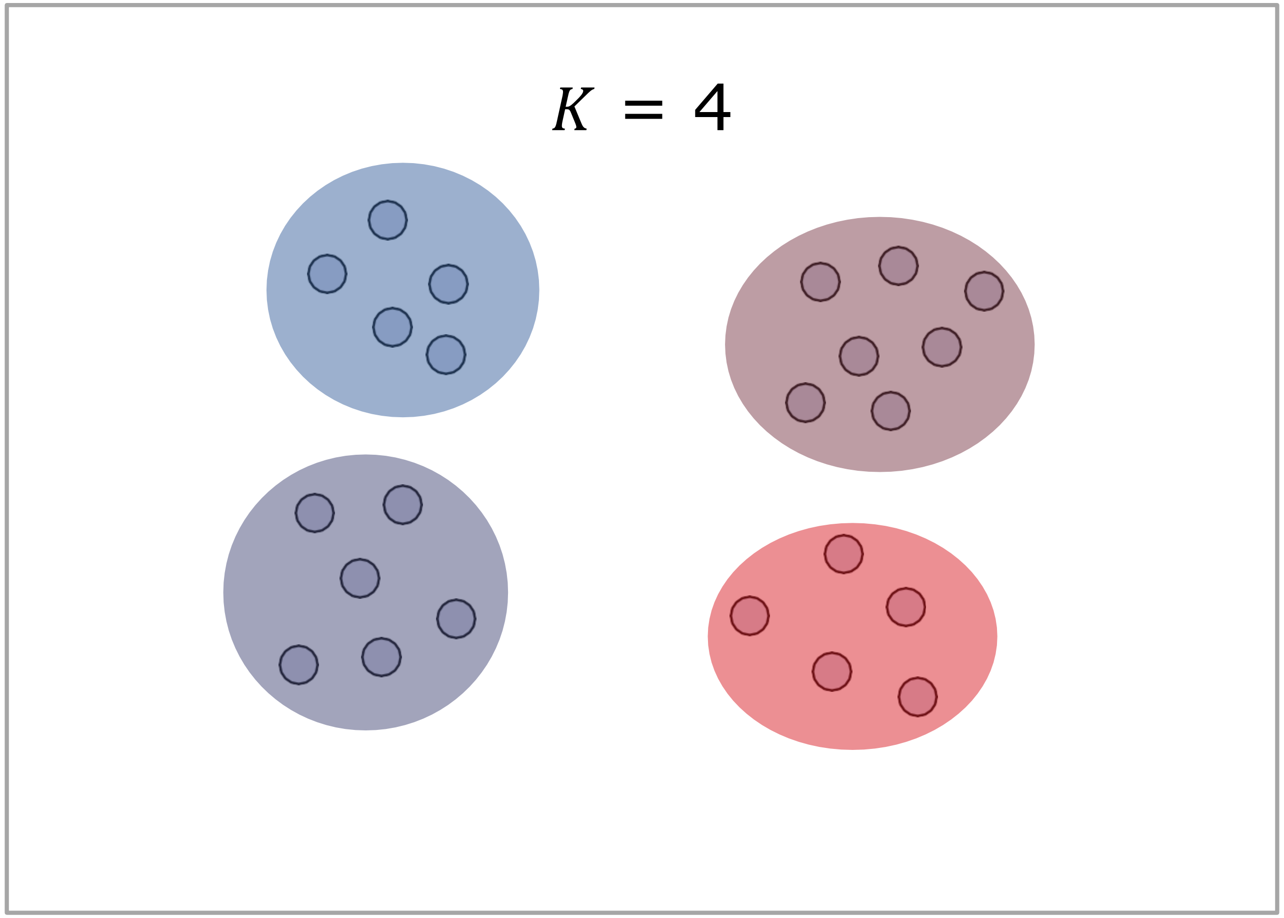


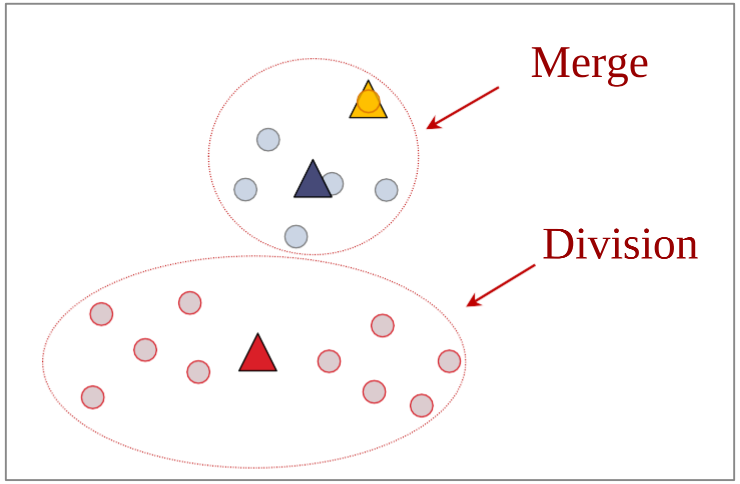
Determining the appropriate number of clusters: Elbow Method

Improving clustering

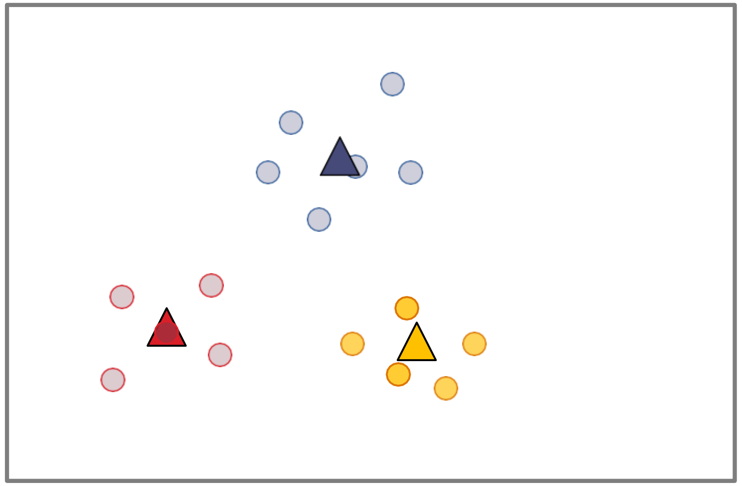
Improving clustering with post-processing of clusters

- **Division.**
  - Splitting a cluster with the highest error into two clusters.

By running the K-means on the data of this cluster with a value of K = 2



- **Merge.**
  - Merge the two closest clusters
  - Merging two clusters with minimal increase in total error.



Algorithm of bipartite generator K-Means

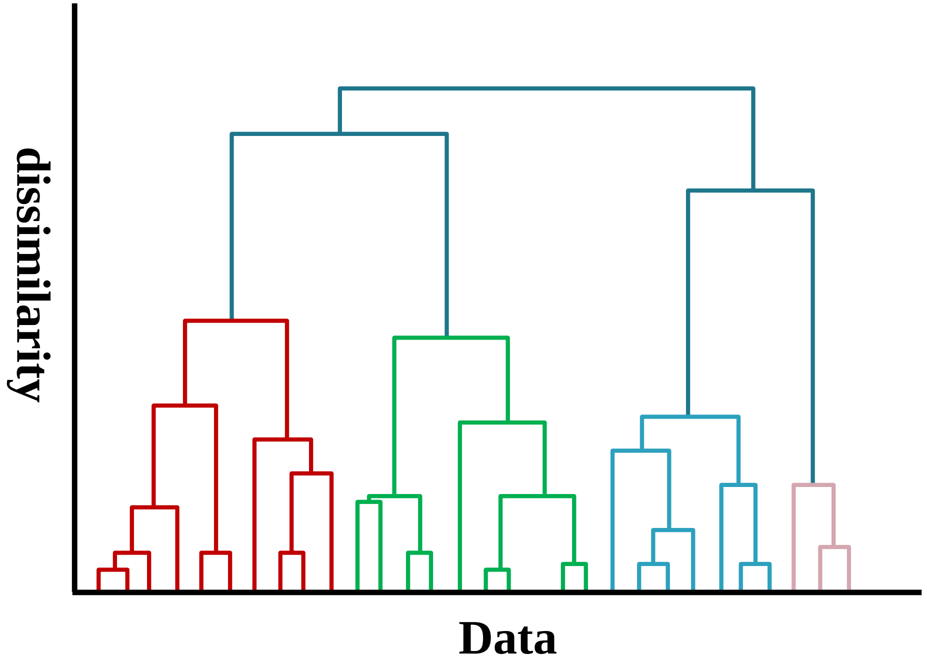
- Bipartite algorithm.
  - Start with a cluster containing all the data.
  - Choose one cluster at a time :
    - Divide the selected cluster into two clusters using K-means algorithm.
    - Calculate the total clustering error.
    - Choose the clustering with the least error.
  - Repeat the process above until you reach the desired number of clusters.

Algorithm of bipartite generator K-Means

Start with all the points in one cluster
while the number of clusters is less than K
    measure the total error
    for every cluster
        perform K-means clustering with $k=2$ on the given cluster
        measure the total error after splitting
    choose the cluster split that gives the lowest error

Hierarchical clustering

- Hierarchical clustering.
  - First, merge very similar data.
  - Gradually create larger clusters by merging smaller clusters.
- Algorithm.
  - At first, each data represents a cluster.
  - Repeat the following steps:
    - Choose the two closest clusters each time.
    - Merge those two clusters into a new cluster.
    - Stop: when only one cluster remains.



- Create a tree diagram containing a wide range of clusters.

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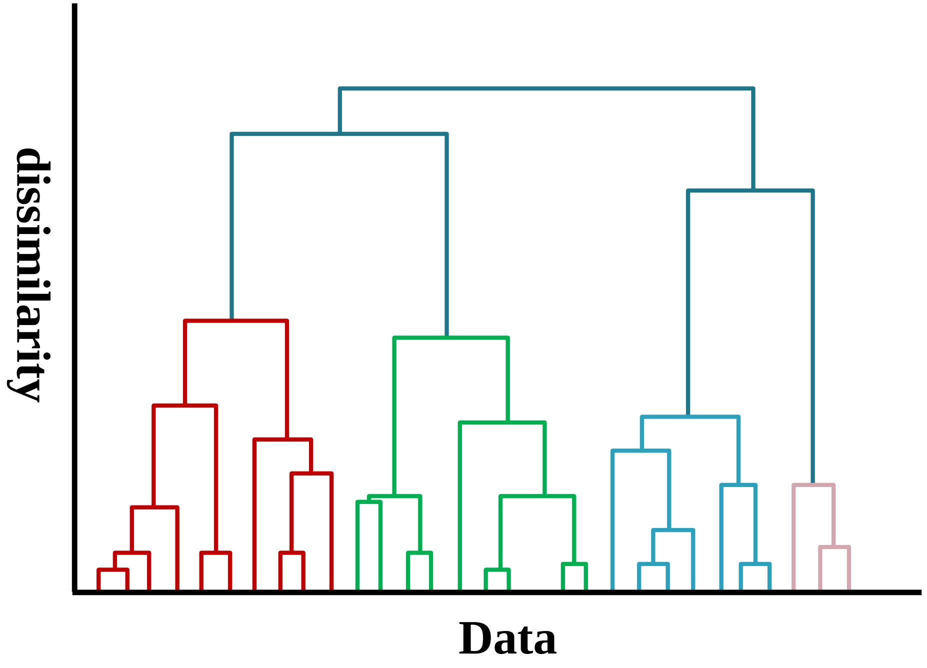

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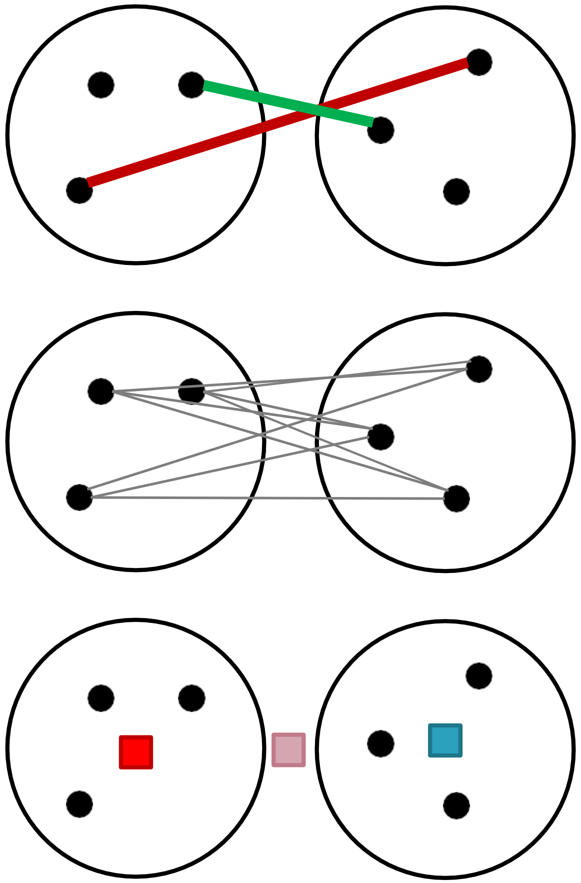
Hierarchical clustering

- How to define the closest two clusters.

- Criteria for determining clusters similarity.
  - Nearest pair (one-link clustering)
  - Farthest pair (all-link clustering)
  - Average distance of all pairs
  - «Enter» method (least variance, like k-means)



- Different criteria create different clusters.

Clustering of digits

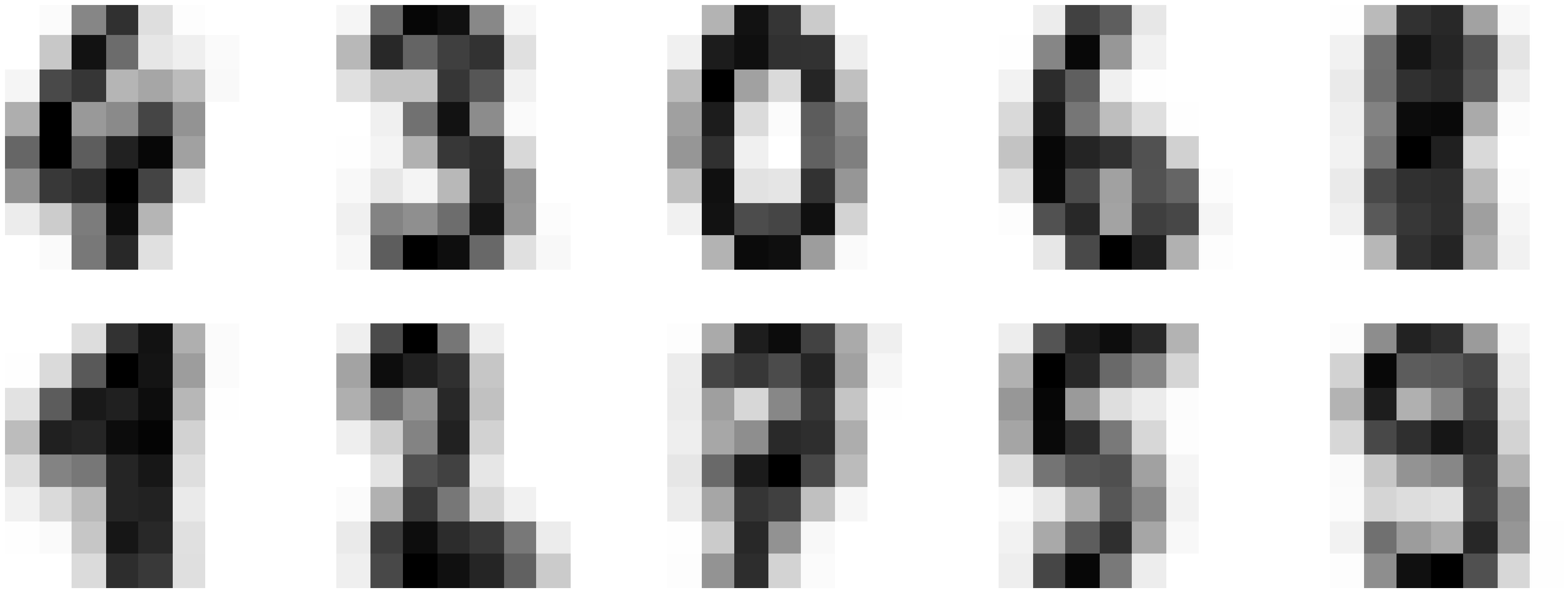
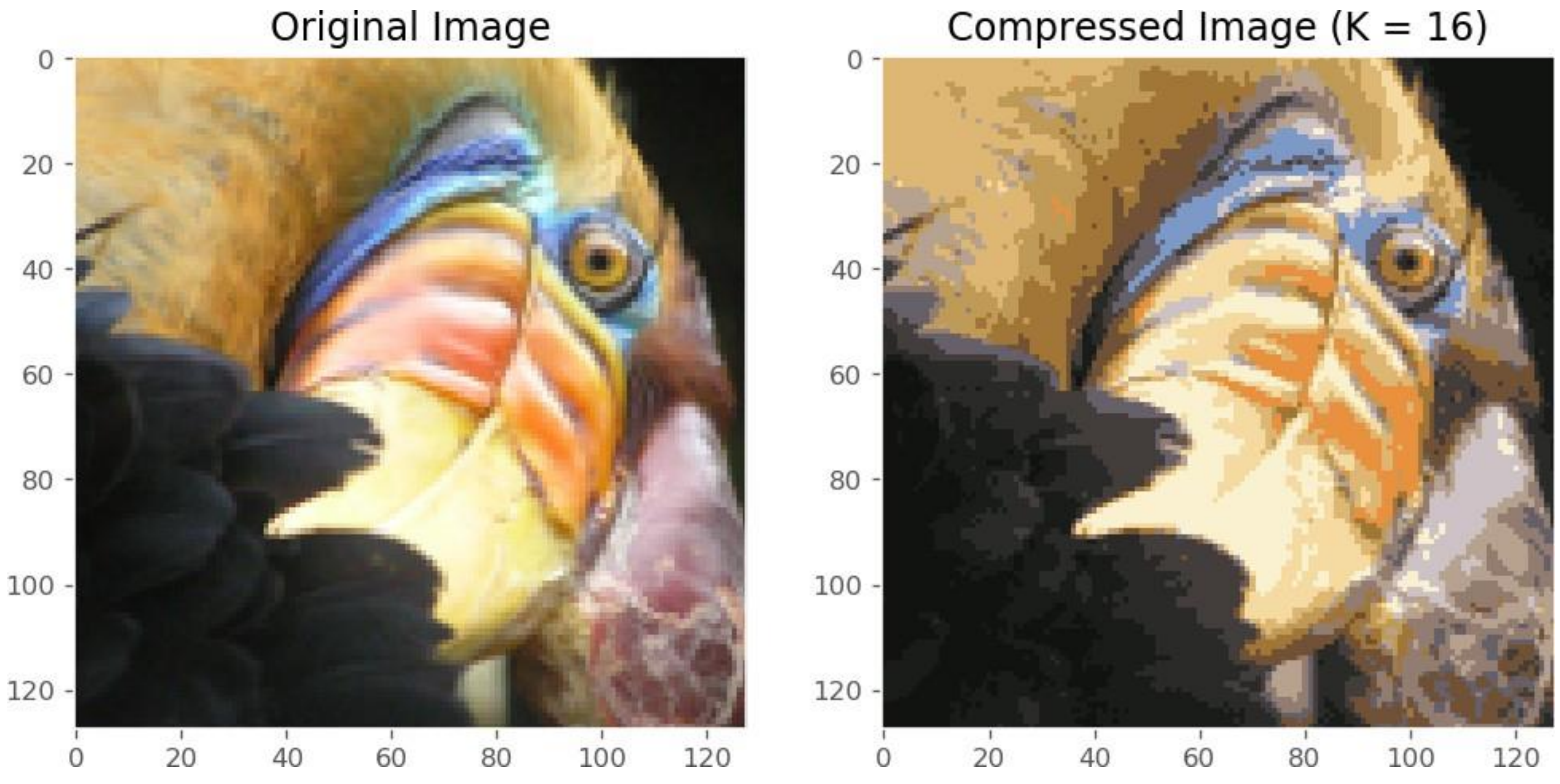


Image compression



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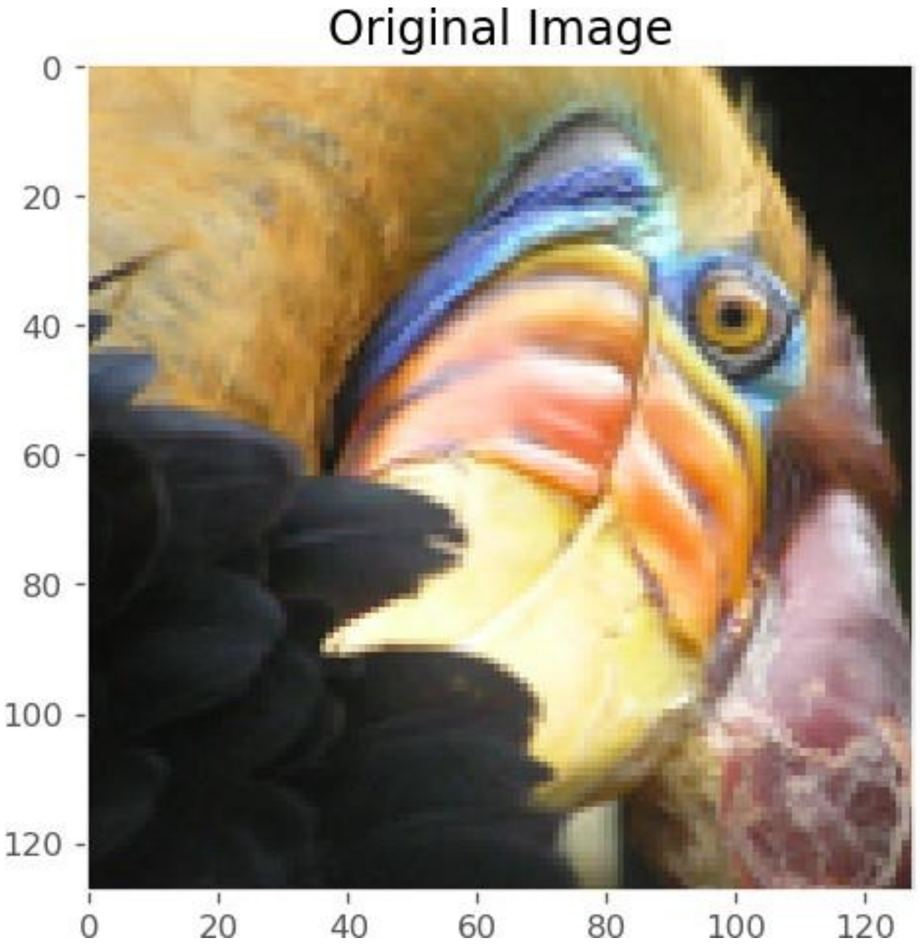

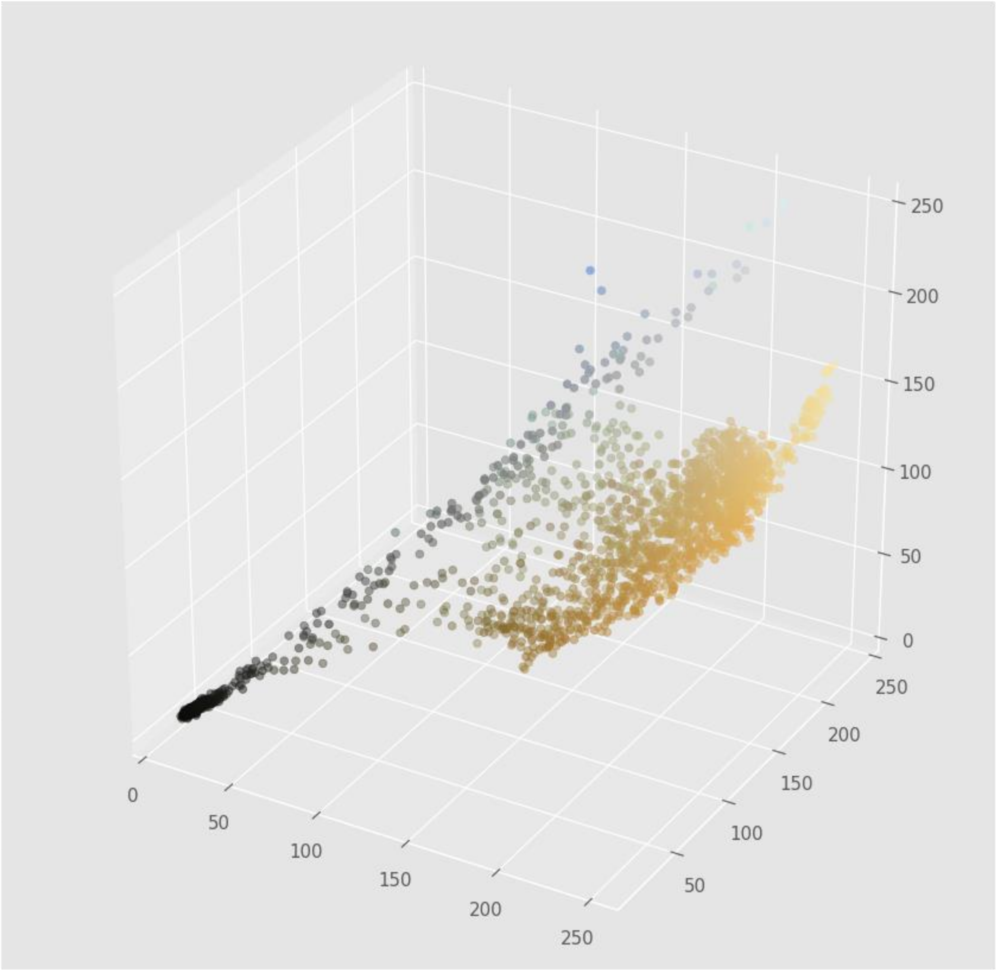

Summary

- Unsupervised learning, Finding structure in data

- Clustering Grouping similar data
  - K-mean Algorithm
    - Easy implementation
    - Slow for very large data sets
    - Possibility of getting stuck in the local optimum
  - Post-processing of clusters : Splitting and merging clusters
  - Algorithm of bipartite generator K-Means
    - Better clustering than the K-Means algorithm
  - Hierarchical clustering algorithms