Lecture1_Clustering

February 1, 2021

1 MATH310 - Lecture 1 (k-means clustering, theory and examples)

In the beginning of this course we will mainly refer to available material for the book "Introduction to Applied Linear Algebra – Vectors, Matrices, and Least Squares" (VMLS) with correspondig available resources.

Linear Algebra requirements and geometric considerations required to understand the k-means Clustering is covered in VMLS, ch. 1-4 and the corresponding VMLS-slides, ch. 1-4.

2 The required key concepts are:

- The Euclidean (standard) inner product and norm in $\mathbf{R}^n$
- Distance in $\mathbf{R}^n$.
- Cauchy-Schwartz inequality.

- Definition of the angle between two vectors in $\mathbf{R}^n$.
- The triangle inequality.
- **Clustering**: The k-means algorithm for grouping unlabelled datapoints (Ch 4.1-4.3 in VMLS)

3 To get started with Julia you should

- Read the Julia language companion, ch. 1-4
- Explore the VMLS Julia resource links here.

4 The standard inner product and norm in $\mathbf{R}^n$ (chapter 1.4 in VMLS)

The the standard inner product (scalar product) between two vectors

$$\mathbf{u} = \begin{bmatrix} u_1 \\ \vdots \\ u_n \end{bmatrix}, \mathbf{v} = \begin{bmatrix} v_1 \\ \vdots \\ v_n \end{bmatrix} \in \mathbf{R}^n$$

is defined as the number

$$\mathbf{u} \cdot \mathbf{v} = \mathbf{u}^t \mathbf{v} = \sum_{i=1}^{n} u_i v_i.$$

The norm of $\mathbf{v}$ in $\mathbf{R}^n$ is defined as

$$\|\mathbf{v}\| = \sqrt{\mathbf{v} \cdot \mathbf{v}} = \sqrt{\sum_{i=1}^{n} v_i v_i},$$

i.e. the square root of the inner product of $\mathbf{v}$ with itself.

5 The distance between vectors in Euclidean space (chapter 3.2 in VMLS)

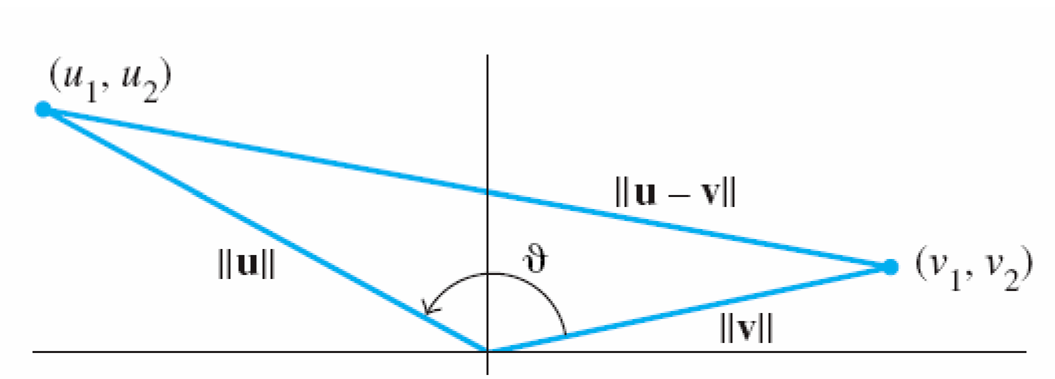
The distance between two vectors $\mathbf{u}, \mathbf{v} \in \mathbf{R}^n$ is defined as the norm of their difference

$$dist(\mathbf{u}, \mathbf{v}) = \|\mathbf{u} - \mathbf{v}\| = \sqrt{(\mathbf{u} - \mathbf{v})^t (\mathbf{u} - \mathbf{v})} = \sqrt{\sum_{i=1}^{n} (u_i - v_i)^2}.$$

6 Angles between vectors

For any pair of vectors $\mathbf{u}, \mathbf{v}$ in $\mathbf{R}^2$ or $\mathbf{R}^3$ in angle ϑ, there is an important relationship given by their norms and the inner product:

$$\mathbf{u} \cdot \mathbf{v} = \|\mathbf{u}\| \|\mathbf{v}\| \cos(\vartheta)$$
$$\Updownarrow$$
$$\cos(\vartheta) = \frac{\mathbf{u} \cdot \mathbf{v}}{\|\mathbf{u}\| \|\mathbf{v}\|}.$$



The angle ϑ between two vectors $\mathbf{u}$ and $\mathbf{v}$.

The cosine-formula can be extended to a general definition of the angle between two vectors $\mathbf{u}, \mathbf{v}$ in $\mathbf{R}^n$:

7 The Cauchy-Schwartz (CS) inequality (chapter 3.4 in VMLS)

Theorem (Cauchy-Schwartz inequality)

If $\mathbf{u}, \mathbf{v} \in \mathbf{R}^n$, then

$$|\mathbf{u} \cdot \mathbf{v}| \leq \|\mathbf{u}\|\|\mathbf{v}\|,$$

and equality only applies when either $\mathbf{u}$ or $\mathbf{v}$ is equal to $\mathbf{0}$, or when $\mathbf{u} = k\mathbf{v}$ for $k \in \mathbf{R}$.

Proof:

If $\mathbf{u}$ or $\mathbf{v}$ is equal to $\mathbf{0}$ equality in the above formula holds by inspection. Therefore we assume that $\mathbf{u}, \mathbf{v} \neq \mathbf{0}$. Let $\mathbf{p} = \mathbf{v}(\mathbf{v}^t\mathbf{v})^{-1}\mathbf{v}^t\mathbf{u} = (\frac{\mathbf{v}\cdot\mathbf{u}}{\mathbf{v}\cdot\mathbf{v}})\mathbf{v}$ be the orthogonal projection of $\mathbf{u}$ onto $\mathbf{v}$. Because $\mathbf{p}$ is orthogonal to the residual vector $(\mathbf{u} - \mathbf{p})$, Pythagoras theorem implies

$$\|\mathbf{p}\|^2 + \|\mathbf{u} - \mathbf{p}\|^2 = \|\mathbf{u}\|^2 \Rightarrow \|\mathbf{p}\|^2 \leq \|\mathbf{u}\|^2.$$

Because $\mathbf{p} = (\frac{\mathbf{v}\cdot\mathbf{u}}{\mathbf{v}\cdot\mathbf{v}})\mathbf{v} = \frac{(\mathbf{v}\cdot\mathbf{u})}{\|\mathbf{v}\|^2}\mathbf{v}$,

$$\|\mathbf{p}\|^2 = \mathbf{p} \cdot \mathbf{p} = \frac{(\mathbf{v} \cdot \mathbf{u})^2}{\|\mathbf{v}\|^4}\|\mathbf{v}\|^2 = \frac{(\mathbf{v} \cdot \mathbf{u})^2}{\|\mathbf{v}\|^2} \leq \|\mathbf{u}\|^2$$

$$\Downarrow$$

$$(\mathbf{v} \cdot \mathbf{u})^2 \leq \|\mathbf{u}\|^2\|\mathbf{v}\|^2,$$

and the CS inequality follows by taking the square root of both sides of this inequality ■

An alternative proof of CS is given on page 57 in VMLS.

8 Definition: Angle between vectors in $\mathbf{R}^n$

We define the cosine of the angle θ between two vectors $\mathbf{u}, \mathbf{v} \in \mathbf{R}^n$ by the formula

$$\cos(\theta) = \frac{\mathbf{u} \cdot \mathbf{v}}{\|\mathbf{u}\|\|\mathbf{v}\|}.$$

This definition is sound because of the CS-inequality:

$$|\mathbf{u} \cdot \mathbf{v}| \leq \|\mathbf{u}\|\|\mathbf{v}\| \Leftrightarrow \frac{|\mathbf{u} \cdot \mathbf{v}|}{\|\mathbf{u}\|\|\mathbf{v}\|} \leq 1 \Leftrightarrow -1 \leq \frac{\mathbf{u} \cdot \mathbf{v}}{\|\mathbf{u}\|\|\mathbf{v}\|} \leq 1 \Rightarrow -1 \leq \cos(\theta) \leq 1.$$

Finally we define the angle θ between $\mathbf{u}$ and $\mathbf{v}$ as

$$\theta = \arccos\left(\frac{\mathbf{u} \cdot \mathbf{v}}{\|\mathbf{u}\|\|\mathbf{v}\|}\right)$$

where arccos denotes the inverse cosine, normalized to lie in the interval $[0, \pi]$.

9 The triangle inequality

Theorem (the triangle inequality)

For all $\mathbf{u}, \mathbf{v} \in \mathbf{R}^n$ the following inequality holds:

$$\|\mathbf{u}+\mathbf{v}\| \leq \|\mathbf{u}\| + \|\mathbf{v}\|$$

Proof:

$$\begin{aligned}
\|\mathbf{u}+\mathbf{v}\|^2 = (\mathbf{u}+\mathbf{v})\cdot(\mathbf{u}+\mathbf{v}) &= \mathbf{u}\cdot\mathbf{u} + 2\mathbf{u}\cdot\mathbf{v} + \mathbf{v}\cdot\mathbf{v} \\
&\leq \|\mathbf{u}\|^2 + 2|\mathbf{v}\cdot\mathbf{u}| + \|\mathbf{v}\|^2 \\
&\text{(use CS here)} \\
&\leq \|\mathbf{u}\|^2 + 2\|\mathbf{u}\|\|\mathbf{v}\| + \|\mathbf{v}\|^2 \\
&= (\|\mathbf{u}\| + \|\mathbf{v}\|)^2.
\end{aligned}$$

The 2nd inequality holds due to the Cauchy-Schwartz inequality. The result follows by taking the square root of both sides of this inequality■

10 k-means clustering material

- The VMLS lecture slides on clustering (page 73) and Chapter 4 on clustering in VMLS.
- A visualization tool for k-Means Clustering.
- VMLS-slides on image compression by k-means clustering.

11 The computational basics of k-means clustering

Cluster analysis by the k-means clustering is a popular method for grouping high-dimensional unlabelled data.

In the following 5 videos from the Coursera-course on Machine learning, Stanford-professor Andrew Ng explains the key aspects of k-means clustering:

- Clustering - Unsupervised Learning - the basic ideas (3min18sec)
- Clustering - the k-means algorithm - how the algorithm works (12min33sec)
- Clustering - the optimization objective - for measuring and comparing the goodness of solution candidates (7min05sec)
- Clustering - random initialization - heuristics on how to initialize (start) the clustering process (7min50sec)
- Clustering - choosing the number of clusters - heuristics on choosing the number of clusters (8min23sec)

Understanding the principle of k-Means Clustering idea becomes easy when playing with an interactive tool for Visualizing the k-means clustering process.

12 Examples with simulated data (Julia code)

In Julia we can do the k-means clustering either by using the VMLS-libray function *kmeans*, or by implementing our own version of the k-means algorithm, see *mykmeans* below.

12.1 Lets start by generating a random "artificial" dataset X containing 3 point-clouds in 2 dimensions:

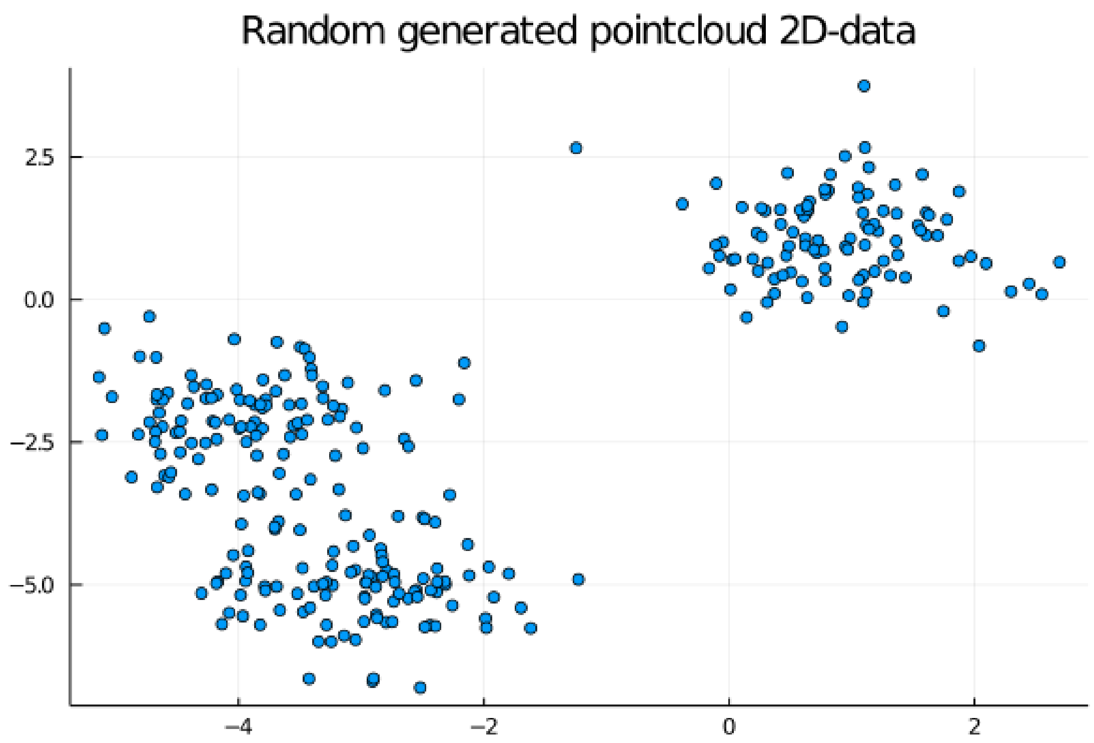
[1]:
```julia
using Random
Random.seed!(1234) # This line assures the same random dataset to be generated␣
↪each time.

nn = 100;     # Generate 3 random "clouds" of datapoints (samples), each of␣
↪size nn.
X = [randn((nn,2))*0.7 .+ [ 1  1];
    randn((nn,2))*0.7  .+ [-3 -5];
    randn((nn,2))*0.7  .+ [-4 -2]];
# Each row of X corresponds to a datapoint
```

12.1.1 A scatterplot shows the generated dataset:

[2]:
```julia
using Plots #b Precompiles on every startup (~20 secondss)
gr() # Needs modules Plots and GR to be installed, may need a rebuild of GR␣
↪with ']build GR'
default(size=(600, 400), fmt = :png) # Default plot size, change output format␣
↪to png
```

[3]:
```julia
# Define and display a plot of the raw random data
sp = scatter(X[:,1],X[:,2], title = "Random generated pointcloud 2D-data",␣
↪legend = false)
display(sp)
```

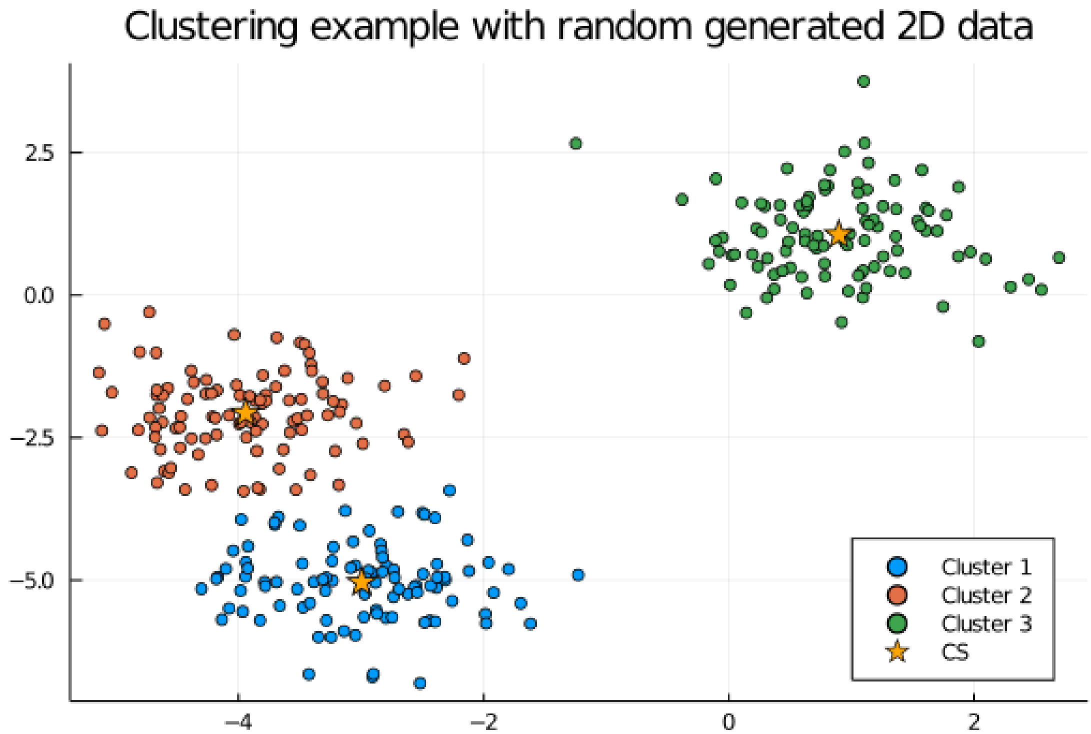


12.1.2 Apply the k-means clustering algorithm (mykmeans.jl) to seach for clusters in the generated dataset X

[4]:
```
include("mykmeans.jl")
k = 3;     # The suggested number of clusters (you should also repeatedly try k␣
↪= 2, 4 and 5)
Cid, CS, J = mykmeans(X, k);
```

12.1.3 We plot the solution with coloring of each identified cluster

[6]:
```
# Define and display a plot of the clustered data and the cluster centers(CS):
p = plot(title = "Clustering example with random generated 2D data",
    label = " ", legend = :bottomright, size = (600, 400))
for i=1:k
    snr = vec(Cid.==i) # the sample numbers of the j-th cluster
    scatter!(p, X[snr,1], X[snr,2], label = string("Cluster ",i))
end
scatter!(p, CS[:,1],CS[:,2], marker = :star, markersize = 8, color = :orange,␣
↪label = "CS")
display(p)
```



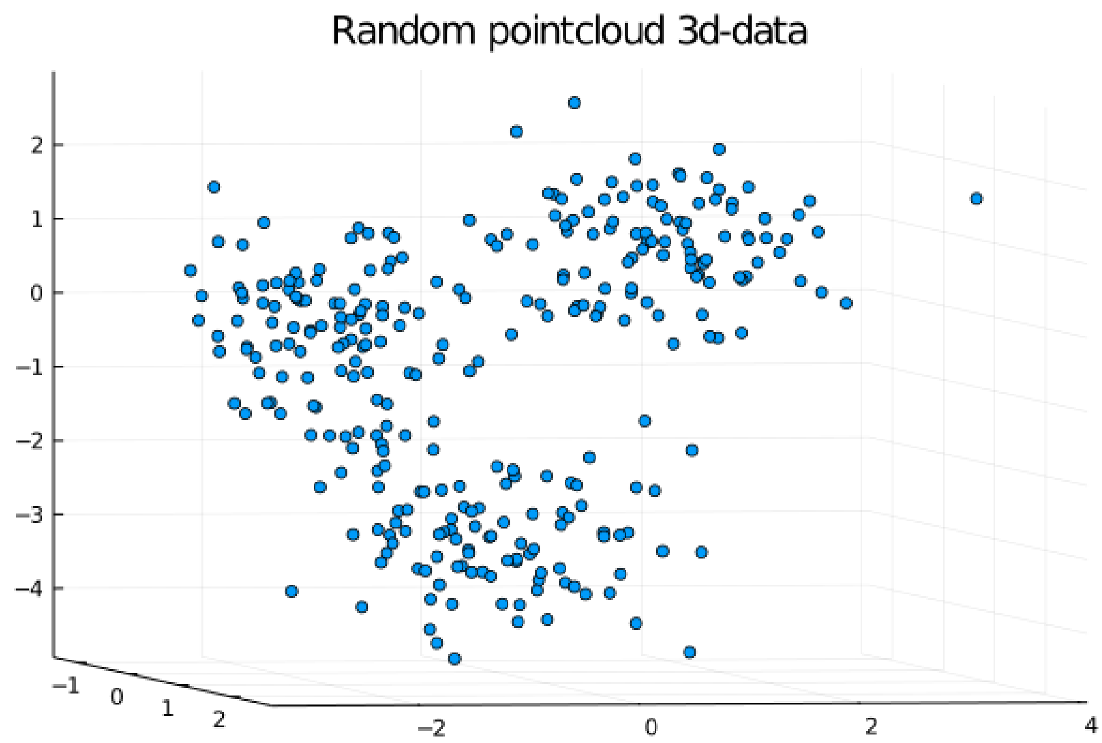
12.1.4 Plotting the objective function values for the iteratrive clustering process

[7]:
```
# Define and display a plot of the objective function values reflecting the␣
↪clustering process
Jp =plot(J, linestyle = :dashdot, title = "Objective function (J) values -␣
↪monitoring the clustering process",
    ylabel = "J (the mean squared distace)", xlabel = "Interations", label =␣
↪"J")
display(Jp)
```

12.2 A random "artificial" dataset X containing 3 point-clouds in 3 dimensions:

[8]:
```
## Visualization for 3D data
# Here is a corresponding 3-dimensional dataset:
Random.seed!(1234) # This line assures the same random dataset to be generated␣
↪each time.
nn = 100;
X = [randn(nn,3)*0.7  .+ [1  1  1];
     randn(nn,3)*0.7  .+ [1 -2 -0];
     randn(nn,3)*0.7  .+ [0  0 -3]];
```

[9]:
```
# Define and display a plot of the raw random data
sp = scatter(X[:,1],X[:,2],X[:,3], title = "Random pointcloud 3d-data", legend␣
↪= false, camera = (75,10))
display(sp)
```

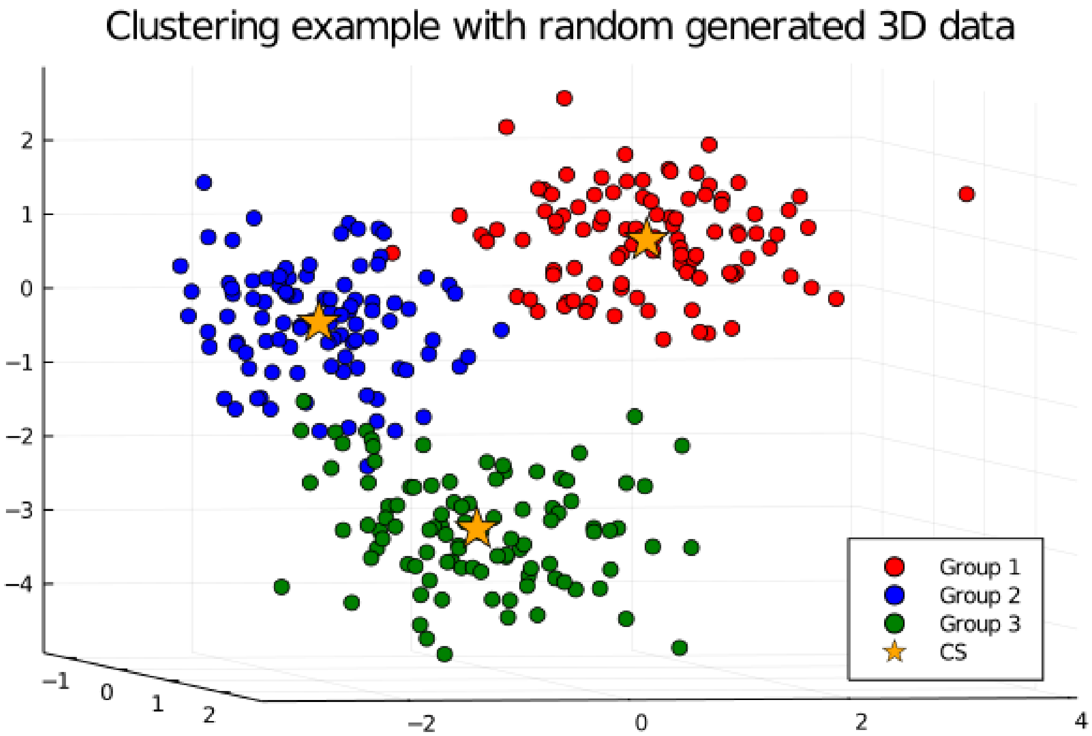


12.2.1 We use our k-means algorithm to cluster the 3d-data.

[10]:
```
k = 3;     # The suggested number of clusters (you should also repeatedly try k␣
↪= 3, 4 and 5)
Cid, CS, J = mykmeans(X, k);
```

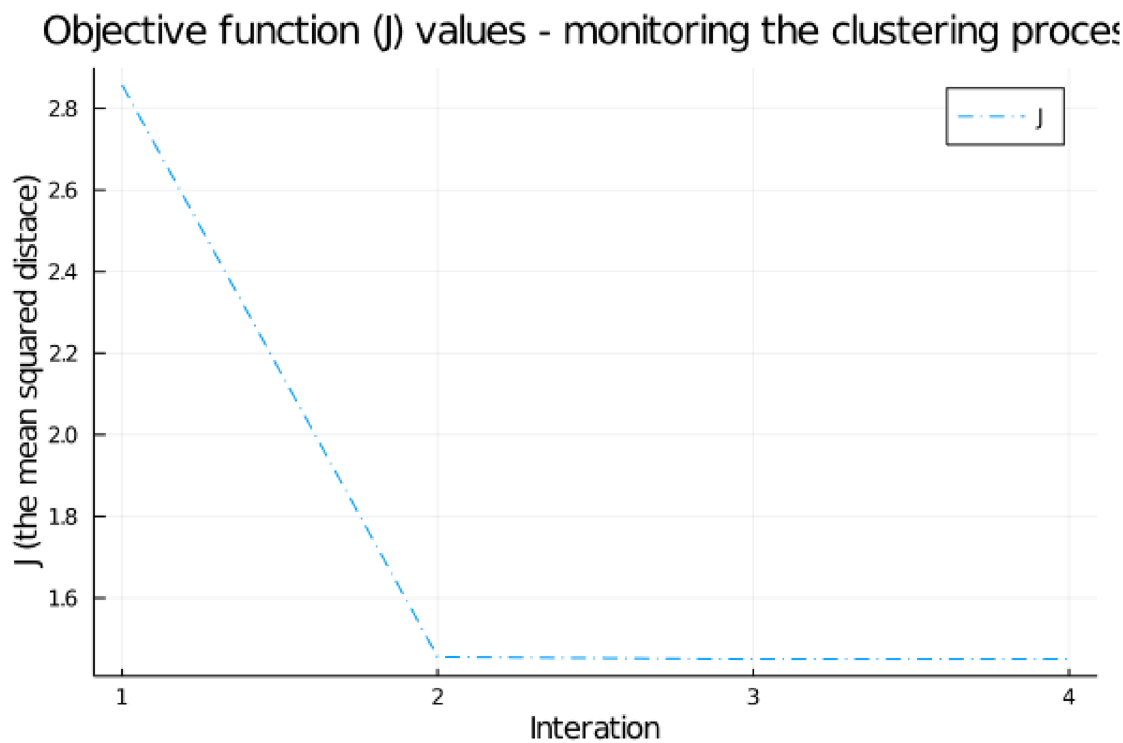
[11]:
```
##
# Plotting the clustered data and the cluster-centers:
colors = [:red, :blue, :green, :cyan, :magenta, :black];

# Define and display a plot of the clustered data and the cluster centers(CS):
p = plot(legend = :bottomright, title = "Clustering example with random␣
↪generated 3D data", size = (600,400))
for j = 1:k
    snr = vec(Cid.==j); # the sample numbers of the j-th cluster
    # Plot only this group:
    scatter!(p, X[snr,1],X[snr,2],X[snr,3],color = colors[j], markersize = 5,␣
↪label = string("Group ", j))
end
scatter!(p, CS[:,1],CS[:,2], CS[:,3], marker = :star, markersize = 12, color = :
↪orange, label = "CS", camera = (75,10)) # Plotting the cluster centers
display(p)
```



12.2.2 Plotting the objective function values for the iteratrive clustering process

[12]:
```
# Define and display a plot of the objective function values reflecting the␣
↪clustering process
Jp = plot(J, linestyle = :dashdot, title = "Objective function (J) values -␣
↪monitoring the clustering process",
    ylabel = "J (the mean squared distace)", xlabel="Interation", label="J")
display(Jp)
```



13 Exercises

- Make an extension of the **mykmeans** algorithm by considering ($r \geq 2$) repeated random initializations of the cluster centers. The new algorithm should return the cluster centers of the best among the R solutions in terms of J-value.

An alternative measure of similarity between vectors is obtained by considering angles rather than distances.

- Figure out, and implement a modification of mykmeans that measure similarity by the angle between vectors.

14 Other clustering techniques:

See Wikipedia-review on Cluster analysis.