PRACTICE 6 - OPTIMIZATION TECHNIQUES

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Exercise

Let the classification problem be identified by `square4.txt` (in text format) or `square4.xlsx` (Excel format). In this problem, a set of data is identified by the cartesian coordinates (first two values) and a category (third value) that takes the values {0, 1, 2, 3}.

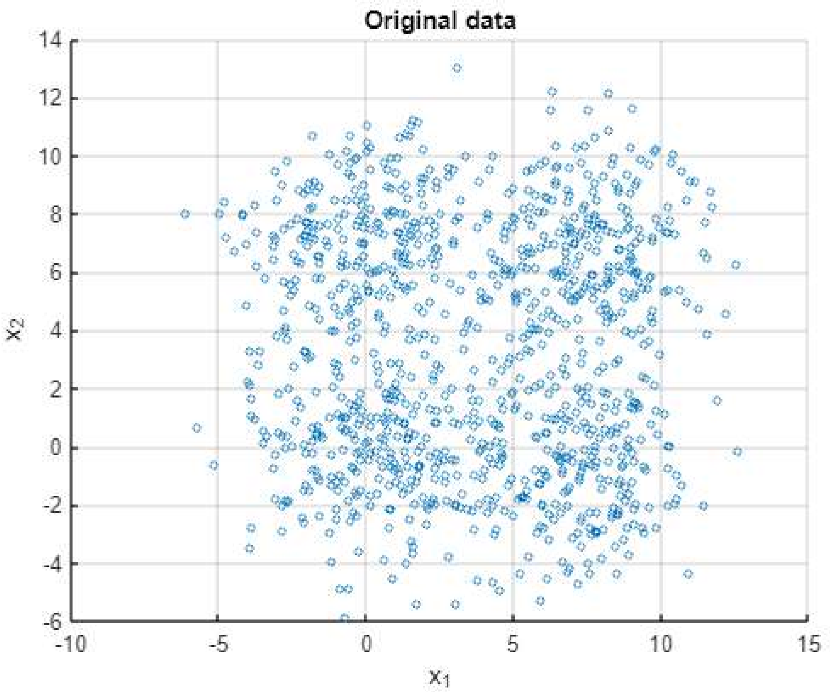
The objective of the practice is to become familiar with the heuristic optimization procedures, so a grouping or clustering problem will arise if the category variable is not used; therefore, in subsequent implementations you should NOT use the third variable, which is only provided for later checks.

Then, the following is requested:

1. Problem comprehension and modelization.

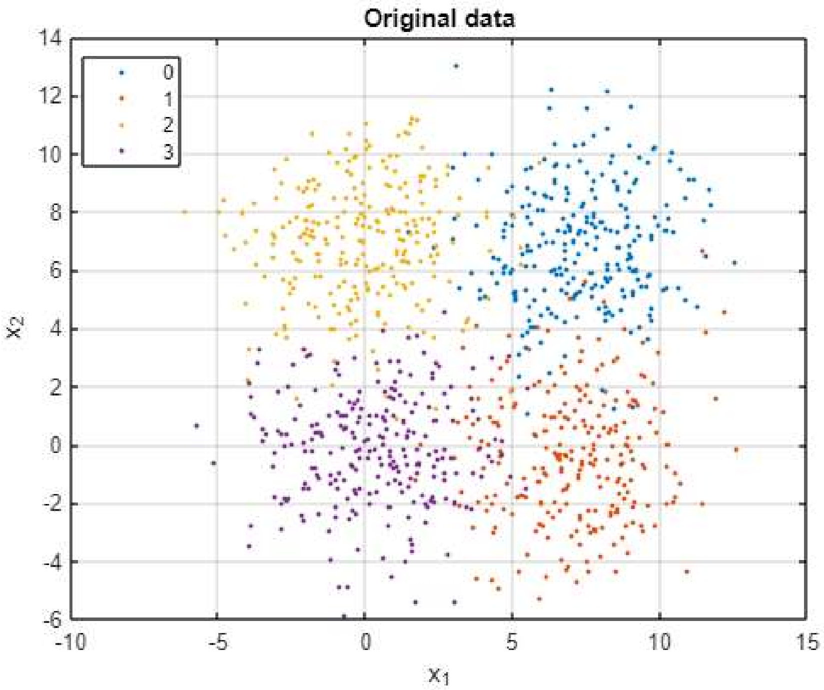
a) Plot the data (filtering by category)

```
clc, clear, clf
cd 'C:\Users\andre\Documents\UNIVERSIDAD\MUTECI\BLOQUE 2\TOPT\lab\P6'
data = importdata('square4.txt', ',',1);
X1 = data.data(:, 1); X2 = data.data(:, 2); Y = data.data(:,3); % category;

figure(1)
scatter(X1, X2, 'SizeData', 10)
grid on
xlabel("x_1")
ylabel("x_2")
title('Original data')
```



Filtering by category...

```
figure(2)
gscatter(X1, X2, Y)
grid on
xlabel("x_1")
ylabel("x_2")
title('Original data')
```



b) If the number of categories is unkwown, try to figure out which is the most appropiate number of clusters for this problem: think about 2, 3 and 4 categories.

Two clusters

With two clusters, the data can be discriminated in horizontal and vertical ways. Since data seems to spread normally distributed over the plane, we can assume that a linear discriminator that passes through the mean of each point could be adapted to the problem.

```
mean(X1)
```

```
ans = 3.6822
```

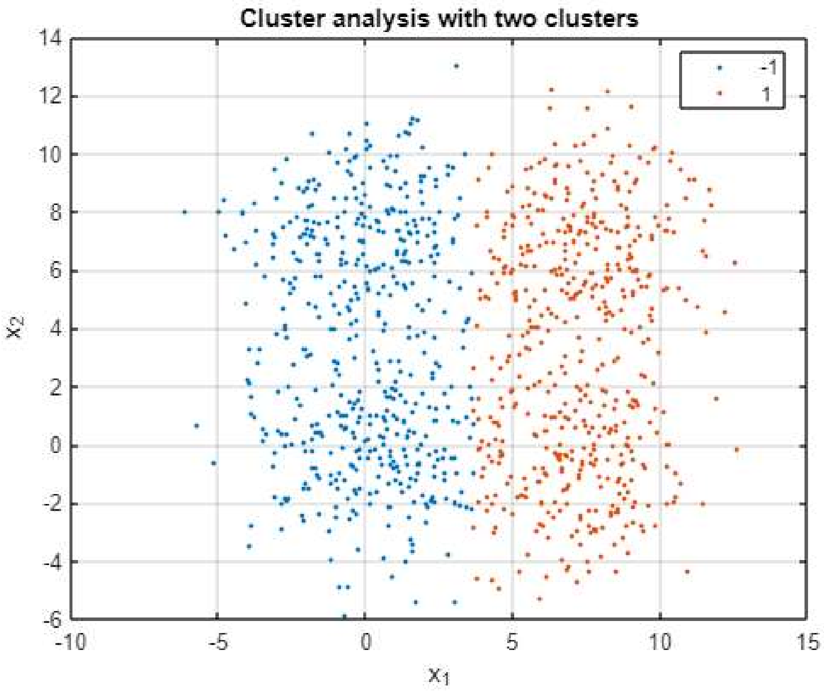
```
mean(X2)
```

```
ans = 3.3593
```

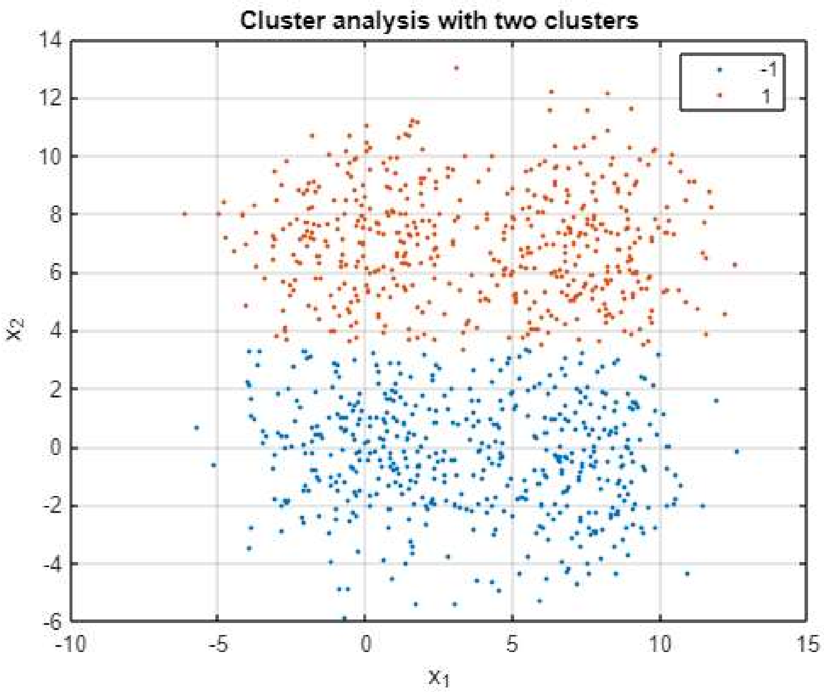
Then, two possible groups could be:

- One group above the line $x_2 = 3.6822$, and another below that line.
- One group on the right of $x_1 = 3.3593$, and one is on the left.

```
C = zeros(1,length(X1));
idxa = X1>=mean(X1);
idxb = X1<mean(X1);

C(idxa) = 1;
C(idxb) = -1;

figure(3)
gscatter(X1, X2, C)
grid on
xlabel("x_1")
ylabel("x_2")
title('Cluster analysis with two clusters')
```




```
idxc = X2>=mean(X2);
idxd = X2<mean(X2);
C(idxc) = 1;
C(idxd) = -1;

figure(4)
gscatter(X1, X2, C)
grid on
xlabel("x_1")
ylabel("x_2")
title('Cluster analysis with two clusters')
```



Both models fit well, but they can be combined in 4 groups instead of 2-by-2. So, two clusters are not a suitable number of groups for this problem.

Three clusters

It does not makes sense to distribute the data across 3 groups because the shape of all data joined it seems like a "window" with 4 squares, or a big square, and the number of points is equally distributed only in pair groups.

Four clusters

As we aforementioned, four groups seems to be a good approximation for our data distribution.

c) Propose a distance or difference measure for the data.

Since we are working in a cartesian plane, we could make use of the eculidean distance, i.e., $d_{i,j} = \sqrt{x_j^2 - x_i^2}$. This distance suits with every kind of data that works with a canonical vectorial kernel. But, since our data is distributed in a shape of a square, a better solution could pass by considering the Mikowski distance of infinite order, this is, **the Chebysev distance**.

The Minkowski distance of order p (where p is an integer) between two points

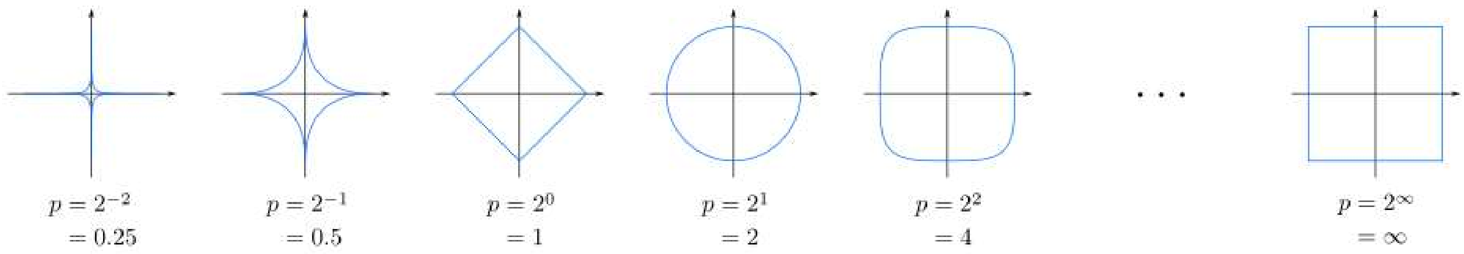
$X = (x_1, x_2, \dots, x_n), Y = (y_1, y_2, \dots, y_n)$, where $X, Y \in \mathbb{R}^n$

is defined as:

$$\left(\sum_{i=1}^{n} |x_i - y_i|^p\right)^{\frac{1}{p}}$$

We obtain the classical Euclidean distance when $p = 2$, and we obtain the manhattan distance when $p = 1$. But, when $p \to \infty$, the distance over a circle unit plots a square.

The following figure shows unit circles (the level set of the distance function where all points are at the unit distance from the center) with various values of p:



So, our choosen distance is the Cherbysev distance:

$$\lim_{p\to\infty}\left(\sum_{i=1}^{2} |x_i - y_i|^p\right)^{\frac{1}{p}}$$

d) Identify the problem as an optimization problem indicating the decision variable, objective function and restrictions.

A data set consists of $d_i = \{(x_1, y_1), (x_2, y_2), \dots, (x_n, y_n)\}$, data points which will be distributed among $c_j = \{c_1, c_2, \dots, c_i\}, c_j = (x_j^{'}, y_j^{'})$ clusters. The data points are assigned to the correct clusters by minimizing the sum of the Cherbysev distance between each data point and cluster centroid. This distance is denoted r_i for $i = 1, 2, \dots, n$.

Then, the problem can be formulated as follows:

$$\begin{array}{ll} \min & \sum_{i=1}^{n} r_i \\ \text{s.t.} & \lim_{p\to\infty}\left(|d_1 - c_1|^p\right)^{\frac{1}{p}} \le r_1 \vee \dots \vee \lim_{p\to\infty}\left(|d_1 - c_K|^p\right)^{\frac{1}{p}} \le r_1 \\ \vdots & \qquad\qquad\qquad\qquad\qquad\qquad \vdots \\ & \lim_{p\to\infty}\left(|d_n - c_1|^p\right)^{\frac{1}{p}} \le r_n \vee \dots \vee \lim_{p\to\infty}\left(|d_n - c_K|^p\right)^{\frac{1}{p}} \le r_n \end{array}$$

Where de decission variable is k, the number of clusters.

Since the data point can only belong to one cluster, we introduce the logicals or statement that we can see in the expression.

2. Propose a voracious constructive procedure to obtain an initial solution quickly.

1. **Initialize centers:** we select the K initial clusters centers $c_1, c_2, \dots, c_K$ taking randomly k different data points.
2. **Assign Points to Clusters:** For each point d_i, calculate the distances to all cluster centers using the expression:

   $\lim_{p\to\infty}\left(|d_1 - c_1|^p\right)^{\frac{1}{p}}, \dots, \lim_{p\to\infty}\left(|d_1 - c_K|^p\right)^{\frac{1}{p}}$. Assign d_i to the cluster whose distance is the smallest among all clusters.
3. **Update centers:** recalculate the cluster centers by taking the mean of all points assigned to each cluster:

   $c_K = \frac{1}{\text{points in cluster k}} \sum_i d_i$.
4. **Repeat steps 2 and 3:** repeat the assignment and update steps until convergence or a predetermined number of iterations.
5. **Calculate Objective Function:** Calculate the objective function value based on the obtained solution.

3. Based on the proposed model, given a generic solution, define a set of neighbors of said solution.

Little modifications of the previous problem can be made in order to obtain the neighbours of the solution. The following are proposed:

1. Perturbation of Cluster Centers:

- Randomly select one or more cluster centers.
- Perturb (add or subtract a certain amount to each cluster center initialization).

2. Combination of Center and Radius Perturbations:

- Combine the above two perturbations, i.e., perturb both cluster centers and radii simultaneously.

3. Swap Points between Clusters:

- Randomly select two clusters.
- Swap a random point between the selected clusters.

4. Add or Remove Cluster:

- Randomly add a new cluster with a random center and radius.
- Randomly remove one of the existing clusters.

5. Local Search Neighborhood:

- Perform a local search around the current solution by iteratively moving towards improving solutions within a local radius.