"Clustering algorithms"

1st Homework

Exercise 1:

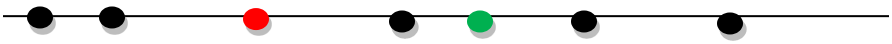
Let $x_1, x_2, \dots, x_n \in R$, with $x_1, < x_2 < \cdots < x_n$. Consider the quantity

$$A = \sum_{i=1}^{n} |x_i - \mu|.$$

Prove that A is minimized when μ is chosen as the median of $x_1, x_2, \dots, x_n$, i.e.

$$\mu = med(x_1, x_2, \dots, x_n).$$

Hints: (a) Let n be odd and $x_q \equiv \mu = med(x_1, x_2, \dots, x_n)$. Consider a number $k > x_q$ so that



$$x_1 < x_2 < \cdots < x_q < \cdots < x_r < k < \quad x_{r+1} < \cdots < x_n.$$

Let

$$A_1 = \sum_{i=1}^{n} |x_i - x_q|,$$

and

$$A_2 = \sum_{i=1}^{n} |x_i - k|.$$

The aim then is to prove that A_2 can be written as $A_2 = A_1 + \Lambda$, where Λ is a positive quantity. To this end, express **each term** $|x_i - k|$ in A_2 in terms of $|x_i - x_q|$ and $|x_q - k|$, separating three cases: (a) $x_i < x_q$, (b) $x_q < x_i < k$, (c) $k < x_i$.

Finally, utilize the fact that $|x_q - k| > |x_q - x_i|, for\ i = q + 1, \dots, r$.

(b) The case where $k < x_q$ (n odd) is treated similarly.

(c) In the case where n is even, the median minimizes A but it is not the only minimizer.

$$x_1 < x_2 < \cdots < x_q < x_{q+1} \dots < x_r < k < \quad x_{r+1} < \cdots < x_n.$$

More specifically, in terms of the above figure, **all the points in** the range $[x_q, x_{q+1}]$ are minimizers of A. Clearly, the **median** $\frac{x_q+x_{q+1}}{2}$ (denoted by the red dot) belongs to this range.

Exercise 2:

(I) Derive the cost function optimization algorithm **hard k-medians** that belongs to the Generalized Hard Algorithmic Scheme (GHAS), where

(a) the clusters are represented by point representatives

(b) the cost function that is minimized is

$$J(U, \Theta) = \sum_{i=1}^{N} \sum_{j=1}^{m} u_{ij} \, ||\boldsymbol{x}_i - \boldsymbol{\theta}_j||_1$$

where $\boldsymbol{x}_i = [x_{i1}, \ldots, x_{il}]^T \in R^l, i = 1, \ldots, N$, are the N l-dimensional data vectors, $\boldsymbol{\theta}_j = [\theta_{j1}, \ldots, \theta_{jl}]^T, j = 1, \ldots, m$, are the m l-dimensional point representatives of the clusters, and

$$||\boldsymbol{x}_i - \boldsymbol{\theta}_j||_1 = \sum_{r=1}^{l} |x_{ir} - \theta_{jr}|.$$

Give the algorithm in pseudocode (following the template given in the lecture slides).

(II) Derive the cost function optimization algorithm **possibilistic k-medians** that belongs to the Generalized Possibilistic Algorithmic Scheme (GPAS), where

(a) the clusters are represented by point representatives

(b) the cost function that is minimized is

$$J(U, \Theta) = \sum_{i=1}^{N} \sum_{j=1}^{m} {u_{ij}}^q \, ||\boldsymbol{x}_i - \boldsymbol{\theta}_j||_1 + \sum_{j=1}^{m} \eta_j \sum_{i=1}^{N} (1 - u_{ij})^q \;, \quad q > 1$$

where $\boldsymbol{x}_i = [x_{i1}, \ldots, x_{il}]^T \in R^l, i = 1, \ldots, N$, are the N l-dimensional data vectors, $\boldsymbol{\theta}_j = [\theta_{j1}, \ldots, \theta_{jl}]^T, j = 1, \ldots, m$, are the m l-dimensional point representatives of the clusters, and

$$||\boldsymbol{x}_i - \boldsymbol{\theta}_j||_1 = \sum_{r=1}^{l} |x_{ir} - \theta_{jr}|.$$

Give the algorithm in pseudocode (following the template given in the lecture slides).

Exercise 3:

Consider the data set $Y = \{\boldsymbol{x}_1, \boldsymbol{x}_2, \boldsymbol{x}_3, \boldsymbol{x}_4, \boldsymbol{x}_5\}$, where $\boldsymbol{x}_1 = [0,0]^{\mathrm{T}}$, $\boldsymbol{x}_2 = [0,3]^{\mathrm{T}}$, $\boldsymbol{x}_3 = [6,0]^{\mathrm{T}}$, $\boldsymbol{x}_4 = [7,0]^{\mathrm{T}}$, $\boldsymbol{x}_5 = [7,-3]^{\mathrm{T}}$.

(a) Run the k-means and the k-medians clustering algorithm, for two representatives, $\boldsymbol{\theta}_1$and $\boldsymbol{\theta}_2$, whose initial positions are $\boldsymbol{\theta}_1(0) = [6,1]^{\mathrm{T}}$ and $\boldsymbol{\theta}_2(0) = [8,0]^{\mathrm{T}}$, respectively. At each iteration report the (i) $U = [u_{ij}]$ matrix, (ii) $\boldsymbol{\theta}_j$'s and (iii) the formed clusters.

(b) What would be the clustering result for the case where $\boldsymbol{\theta}_2(0) = [20,0]^{\mathrm{T}}$?

How many clusters will be obtained if three representatives where employed?

Note: For this exercise use only paper, pencil and a pocket calculator (if necessary).

Exercise 4 (code):

(a) Generate a data set consisting of 400 2-dimensional points. The 1st, 2nd, 3rd and 4th groups of 100 points stem from 2-dimensional normal distributions with means $m_1 = [0,0]^T, m_2 = [10,0]^T, m_3 = [0,9]^T, m_4 = [9,8]^T$, and covariance matrices $\Sigma_1 = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}, \Sigma_2 = \begin{bmatrix} 1 & -0.2 \\ -0.2 & 1.5 \end{bmatrix}, \Sigma_3 = \begin{bmatrix} 1 & -0.4 \\ -0.4 & 1.1 \end{bmatrix}, \Sigma_4 = \begin{bmatrix} 0.3 & 0.2 \\ 0.2 & 0.5 \end{bmatrix}$, respectively. Plot the data points using different colors for points stemming from different distributions.

(b) Run the k-means and the k-medians algorithms on the above data set and plot the data points that belong to different clusters with different colors.

(c) Compare quantitatively the estimates of the representatives with the respective means of the distributions.

Hints: (a) To generate the data set use the following MATLAB code

```
randn('seed',0)
m=[0 0; 10 0; 0 9; 9 8];
S(:,:,1)=eye(2);
S(:,:,2)=[1.0 -.2; -.2 1.5];
S(:,:,3)=[1.0 -.4; -.4 1.1];
S(:,:,4)=[.3 .2; .2 .5];
n_points=100*ones(1,4);
X=[];
for i=1:4
    X=[X; mvnrnd(m(i,:),S(:,:,i),n_points(i))];
end
X=X';
```

(b) To plot the data set use the following MATLAB code

```
figure(1), plot(X(1,:),X(2,:),'.b')
figure(1), axis equal
```

(c) To plot the points of different clusters with different colors, as well as to plot the cluster representatives, use the following MATLAB code

```
% Plot the clusters
figure(2), hold on
figure(2), plot(X(1,bel==1),X(2,bel==1),'r.',...
X(1,bel==2),X(2,bel==2),'g*',X(1,bel==3),X(2,bel==3),'bo',...
X(1,bel==4),X(2,bel==4),'cx',X(1,bel==5),X(2,bel==5),'md',...
X(1,bel==6),X(2,bel==6),'yp',X(1,bel==7),X(2,bel==7),'ks')
figure(2), plot(theta(1,:),theta(2,:),'k+')
figure(2), axis equal
```

Exercise 5 (code):

(a) Implement in MATLAB the above derived algorithm.

(b) Generate a data set consisting of 500 2-dimensional points. The first 400 points are generated as in exercise 3. The next 99 points are noisy points that are uniformly spread among the points resulting from the above four distributions and the last point is the $\boldsymbol{x}_{500} = [100, 100]^T$. Plot the data points using different colors for the points stemming from different distributions as well as the noisy points.

(c) Run the k-means and the k-medians algorithms on the above data set and plot the data points that belong to different clusters with different colors.

(d) Compare quantitatively the estimates of the representatives with the respective means of the distributions.

Hint: To generate the additional 99 noisy points add after the code generating the 400 points from the distributions, the following MATLAB code

```
% Generate the remaining 100 points
noise=rand(2,99)*14-2;
X=[X noise];
```

Exercise 6:

Discuss the results obtained in exercises 4 and 5.