7 - Clustering problems

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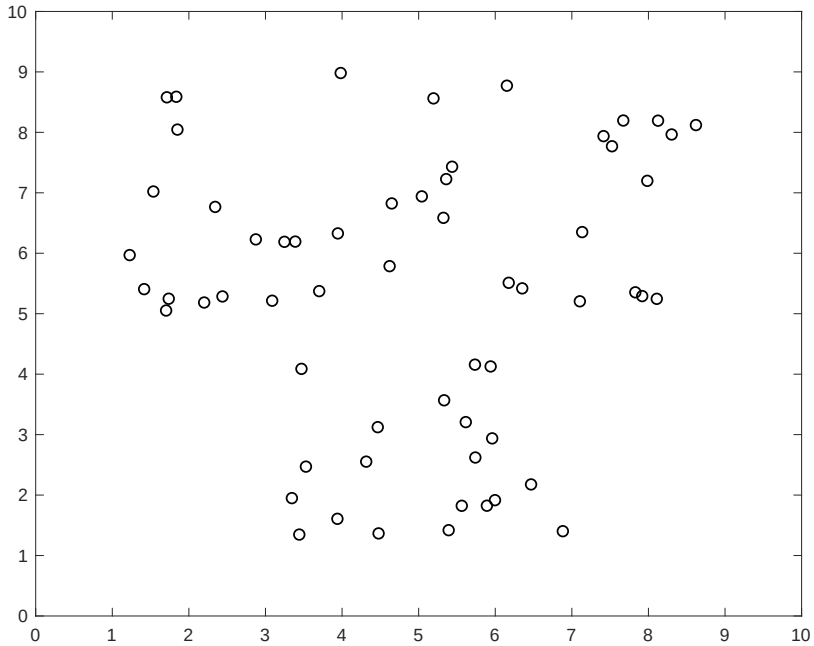
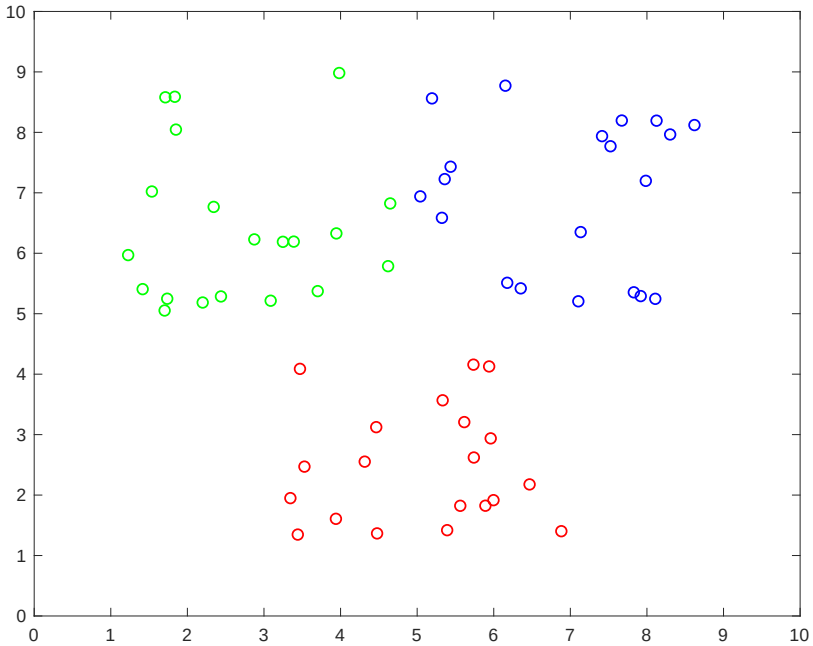
Definition

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





Clustering problem is of interest in unsupervisioned machine learning.

The optimization model

- Assume that patterns are vectors $p_1, \ldots, p_\ell \in \mathbb{R}^n$.
- Consider a distance $d : \mathbb{R}^n \times \mathbb{R}^n \to \mathbb{R}$ 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

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

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

Consider the square distance $d(x, y) = \|x - y\|_2^2$.
The optimization problem to solve is

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

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

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

The global optimum is the stationary point:

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

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

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

$$\begin{cases} \min\limits_{x} \sum\limits_{i=1}^{\ell} \min\limits_{j=1,\dots,k} \|p_i - x_j\|_2^2 \\ x_j \in \mathbb{R}^n \qquad \forall\, j = 1, \dots, k \end{cases} \tag{2}$$

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

$$\min_{j=1,\dots,k} \|p_i - x_j\|_2^2 = \begin{cases} \min \sum\limits_{j=1}^{k} \alpha_{ij} \|p_i - x_j\|_2^2 \\ \sum\limits_{j=1}^{k} \alpha_{ij} = 1 \\ \alpha_{ij} \geq 0 \qquad \forall\ \ j = 1, \dots, k \end{cases} \tag{3}$$

Remark

It is enough to notice that $\min\limits_{j=1,\dots,k} \{a_j\} = \min \left\{ \sum\limits_{j=1}^{k} \alpha_j a_j : \ \sum\limits_{j=1}^{k} \alpha_j = 1,\ \alpha \geq 0 \right\}$.

An optimal solution of (3) is given by

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

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:

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

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 $i = 1, \ldots, \ell$, the optimal solution is

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

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

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

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

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

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

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

1. (Update centroids) For each $j = 1, \ldots, k$ 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 $i = 1, \ldots, \ell$ compute

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

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

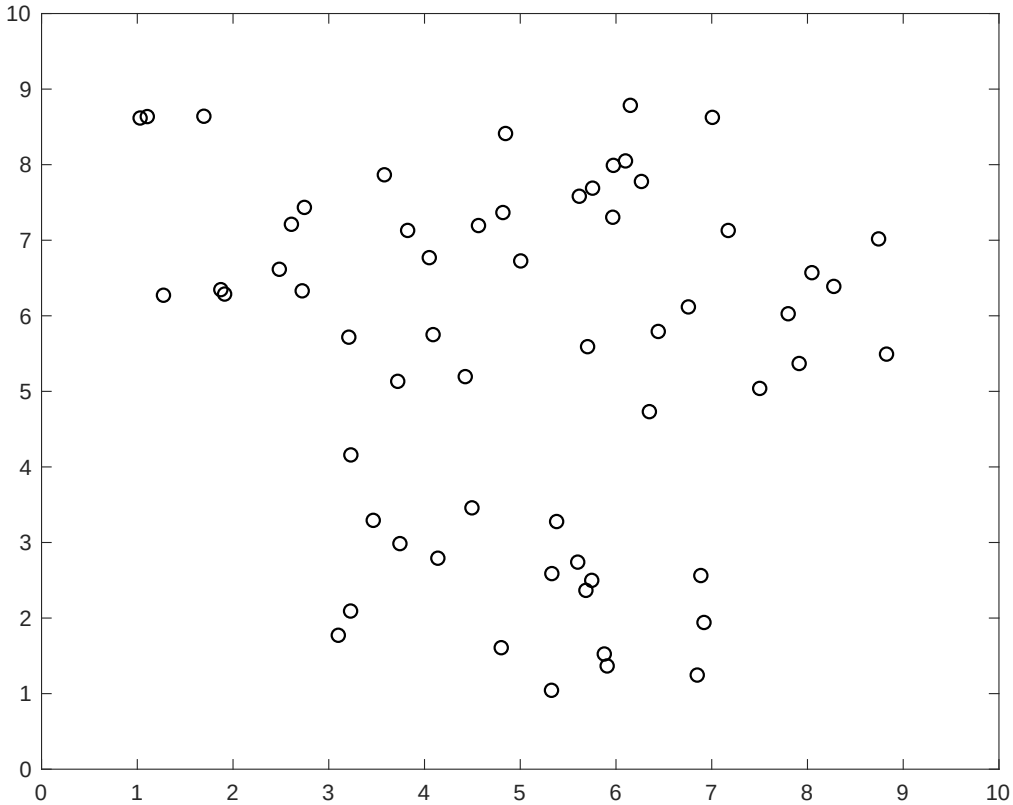
$$f(x^*, \alpha^*) \leq f(x^*, \alpha), \qquad \forall\ \alpha \geq 0 \ \text{ s.t. } \sum_{j=1}^{k} \alpha_{ij} = 1 \quad \forall\ i = 1, \ldots, \ell,$$

$$f(x^*, \alpha^*) \leq f(x, \alpha^*), \qquad \forall\ x \in \mathbb{R}^{kn}.$$

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

$$\begin{pmatrix} 1.2734 & 6.2721 \\ 2.7453 & 7.4345 \\ 1.6954 & 8.6408 \\ 1.1044 & 8.6364 \\ 4.8187 & 7.3664 \\ 2.7224 & 6.3303 \\ 4.8462 & 8.4123 \\ 4.0497 & 6.7696 \\ 1.0294 & 8.6174 \\ 3.7202 & 5.1327 \\ 3.8238 & 7.1297 \\ 3.5805 & 7.8660 \\ 3.2092 & 5.7172 \\ 1.8724 & 6.3461 \\ 4.0895 & 5.7509 \\ 1.9121 & 6.2877 \\ 2.4835 & 6.6154 \\ 4.5637 & 7.1943 \\ 4.4255 & 5.1950 \\ 2.6097 & 7.2109 \end{pmatrix} \quad \begin{pmatrix} 6.0992 & 8.0496 \\ 5.9660 & 7.3042 \\ 5.9726 & 7.9907 \\ 5.6166 & 7.5821 \\ 8.8257 & 5.4929 \\ 8.7426 & 7.0176 \\ 8.2749 & 6.3890 \\ 7.9130 & 5.3686 \\ 5.7032 & 5.5914 \\ 6.4415 & 5.7927 \\ 5.7552 & 7.6891 \\ 5.0048 & 6.7260 \\ 6.2657 & 7.7776 \\ 7.7985 & 6.0271 \\ 7.5010 & 5.0390 \\ 7.1722 & 7.1291 \\ 6.7561 & 6.1176 \\ 6.1497 & 8.7849 \\ 7.0066 & 8.6258 \\ 8.0462 & 6.5707 \end{pmatrix} \quad \begin{pmatrix} 3.0994 & 1.7722 \\ 5.6857 & 2.3666 \\ 6.3487 & 4.7316 \\ 6.8860 & 2.5627 \\ 3.2277 & 2.0929 \\ 4.8013 & 1.6078 \\ 5.3299 & 2.5884 \\ 5.7466 & 2.4989 \\ 5.8777 & 1.5245 \\ 5.6002 & 2.7402 \\ 5.9077 & 1.3661 \\ 4.4954 & 3.4585 \\ 5.3263 & 1.0439 \\ 3.4645 & 3.2930 \\ 3.2306 & 4.1589 \\ 6.9191 & 1.9415 \\ 4.1393 & 2.7921 \\ 5.3799 & 3.2774 \\ 6.8486 & 1.2456 \\ 3.7431 & 2.9852 \end{pmatrix}$$



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)?

Matlab commands

```
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

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

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

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

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

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

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

The objective function is convex and piecewise linear:

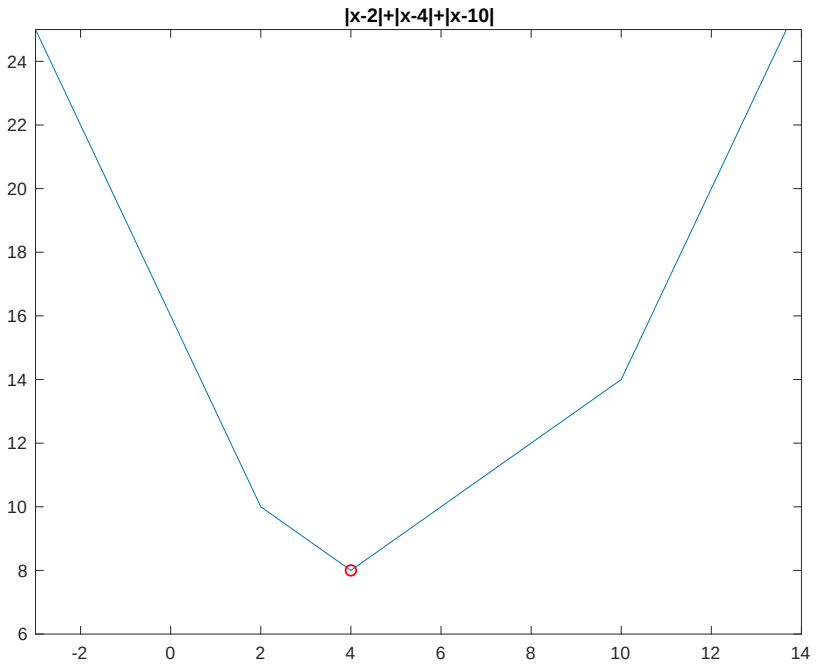
$$f(x) = \begin{cases} -\ell x + \sum_{i=1}^{\ell} a_i & \text{if } x < a_1 \\ (2-\ell)x + \sum_{i=2}^{\ell} a_i - a_1 & \text{if } x \in [a_1, a_2] \\ \dots & \dots \\ (2r-\ell)x + \sum_{i=r+1}^{\ell} a_i - \sum_{i=1}^{r} a_1 & \text{if } x \in [a_r, a_{r+1}] \\ \dots & \dots \\ (\ell-2)x + a_\ell -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

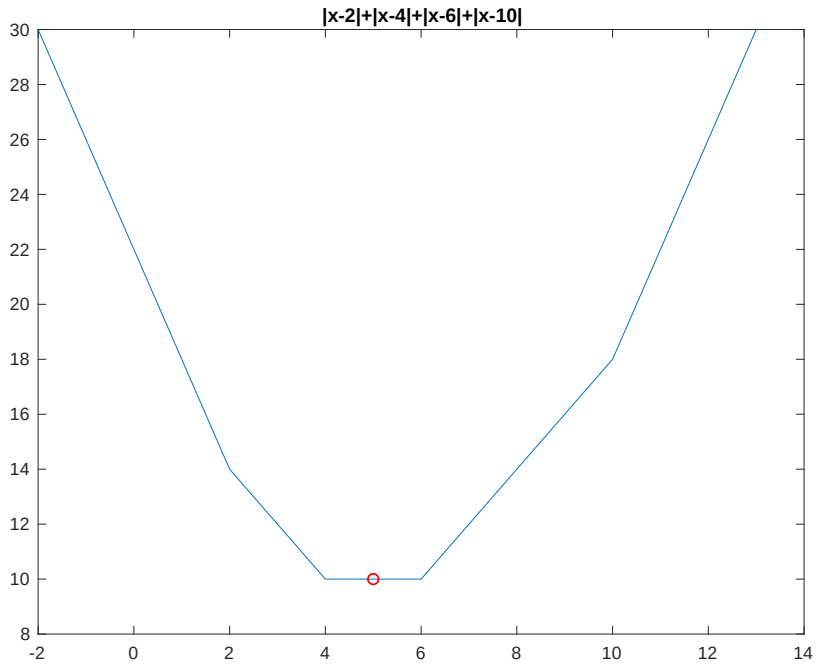
The global optimum is $\text{median}(a_1, \dots, a_\ell) = \begin{cases} a_{(\ell+1)/2} & \text{if } \ell \text{ is odd,} \\ \dfrac{a_{\ell/2} + a_{1+\ell/2}}{2} & \text{if } \ell \text{ is even.} \end{cases}$

Example

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

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





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

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

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

$$\begin{cases} \min\limits_{x} \sum\limits_{i=1}^{\ell} \min\limits_{j=1,\dots,k} \|p_i - x_j\|_1 \\ x_j \in \mathbb{R}^n \qquad \forall\, j = 1, \dots, k \end{cases} \tag{8}$$

Theorem

Problem (8) is equivalent to the following problem:

$$\begin{cases} \min\limits_{x,\alpha} \sum\limits_{i=1}^{\ell} \sum\limits_{j=1}^{k} \alpha_{ij} \|p_i - x_j\|_1 \\ \sum\limits_{j=1}^{k} \alpha_{ij} = 1 \quad \forall\, i = 1, \dots, \ell \\ \alpha_{ij} \geq 0 \qquad \forall\, i = 1, \dots, \ell,\ j = 1, \dots, k \\ x_j \in \mathbb{R}^n \qquad \forall\, j = 1, \dots, k. \end{cases} \tag{9}$$

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:

$$\begin{cases} \min\limits_{x,\alpha,u} \sum\limits_{i=1}^{\ell}\sum\limits_{j=1}^{k}\sum\limits_{h=1}^{n} \alpha_{ij}\, u_{ijh} \\ u_{ijh} \geq (p_i)_h - (x_j)_h \qquad \forall\ i = 1,\dots,\ell,\ j = 1,\dots,k,\ h = 1,\dots,n \\ u_{ijh} \geq (x_j)_h - (p_i)_h \qquad \forall\ i = 1,\dots,\ell,\ j = 1,\dots,k,\ h = 1,\dots,n \\ \sum\limits_{j=1}^{k} \alpha_{ij} = 1 \qquad \forall\ i = 1,\dots,\ell \\ \alpha_{ij} \geq 0 \qquad \forall\ i = 1,\dots,\ell,\ j = 1,\dots,k \\ x_j \in \mathbb{R}^n \qquad \forall\ j = 1,\dots,k. \end{cases} \tag{10}$$

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 $i = 1, \ldots, \ell$, the optimal solution is

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

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

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

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

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

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

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

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

$$f(x^*, \alpha^*) \leq f(x^*, \alpha), \qquad \forall\ \alpha \geq 0 \ \text{ s.t. } \sum_{j=1}^{k} \alpha_{ij} = 1 \quad \forall\ i = 1, \ldots, \ell,$$

$$f(x^*, \alpha^*) \leq f(x, \alpha^*), \qquad \forall\ x \in \mathbb{R}^{kn}.$$

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)?

Matlab commands

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
```