

7 - Clustering problems

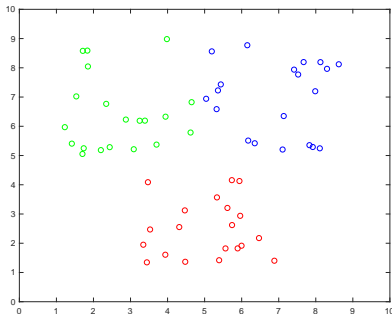
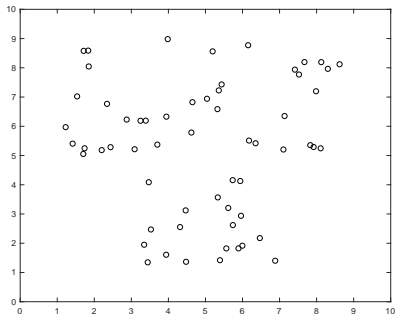
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Definition

Given a set S of patterns and an integer number k , a clustering problem consists in finding a partition of S in k subsets S_1, \dots, S_k (clusters) that are homogeneous and well separated.



Clustering problem is of interest in **unsupervised** machine learning.

The optimization model

- Assume that patterns are vectors $p_1, \dots, p_\ell \in \mathbb{R}^n$.
- Consider a distance $d : \mathbb{R}^n \times \mathbb{R}^n \rightarrow \mathbb{R}$ between vectors in \mathbb{R}^n .
In what follows we will consider the square distance $d(x, y) = \|x - y\|_2^2$ or $d(x, y) = \|x - y\|_1$.
- For each cluster S_j introduce a centroid $x_j \in \mathbb{R}^n$ (unknown).
- Define clusters so that each pattern is associated to the closest centroid.

We aim to find k centroids in order to minimize the sum of the distances between each pattern and the closest centroid.

The model

$$\begin{cases} \min \sum_{i=1}^{\ell} \min_{j=1, \dots, k} d(p_i, x_j) \\ x_j \in \mathbb{R}^n \quad \forall j = 1, \dots, k \end{cases}$$

The optimization model with $\|\cdot\|_2$

Consider the square distance $d(x, y) = \|x - y\|_2^2$.

The optimization problem to solve is

$$\begin{cases} \min \sum_{i=1}^{\ell} \min_{j=1, \dots, k} \|p_i - x_j\|_2^2 \\ x_j \in \mathbb{R}^n \quad \forall j = 1, \dots, k \end{cases}$$

If $k = 1$ (one cluster), then it is a **convex** quadratic programming problem without constraints:

$$\begin{cases} \min \sum_{i=1}^{\ell} \|p_i - x\|_2^2 = \min \sum_{i=1}^{\ell} (x - p_i)^T (x - p_i) \\ x \in \mathbb{R}^n \end{cases} \quad (1)$$

The global optimum is the stationary point:

$$2\ell x - 2 \sum_{i=1}^{\ell} p_i = 0 \quad \Longleftrightarrow \quad x = \frac{\sum_{i=1}^{\ell} p_i}{\ell} \quad (\text{mean or baricenter})$$

If $k > 1$ (at least two clusters), then the problem is **nonconvex and nondifferentiable**:

$$\begin{cases} \min_x \sum_{i=1}^{\ell} \min_{j=1, \dots, k} \|p_i - x_j\|_2^2 \\ x_j \in \mathbb{R}^n \quad \forall j = 1, \dots, k \end{cases} \quad (2)$$

We observe that for fixed p_i and x_j , $j = 1, \dots, k$,

$$\min_{j=1, \dots, k} \|p_i - x_j\|_2^2 = \begin{cases} \min \sum_{j=1}^k \alpha_{ij} \|p_i - x_j\|_2^2 \\ \sum_{j=1}^k \alpha_{ij} = 1 \\ \alpha_{ij} \geq 0 \quad \forall j = 1, \dots, k \end{cases} \quad (3)$$

Remark

It is enough to notice that, fixed a_1, a_2, \dots, a_k , we have that

$$\min_{j=1, \dots, k} \{a_j\} = \min \left\{ \sum_{j=1}^k \alpha_j a_j : \sum_{j=1}^k \alpha_j = 1, \alpha \geq 0 \right\}.$$

An optimal solution of (3) is given by

$$\alpha_{ij}^* = \begin{cases} 1 & \text{if } \|p_i - x_j\|_2 = \min_{h=1,\dots,k} \|p_i - x_h\|_2 \\ 0 & \text{otherwise.} \end{cases} \quad (4)$$

Remark

Observe that $\alpha_{ij}^* = 1$ if pattern i is assigned to cluster j .

Theorem

Problem (2) is equivalent to the following **nonconvex differentiable** problem:

$$\begin{cases} \min_{x, \alpha} f(x, \alpha) := \sum_{i=1}^{\ell} \sum_{j=1}^k \alpha_{ij} \|p_i - x_j\|_2^2 \\ \sum_{j=1}^k \alpha_{ij} = 1 \quad \forall i = 1, \dots, \ell \\ \alpha_{ij} \geq 0 \quad \forall i = 1, \dots, \ell, j = 1, \dots, k \\ x_j \in \mathbb{R}^n \quad \forall j = 1, \dots, k. \end{cases} \quad (5)$$

Clustering problem – k -means algorithm

The k -means algorithm is based on the following properties of problem (5):

- If x_j are fixed, then (5) is decomposable into ℓ simple **LP problems** of the form (3) : for any $i = 1, \dots, \ell$, the optimal solution is

$$\alpha_{ij}^* = \begin{cases} 1 & \text{if } j \text{ is the first index s.t. } \|p_i - x_j\|_2 = \min_{h=1, \dots, k} \|p_i - x_h\|_2 \\ & (x_j \text{ is the first closest centroid to } p_i), \\ 0 & \text{otherwise.} \end{cases}$$

- If α_{ij} are fixed, then (5) is decomposable into k **convex QP problems** (in the unknown x_j) similar to (1), i.e.,

$$\begin{cases} \min \sum_{i=1}^{\ell} \alpha_{ij} \|p_i - x_j\|_2^2 = \min \sum_{i=1}^{\ell} \alpha_{ij} (x_j - p_i)^T (x_j - p_i) \\ x_j \in \mathbb{R}^n \end{cases} \quad (6)$$

For any $j = 1, \dots, k$, the optimal solution of (6) is

$$x_j^* = \frac{\sum_{i=1}^{\ell} \alpha_{ij} p_i}{\sum_{i=1}^{\ell} \alpha_{ij}} \quad (\text{mean of patterns}).$$

Clustering problem – k -means algorithm

The k -means algorithm consists in an **alternating minimization** of

$f(x, \alpha) = \sum_{i=1}^{\ell} \sum_{j=1}^k \alpha_{ij} \|p_i - x_j\|_2^2$ with respect to the two blocks of variables x and α .

0. (Initialization) Set $t = 0$, choose centroids $x_1^0, \dots, x_k^0 \in \mathbb{R}^n$ and assign patterns to clusters: for any $i = 1, \dots, \ell$

$$\alpha_{ij}^0 = \begin{cases} 1 & \text{if } j \text{ is the first index s.t. } \|p_i - x_j^0\|_2 = \min_{h=1, \dots, k} \|p_i - x_h^0\|_2 \\ 0 & \text{otherwise.} \end{cases}$$

1. (Update centroids) For each $j = 1, \dots, k$ compute the mean

$$x_j^{t+1} = \left(\sum_{i=1}^{\ell} \alpha_{ij}^t p_i \right) / \left(\sum_{i=1}^{\ell} \alpha_{ij}^t \right).$$

2. (Update clusters) For any $i = 1, \dots, \ell$ compute

$$\alpha_{ij}^{t+1} = \begin{cases} 1 & \text{if } j \text{ is the first index s.t. } \|p_i - x_j^{t+1}\|_2 = \min_{h=1, \dots, k} \|p_i - x_h^{t+1}\|_2 \\ 0 & \text{otherwise.} \end{cases}$$

3. (Stopping criterion) If $f(x^{t+1}, \alpha^{t+1}) = f(x^t, \alpha^t)$ then STOP
else $t = t + 1$, go to Step 1.

Theorem

The k -means algorithm stops after a finite number of iterations at a solution (x^*, α^*) of the KKT system of problem (5) such that

$$\begin{aligned} f(x^*, \alpha^*) &\leq f(x^*, \alpha), & \forall \alpha \geq 0 \text{ s.t. } \sum_{j=1}^k \alpha_{ij} = 1 \quad \forall i = 1, \dots, \ell, \\ f(x^*, \alpha^*) &\leq f(x, \alpha^*), & \forall x \in \mathbb{R}^{kn}. \end{aligned}$$

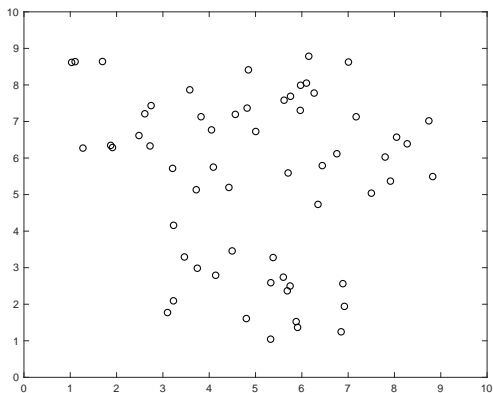
Remark. The k -means algorithm **does not guarantee** to find a **global optimum**.

Exercise 7.1. Consider the k -means algorithm, with $k = 3$, for the following set of patterns

1.2734	6.2721
2.7453	7.4345
1.6954	8.6408
1.1044	8.6364
4.8187	7.3664
2.7224	6.3303
4.8462	8.4123
4.0497	6.7696
1.0294	8.6174
3.7202	5.1327
3.8238	7.1297
3.5805	7.8660
3.2092	5.7172
1.8724	6.3461
4.0895	5.7509
1.9121	6.2877
2.4835	6.6154
4.5637	7.1943
4.4255	5.1950
2.6097	7.2109

6.0992	8.0496
5.9660	7.3042
5.9726	7.9907
5.6166	7.5821
8.8257	5.4929
8.7426	7.0176
8.2749	6.3890
7.9130	5.3686
5.7032	5.5914
6.4415	5.7927
5.7552	7.6891
5.0048	6.7260
6.2657	7.7776
7.7985	6.0271
7.5010	5.0390
7.1722	7.1291
6.7561	6.1176
6.1497	8.7849
7.0066	8.6258
8.0462	6.5707

3.0994	1.7722
5.6857	2.3666
6.3487	4.7316
6.8860	2.5627
3.2277	2.0929
4.8013	1.6078
5.3299	2.5884
5.7466	2.4989
5.8777	1.5245
5.6002	2.7402
5.9077	1.3661
4.4954	3.4585
5.3263	1.0439
3.4645	3.2930
3.2306	4.1589
6.9191	1.9415
4.1393	2.7921
5.3799	3.2774
6.8486	1.2456
3.7431	2.9852



- a) Run the algorithm starting from centroids $x_1 = (5, 7)$, $x_2 = (6, 3)$, $x_3 = (4, 3)$.
- b) Run the algorithm starting from centroids $x_1 = (5, 7)$, $x_2 = (6, 3)$, $x_3 = (4, 4)$.
- c) Is it possible to improve the solutions obtained in a) and b)?

```
data=[...];  
  
k=3;  % number of clusters  
  
InitialCentroids=[5,7;6,3;4,3];  
  
[x,cluster,v] = kmeans1(data,k,InitialCentroids)  
  
% plot centroids  
plot(x(1,1),x(1,2),'b*',x(2,1),x(2,2),'r*',x(3,1),x(3,2),'g*');  
  
hold on  
  
% plot clusters  
  
c1 = data(cluster==1,:);  
c2 = data(cluster==2,:);  
c3 = data(cluster==3,:);  
  
plot(c1(:,1),c1(:,2),'bo',c2(:,1),c2(:,2),'ro',c3(:,1),c3(:,2),'go');
```

```
function [x,cluster,v] = kmeans1(data,k,InitialCentroids)
```

```
l = size(data,1); % number of patterns
```

```
x = InitialCentroids; % initialize centroids
```

```
% initialize clusters
```

```
cluster = zeros(l,1);
```

```
for i = 1 : l
```

```
    d = inf;
```

```
    for j = 1 : k
```

```
        if norm(data(i,:)-x(j,:)) < d
```

```
            d = norm(data(i,:)-x(j,:));
```

```
            cluster(i) = j;
```

```
        end
```

```
    end
```

```
end
```

```
% compute the objective function value
```

```
vold = 0;
```

```
for i = 1 : l
```

```
    vold = vold + norm(data(i,:)-x(cluster(i),:))^ 2 ;
```

```
end
```

```
while true
```

% update centroids

```
for j = 1 : k
    ind = find(cluster == j);
    if isempty(ind)==0
        x(j,:) = mean(data(ind,:),1);
    end
end
```

% update clusters

```
for i = 1 : l
    d = inf;
    for j = 1 : k
        if norm(data(i,:)-x(j,:)) < d
            d = norm(data(i,:)-x(j,:));
            cluster(i) = j;
        end
    end
end
```

% update objective function

```
v = 0;
for i = 1 : l
    v = v + norm(data(i,:)-x(cluster(i),:))^ 2 ;
end
```

% stopping criterion

if $vold - v < 1e-5$

 break

else

$vold = v;$

end

end

end

Clustering problem – optimization model with $\|\cdot\|_1$

Consider now the distance $d(x, y) = \|x - y\|_1$.

The optimization problem to solve is

$$\begin{cases} \min \sum_{i=1}^{\ell} \min_{j=1, \dots, k} \|p_i - x_j\|_1 \\ x_j \in \mathbb{R}^n \quad \forall j = 1, \dots, k \end{cases}$$

If $k = 1$ (one cluster), then it is a **convex** problem decomposable into n convex problems of one variable:

$$\begin{cases} \min \sum_{i=1}^{\ell} \|p_i - x\|_1 = \min \sum_{i=1}^{\ell} \sum_{h=1}^n |x_h - (p_i)_h| = \min \sum_{h=1}^n \underbrace{\sum_{i=1}^{\ell} |x_h - (p_i)_h|}_{f_h(x_h)} \\ x \in \mathbb{R}^n \end{cases} \quad (7)$$

Clustering problem – optimization model with $\|\cdot\|_1$

Given ℓ real numbers $a_1 < a_2 < \dots < a_\ell$, what is the optimal solution of

$$\begin{cases} \min \sum_{i=1}^{\ell} |x - a_i| = f(x) \\ x \in \mathbb{R} \end{cases} \quad ?$$

The objective function is convex and piecewise linear:

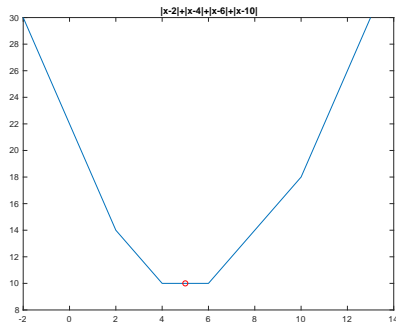
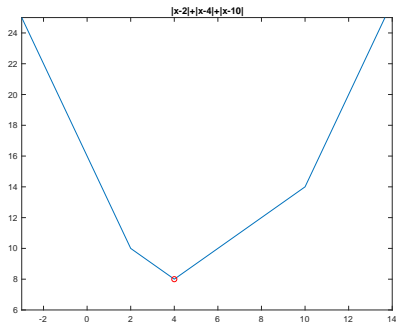
$$f(x) = \begin{cases} -\ell x + \sum_{i=1}^{\ell} a_i & \text{if } x < a_1 \\ (2 - \ell)x + \sum_{i=2}^{\ell} a_i - a_1 & \text{if } x \in [a_1, a_2] \\ \dots & \dots \\ (2r - \ell)x + \sum_{i=r+1}^{\ell} a_i - \sum_{i=1}^r a_i & \text{if } x \in [a_r, a_{r+1}] \\ \dots & \dots \\ (\ell - 2)x + a_\ell - \sum_{i=1}^{\ell-1} a_i & \text{if } x \in [a_{\ell-1}, a_\ell] \\ \ell x - \sum_{i=1}^{\ell} a_i & \text{if } x > a_\ell \end{cases}$$

The global optimum is $\text{median}(a_1, \dots, a_\ell) = \begin{cases} a_{(\ell+1)/2} & \text{if } \ell \text{ is odd,} \\ \frac{a_{\ell/2} + a_{1+\ell/2}}{2} & \text{if } \ell \text{ is even.} \end{cases}$

Example

(a) $f(x) = |x - 2| + |x - 4| + |x - 10|$, $\ell = 3$;

(b) $f(x) = |x - 2| + |x - 4| + |x - 6| + |x - 10|$, $\ell = 4$;



The global optimum is $\text{median}(a_1, \dots, a_\ell) = \begin{cases} a_{(\ell+1)/2} & \text{if } \ell = 3, \\ \frac{a_{\ell/2} + a_{1+\ell/2}}{2} & \text{if } \ell = 4. \end{cases}$

If $k > 1$ (at least two clusters), then the problem is **nonconvex and nonsmooth**:

$$\left\{ \begin{array}{ll} \min_x \sum_{i=1}^{\ell} \min_{j=1, \dots, k} \|p_i - x_j\|_1 & \\ x_j \in \mathbb{R}^n & \forall j = 1, \dots, k \end{array} \right. \quad (8)$$

Theorem

Problem (8) is equivalent to the following problem:

$$\left\{ \begin{array}{ll} \min_{x, \alpha} \sum_{i=1}^{\ell} \sum_{j=1}^k \alpha_{ij} \|p_i - x_j\|_1 & \\ \sum_{j=1}^k \alpha_{ij} = 1 & \forall i = 1, \dots, \ell \\ \alpha_{ij} \geq 0 & \forall i = 1, \dots, \ell, j = 1, \dots, k \\ x_j \in \mathbb{R}^n & \forall j = 1, \dots, k. \end{array} \right. \quad (9)$$

Note that

$$f(x, \alpha) := \sum_{i=1}^{\ell} \sum_{j=1}^k \alpha_{ij} \|p_i - x_j\|_1 = \sum_{i=1}^{\ell} \sum_{j=1}^k \sum_{h=1}^n \alpha_{ij} u_{ijh}$$

where we set

$$u_{ijh} = |(x_j)_h - (p_i)_h| = \max\{(x_j)_h - (p_i)_h, (p_i)_h - (x_j)_h\}$$

Consequently, we have the following result.

Theorem

Problem (9) is equivalent to the **nonconvex differentiable (bilinear)** problem:

$$\left\{ \begin{array}{ll} \min_{x, \alpha, u} & \sum_{i=1}^{\ell} \sum_{j=1}^k \sum_{h=1}^n \alpha_{ij} u_{ijh} \\ & u_{ijh} \geq (p_i)_h - (x_j)_h \quad \forall i = 1, \dots, \ell, j = 1, \dots, k, h = 1, \dots, n \\ & u_{ijh} \geq (x_j)_h - (p_i)_h \quad \forall i = 1, \dots, \ell, j = 1, \dots, k, h = 1, \dots, n \\ & \sum_{j=1}^k \alpha_{ij} = 1 \quad \forall i = 1, \dots, \ell \\ & \alpha_{ij} \geq 0 \quad \forall i = 1, \dots, \ell, j = 1, \dots, k \\ & x_j \in \mathbb{R}^n \quad \forall j = 1, \dots, k. \end{array} \right. \quad (10)$$

Clustering problem – k -median algorithm

The k -median algorithm is based on the following properties of problem (9):

- If x_j are fixed, then (9) is decomposable into ℓ simple LP problems: for any $i = 1, \dots, \ell$, the optimal solution is

$$\alpha_{ij}^* = \begin{cases} 1 & \text{if } j \text{ is the first index s.t. } \|p_i - x_j\|_1 = \min_{h=1, \dots, k} \|p_i - x_h\|_1 \\ & (x_j \text{ is the first closest centroid to } p_i), \\ 0 & \text{otherwise.} \end{cases}$$

- If $\alpha_{ij} \in \{0, 1\}$ are fixed, then (9) is decomposable into k simple convex problems similar to (7), i.e.,

$$\begin{cases} \min \sum_{i=1}^{\ell} \alpha_{ij} \|p_i - x_j\|_1 = \min \sum_{i=1}^{\ell} \sum_{h=1}^n \alpha_{ij} |(x_j)_h - (p_i)_h| \\ x_j \in \mathbb{R}^n \end{cases} \quad (11)$$

For any $j = 1, \dots, k$, the optimal solution is

$$x_j^* = \text{median}(p_i : \alpha_{ij} = 1).$$

Clustering problem – k -median algorithm

The k -median algorithm consists in an **alternating minimization** of

$f(x, \alpha) = \sum_{i=1}^{\ell} \sum_{j=1}^k \alpha_{ij} \|p_i - x_j\|_1$ with respect to the two blocks of variables x and α .

0. (Initialization) Set $t = 0$, choose centroids $x_1^0, \dots, x_k^0 \in \mathbb{R}^n$ and assign patterns to clusters: for any $i = 1, \dots, \ell$

$$\alpha_{ij}^0 = \begin{cases} 1 & \text{if } j \text{ is the first index s.t. } \|p_i - x_j^0\|_1 = \min_{h=1, \dots, k} \|p_i - x_h^0\|_1 \\ 0 & \text{otherwise.} \end{cases}$$

1. (Update centroids) For each $j = 1, \dots, k$ compute

$$x_j^{t+1} = \text{median}(p_i : \alpha_{ij}^t = 1).$$

2. (Update clusters) For any $i = 1, \dots, \ell$ compute

$$\alpha_{ij}^{t+1} = \begin{cases} 1 & \text{if } j \text{ is the first index s.t. } \|p_i - x_j^{t+1}\|_1 = \min_{h=1, \dots, k} \|p_i - x_h^{t+1}\|_1 \\ 0 & \text{otherwise.} \end{cases}$$

3. (Stopping criterion) If $f(x^{t+1}, \alpha^{t+1}) = f(x^t, \alpha^t)$ then STOP
else $t = t + 1$, go to Step 1.

Theorem

The k -median algorithm stops after a finite number of iterations at a stationary point (x^*, α^*) of problem (8) such that

$$\begin{aligned} f(x^*, \alpha^*) &\leq f(x^*, \alpha), & \forall \alpha \geq 0 \text{ s.t. } \sum_{j=1}^k \alpha_{ij} = 1 \quad \forall i = 1, \dots, \ell, \\ f(x^*, \alpha^*) &\leq f(x, \alpha^*), & \forall x \in \mathbb{R}^{kn}. \end{aligned}$$

Remark.

The k -median algorithm **does not guarantee** to find a **global optimum**.

Exercise 7.2. Consider the k -median algorithm, with $k = 3$, for the set of patterns given in Exercise 7.1.

- a) Run the algorithm starting from centroids $x_1 = (5, 7)$, $x_2 = (6, 3)$, $x_3 = (4, 3)$.
- b) Run the algorithm starting from centroids $x_1 = (5, 7)$, $x_2 = (6, 3)$, $x_3 = (4, 4)$.
- c) Is it possible to improve the solutions obtained in a) and b)?

Notice that the Matlab implementation of the k-median algorithm is analogous to the one of the k-means algorithm.

The changes with respect to the Matlab solution of Exercise 7.1 are given in [blue](#).

```
data=[...];  
  
k=3;  % number of clusters  
  
InitialCentroids=[5,7;6,3;4,3];  
  
[x,cluster,v] = kmedian2(data,k,InitialCentroids)  
  
% plot centroids  
plot(x(1,1),x(1,2),'b*',x(2,1),x(2,2),'r*',x(3,1),x(3,2),'g*');  
  
hold on  
  
% plot clusters  
  
c1 = data(cluster==1,:);  
c2 = data(cluster==2,:);  
c3 = data(cluster==3,:);  
  
plot(c1(:,1),c1(:,2),'bo',c2(:,1),c2(:,2),'ro',c3(:,1),c3(:,2),'go');
```



```
function [x,cluster,v] = kmedian2(data,k,InitialCentroids)
```

```
l = size(data,1); % number of patterns
```

```
x = InitialCentroids; % initialize centroids
```

```
% initialize clusters
```

```
cluster = zeros(l,1);
```

```
for i = 1 : l
```

```
    d = inf;
```

```
    for j = 1 : k
```

```
        if norm(data(i,:)-x(j,:),1) < d
```

```
            d = norm(data(i,:)-x(j,:),1);
```

```
            cluster(i) = j;
```

```
        end
```

```
    end
```

```
end
```

```
% compute the objective function value
```

```
vold = 0;
```

```
for i = 1 : l
```

```
    vold = vold + norm(data(i,:)-x(cluster(i,:),1) ;
```

```
end
```

```
while true
```

% update centroids

```
for j = 1 : k
    ind = find(cluster == j);
    if isempty(ind)==0
        x(j,:) = median(data(ind,:),1);
    end
end
```

% update clusters

```
for i = 1 : l
    d = inf;
    for j = 1 : k
        if norm(data(i,:)-x(j,:),1) < d
            d = norm(data(i,:)-x(j,:),1);
            cluster(i) = j;
        end
    end
end
```

% update objective function

```
v = 0;
for i = 1 : l
    v = v + norm(data(i,:)-x(cluster(i),:),1) ;
end
```

% stopping criterion

if $vold - v < 1e-5$

 break

else

$vold = v;$

end

end

end