K-means Clustering

In this problem set we will implement and apply the batch K-means algorithm, the online version, and the "soft" clustering procedures. The file `cluster.dat` contains a data set of $p = 500$ (2-dimensional) observations generated from four different Gaussians with four different means.

Exercise 8.1: K-means Clustering – batch version (3 points)

Write a program that implements the *batch* version of K-means clustering and partitions the given data set into M clusters. Repeat the clustering procedure for different initializations of the prototypes and $M = 2, 3, 4, 5, 6, 7, 8$. Include the following steps:

A: Initialization –

1. Set the initial position of each prototype $\underline{\mathbf{w}}_q$ randomly around the mean of the entire dateset.
2. Set the maximum number of iterations: $t_{max} = 5$

B: Optimization –

Implement the K-means update. Each iteration should contain the following two steps

1. Assign all datapoints to their closest prototype.
2. Re-compute the location of the prototypes due to the new assignments.

C: Visualization –

(a) Visualize data points and prototypes for each iteration in a sequence of scatter plots.

(b) For two different initializations, plot the error function E vs. the iteration t

$$E_{\left[\{m_q^{(\alpha)}\},\{\underline{\mathbf{w}}_q\}\right]} = \frac{1}{p}\sum_{\alpha=1}^{p}\sum_{q=1}^{M} m_q^{(\alpha)} \left\|\underline{\mathbf{x}}^{(\alpha)} - \underline{\mathbf{w}}_q\right\|_2^2$$

(c) Create a plot (Voronoi-Tesselation) to show how the resulting solution would potentially assign new data points (i.e. show the decision boundaries that separate the clusters).

Exercise 8.2: Online K-means Clustering (3 points)

Write a program that implements the *online* version of K-means clustering and partitions the given data set into $M = 4$ clusters. Include the following steps:

A: Initialization –

1. Set the initial position of each prototype $\underline{\mathbf{w}}_q$ randomly around the mean of the entire dateset.
2. Select an initial learning step ε_0
3. Set the maximum number of iterations t_{max} equal to the data set size p.

B: Optimization –

1. Choose a suitable $\tau < 1$ and implement online K-means clustering using the following "annealing" schedule for ε:

$$\varepsilon_t = \varepsilon_0 \quad \text{for } t = 0, ..., \frac{t_{max}}{4} \qquad \text{and} \qquad \varepsilon_t = \tau\varepsilon_{t-1} \quad \text{for } t = \frac{t_{max}}{4} + 1, ..., t_{max}$$

C: Visualization –

(a) Visualize the data points and prototypes, where data points are colored according to the cluster they will *finally* be assigned to *after* $t_{\max}$. Additionally, show for each cluster the sequence of prototype positions $\underline{\mathbf{w}}_q$ by connecting them with straight lines (each iteration pair $t \to t+1$ one line per prototype - to trace the position of a prototype over time). Use different colors for the prototype lines than the colours used for the data points.

(b) Plot the error function E (as above) against the iteration t. Is E nonincreasing?

Exercise 8.3: Soft K-means Clustering (4 points)

Implement the *soft* K-means algorithm with squared Euclidean distances (the batch version) and apply it to the same data as before. Proceed as follows:

(a) Set $M = 12$ initial prototypes $\mathbf{w}_q$ randomly around the data set mean and choose a convergence tolerance θ.

(b) For fixed β (no annealing), let the optimization procedure run until convergence, that is $\|\mathbf{w}_q^{new} - \mathbf{w}_q^{old}\|_2 < \theta \; \forall q$. Repeat this for different $\beta \in [0.2, 20]$ e.g. in steps of $\Delta\beta = 0.2$. Use the same initial prototypes for all runs.

(c) Visualize the data set, initial and final prototypes for each (fixed) β in one scatter plot.

(d) In additional simulations, run the optimization using an annealing schedule: increase β after each iteration. E.g. $\beta_0 = 0.2,\ \tau = 1.1,\ \beta_{t+1} = \tau\beta_t$.

(e) Show the data set, initial and final prototypes of the "annealed" clustering solutions in a scatter plot. Additionally, show the position of each prototype (x_2 coordinate only) as a function of t – all in one figure (i.e., $M = 12$ lines). How "soft" are data points assigned now?

Total 10 points.