Final Project, K-Means Clustering

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Clustering

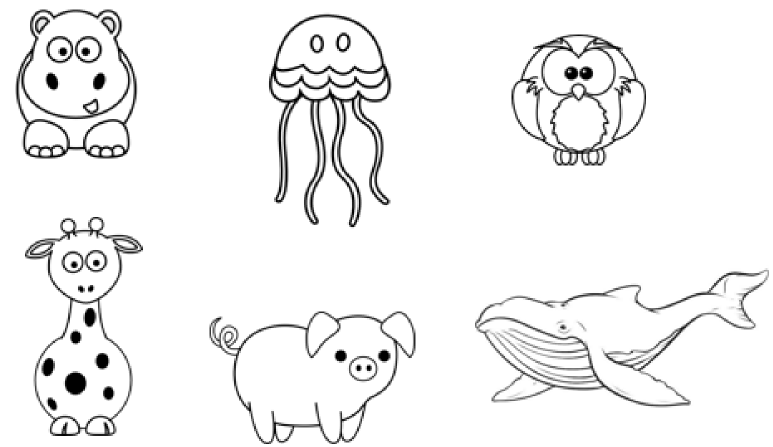
- Clustering is a machine learning task that **groups similar objects together**.
- Given a dataset with n observations, $D := \{\boldsymbol{x}_i\}_{i=1}^n$, we would like to divide D into K disjoint subsets:

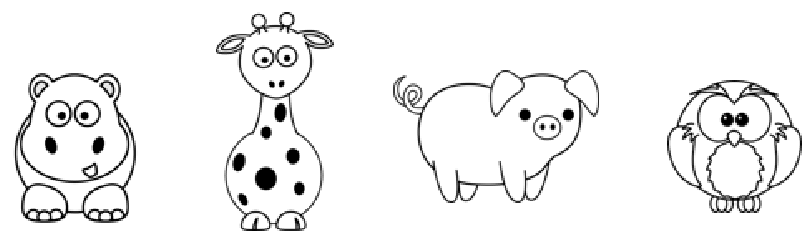
$$D = \cup_{i \in \{1...K\}} D_i \text{ and } \cap_{i \in \{1...K\}} D_i = \emptyset,$$

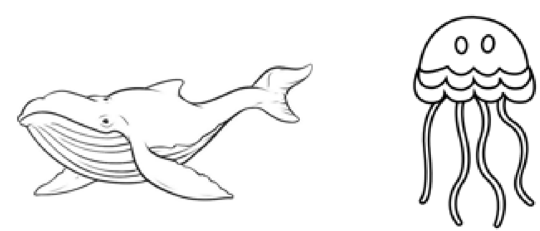
- Such that observations in each subset D_i **are similar** to each other.

Clustering Example

- Clustering of animals: Land vs. Sea.

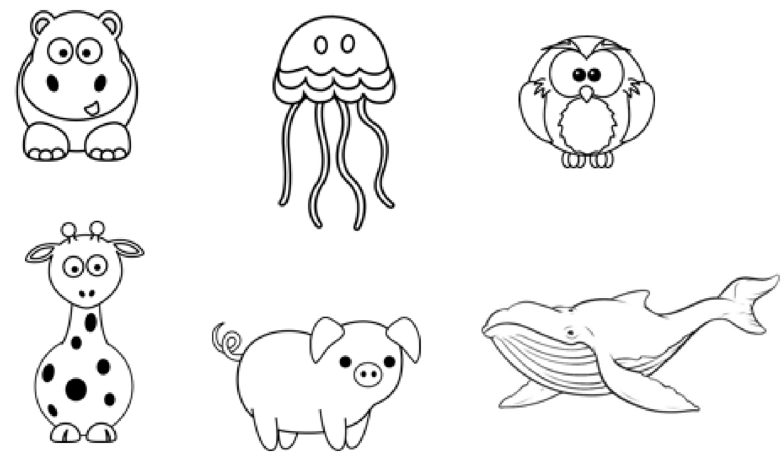
$D := \{$  $\}$

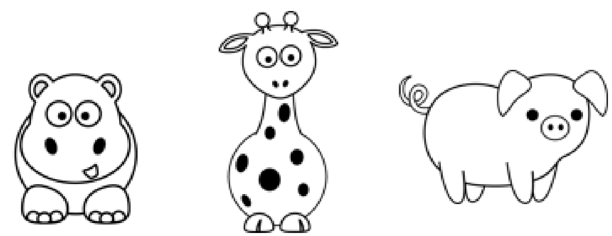
$D_1 = \{$  $\}$

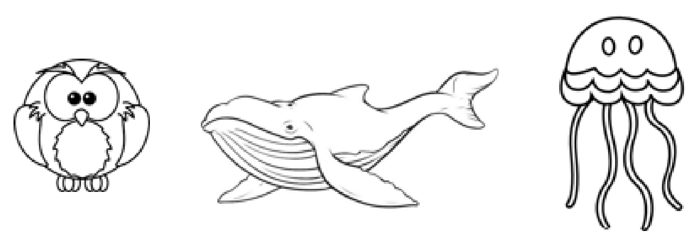
$D_2 = \{$  $\}$

Clustering Example, 2

- Clustering of animals: Mammals vs. Non-mammals.

$D := \{$  $\}$

$D_1 = \{$  $\}$

$D_2 = \{$  $\}$

Clustering Example

- The subsets found by clustering is **not** unique.
    - depending on **how the similarity is defined**, you can get different clustering results.
    - For example, I can also divide the animals in the previous case into mammals and non-mammals.
- You may want to define different types of similarities in different clustering applications.
    - For example, if you would like to group handwritten digits, you may want to consider hand writing features (directions of strokes, etc) when defining similarities between two handwritten digits.

Similarities

- In mathematics, similarities between objects are usually defined by a metric or distance function.
- One classic choice of distance is Euclidean distances.
- If two objects can be expressed as two points $\boldsymbol{a}$ and $\boldsymbol{b}$ in a d-dimensional Euclidean space, the Euclidean distance is

$$\operatorname{dist}(\boldsymbol{a}, \boldsymbol{b}) := \sqrt{\sum_{i \in \{1 \ldots d\}} (a_i - b_i)^2}$$

Similarities

Ronald Fisher created Iris dataset, where he measured the length, width of the sepals and petals 150 iris flowers.

- In this dataset, each flower is a 4-dimensional vector.

```
> iris # load iris dataset in R by typing "iris".
    Sepal.Length Sepal.Width Petal.Length Petal.Width
1            5.1         3.5          1.4         0.2
2            4.9         3.0          1.4         0.2
3            4.7         x3.2          1.3         0.2
...
```

- You can then measure the similarity between flowers by Euclidean distance.
  - The Euclidean distance between the first two observations is:

$$\sqrt{(5.1-4.9)^2+(3.5-3.0)^2+(1.4-1.4)^2+(0.2-0.2)^2}$$

K-Means Clustering Algorithm

Given a dataset and a distance function, how to do clustering?

- K-means is a simple and popular choice.
- It measures the similarity between each observation and "centers" of each subset, thens assign observations to different subsets.
- After the assignments are made, it updates the centers to be the average of observations in all subsets.
- It repeatedly carries out the previous two steps until convergance.

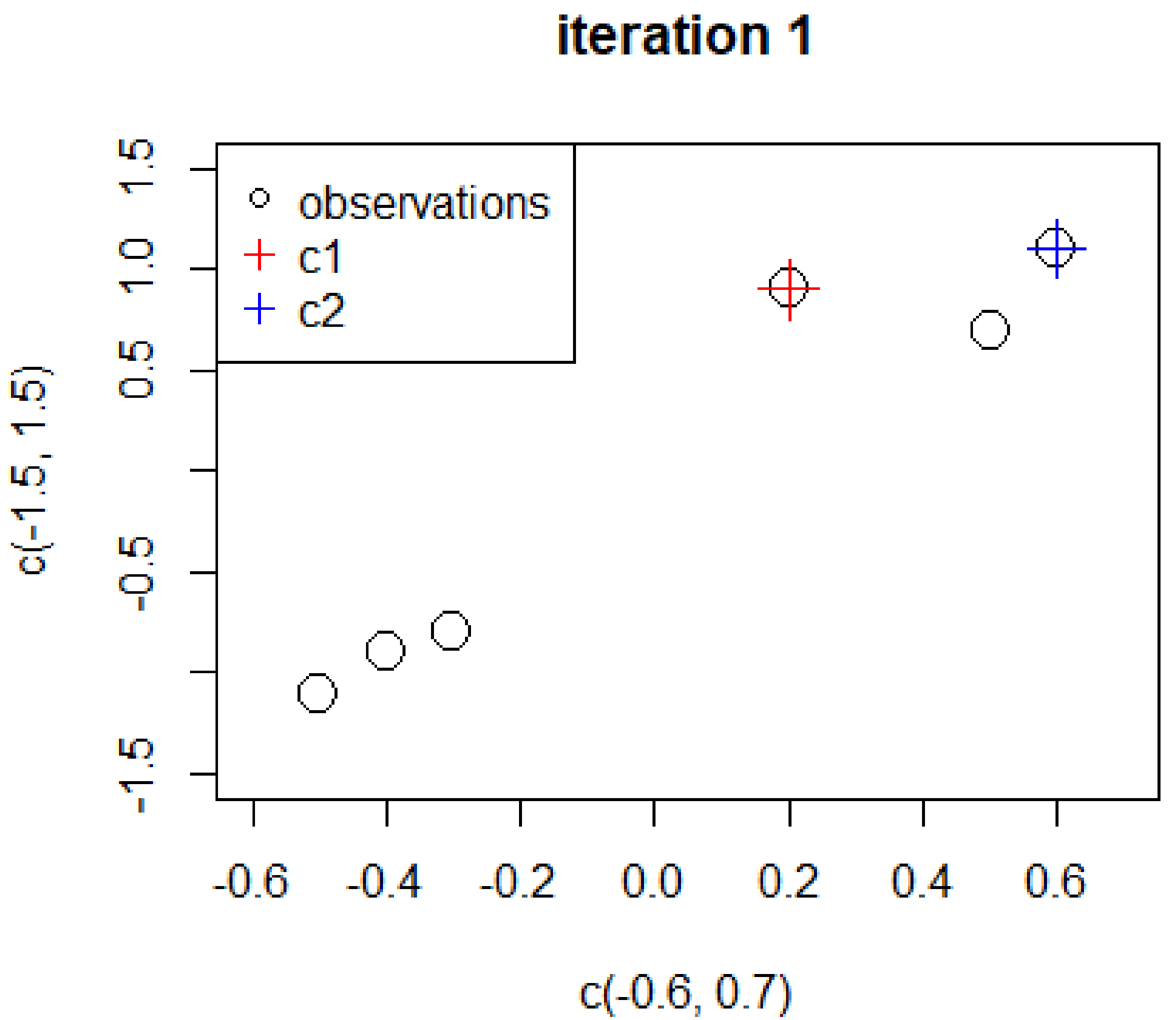
K-Means Clustering Algorithm

Suppose your dataset D contains n observations in d-dimensional space. Then K-Means divides D into $D_1, \ldots, D_K$ subsets using the following algorithm.

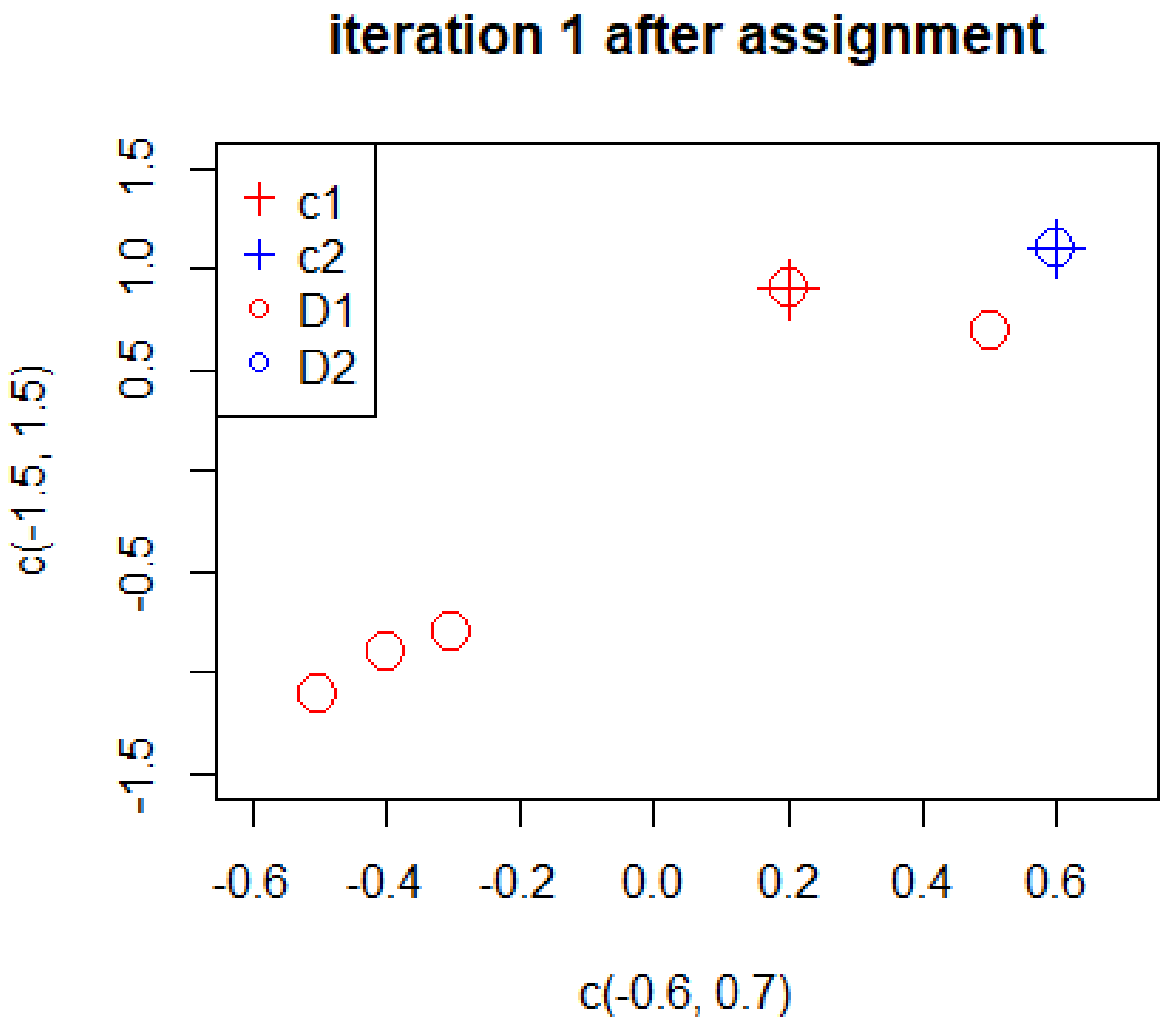
K-Means Clustering Algorithm

1. Randomly pick K observations from your dataset, as K **centers**: $\boldsymbol{c}_1, \ldots, \boldsymbol{c}_K$
2. For each observation $\boldsymbol{x}_i \in D$,
   i. For each $k \in \{1 \ldots K\}$, compute the distance $d_{i,k} = \text{dist}(\boldsymbol{x}_i, \boldsymbol{c}_k)$
   ii. Assign $\boldsymbol{x}_i$ to the subset $D_{k=k'}$, where $k' = \arg\min_k d_{i,k}$
3. Compute the new centers: $\boldsymbol{c}_1, \ldots, \boldsymbol{c}_K$, where $\boldsymbol{c}_k := \frac{1}{|D_k|} \sum_{\boldsymbol{x}_j \in D_k} \boldsymbol{x}_j$, i.e., the average of all observations in subset D_k.
4. Repeat 2 and 3 until the assignment does not change any more.

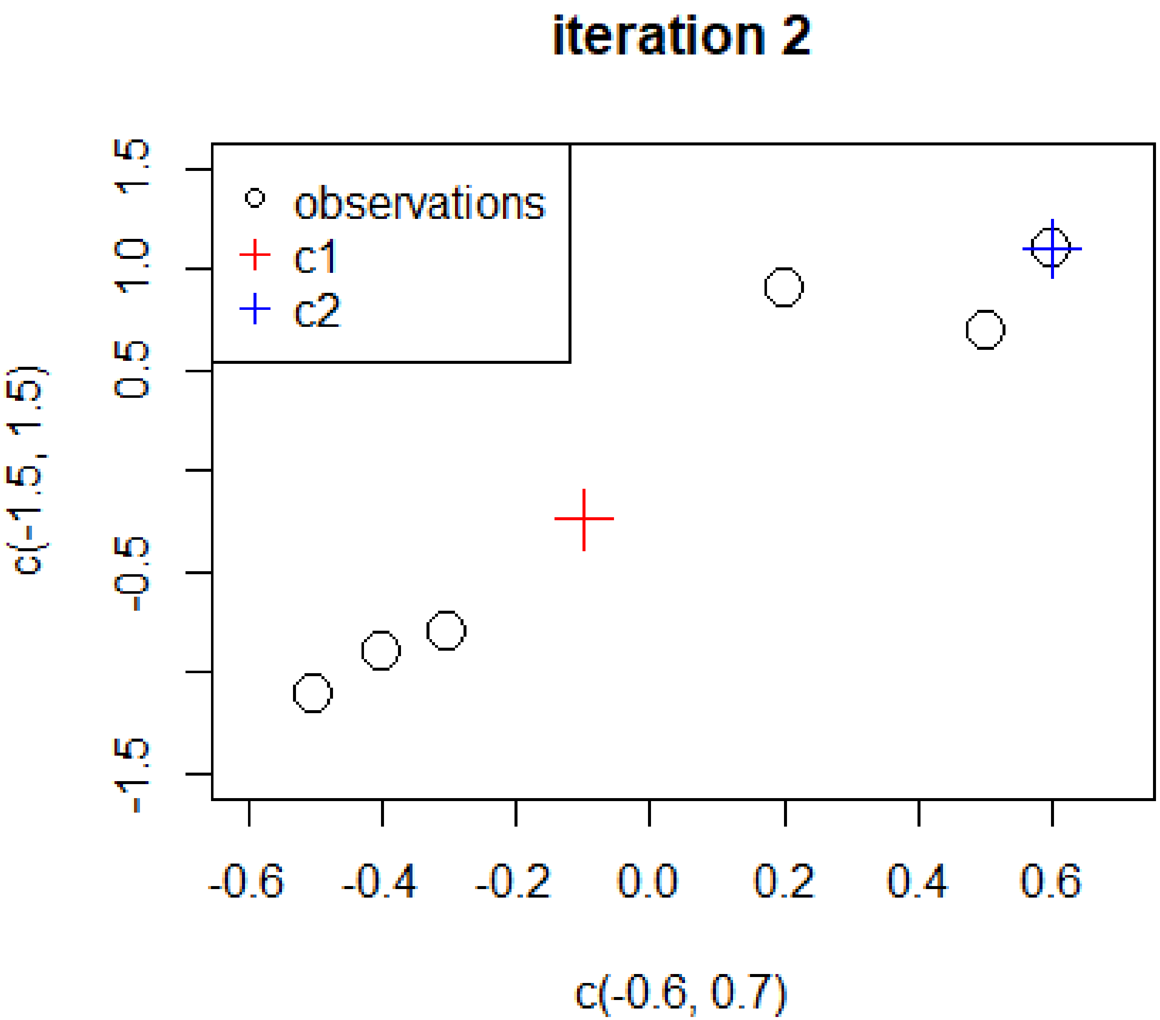
K-Means Clustering Algorithm: Demo



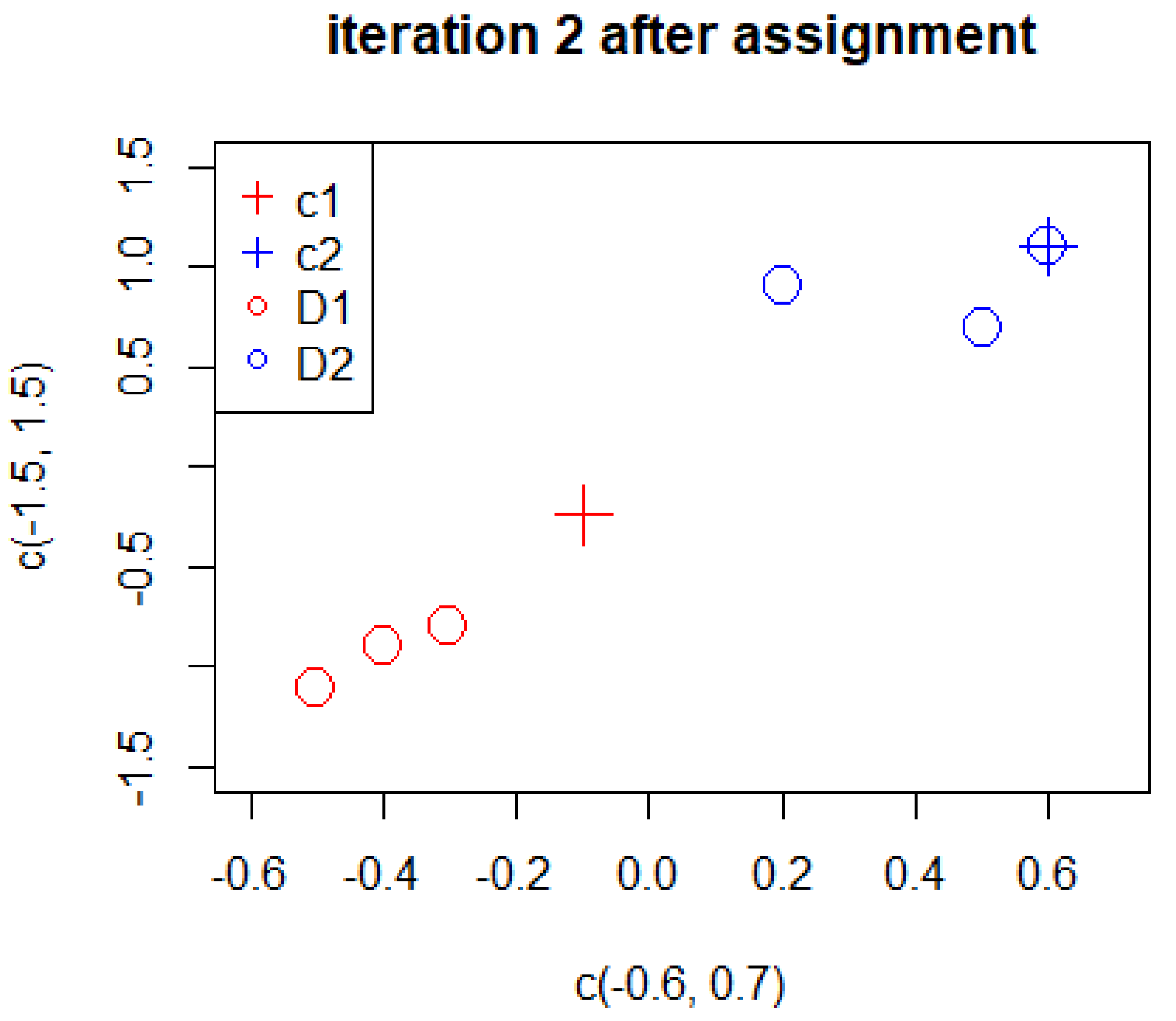
K-Means Clustering Algorithm: Demo



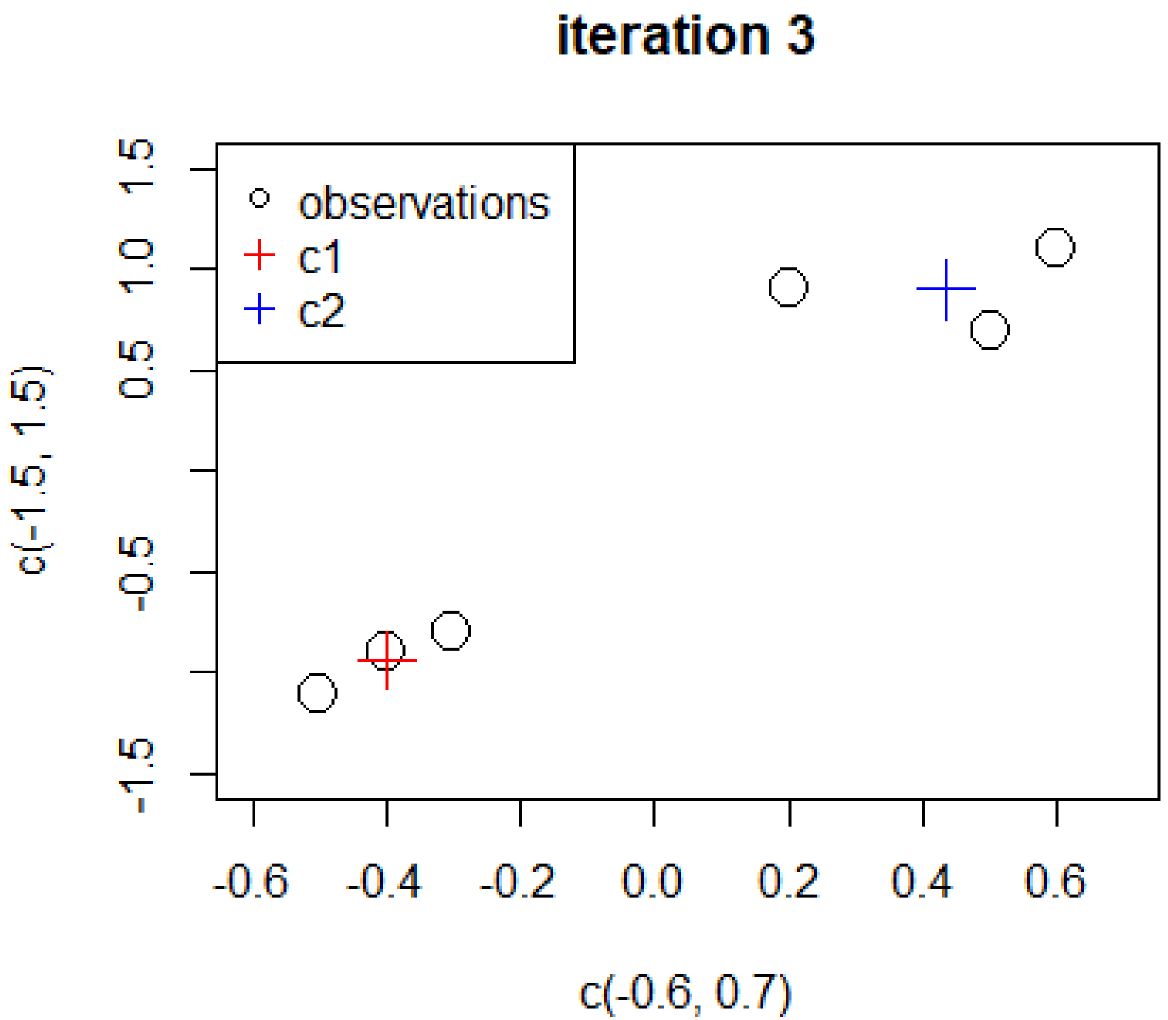
K-Means Clustering Algorithm: Demo



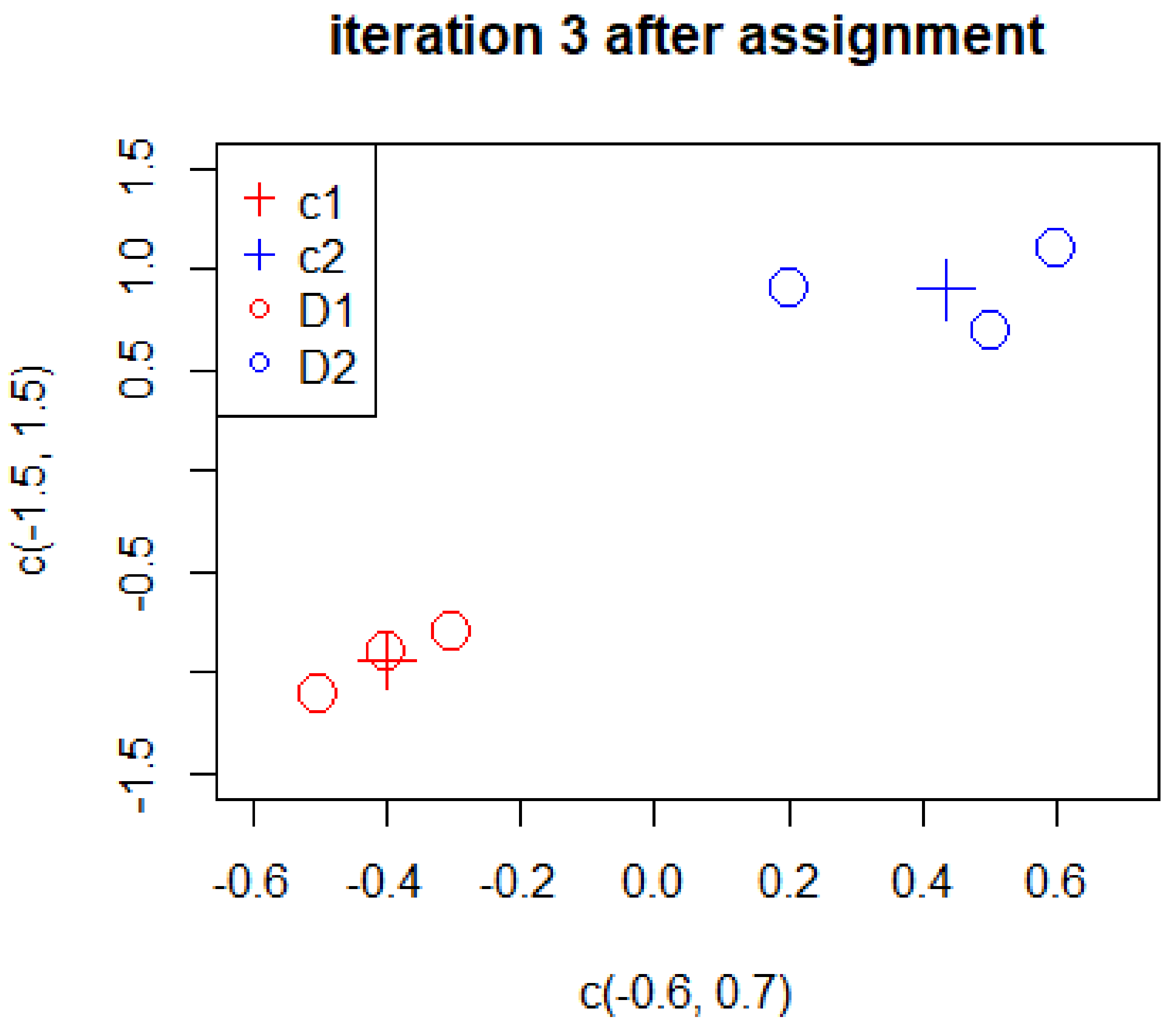
K-Means Clustering Algorithm: Demo



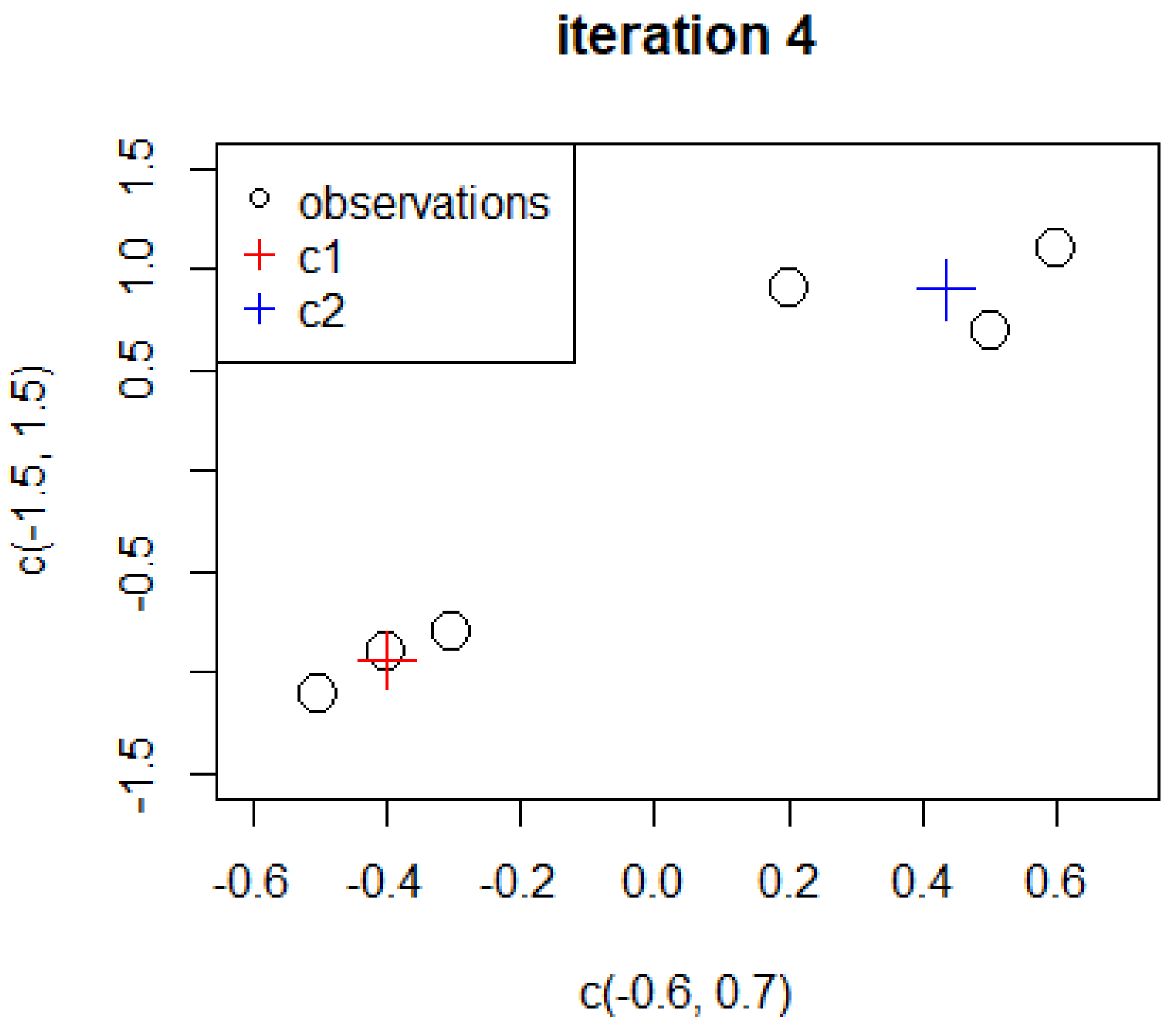
K-Means Clustering Algorithm: Demo



K-Means Clustering Algorithm: Demo



K-Means Clustering Algorithm: Demo



K-Means Clustering Algorithm: Demo

The new centers do not lead to a different assignment comparing to iteration 3.

Stop.

Coursework: Part I (15 points)

The first part of this coursework is generating a toy dataset for our K means algorithm. Let us assume $K = 2$ for now.

Coursework: Part I (15 points)

0. Set the random seed to 1.
1. Generate a dataset D, containing 100 random observations from two **2-dimensional** normal distribution with **different means**.
   - D can be either a matrix or data frame.
   - You should sample 50 observations from one normal distribution and 50 from the other normal distribution.
2. Create $C = \{\boldsymbol{c}_1, \boldsymbol{c}_2\}$ by randomly picking **2 centers** from your dataset.
   - The choice of centers needs to be random.
   - You are not allowed to specify centers yourself.

Coursework: Part I (15 points)

3. Visualize D using `points` function.
    - It is up to you how to visualize your dataset.

Coursework: Part II (30 points)

- Now, let us write the K-means algorithm and test it on the toy dataset.
- Below is a list of suggested steps of writing your code. However, you can write your code differently.

Coursework: Part II (30 points)

1. Write a function `dist` that computes the distance $d_{i,k}$.
2. Write a function `assign` that assigns $\boldsymbol{x}_i$ to $D_{k=k'}$.
3. Find a way to apply `assign` to all observations in D. Obtain an 100-dimensional vector `k_prime` whose i-th component is the assignment k' for the i-th observation.
4. Write a function `update_centers` that updates centers in C with the new assignments stored in `k_prime`.
5. Write a function `visualize` that visualizes $\boldsymbol{c}_1, \boldsymbol{c}_2$ and D_1, D_2.

Coursework: Part II (30 points)

6. Write a loop that calls `assign`, `update_centers` and `visualize` repeatedly until the elements in `k_prime` do not change any more.

Coursework: Part III (15 points)

Now, let us apply K means algorithm to a real-world dataset `iris`.

- Load iris dataset by typing `iris` and inspect the dataset.
- There are 5 variables in this dataset:
  - Sepal.Length
  - Sepal.Width
  - Petal.Length
  - Petal.Width
  - Species
- The first four variables are the properties of flowers. The fifth variable indicates the types of flowers.

Coursework: Part III (15 points)

0. Create a new R file.
1. Create **a list of 6 new datasets** from the iris dataset, by picking any pairs of variables from the first four variables.
2. Find a way to apply the K means algorithm you previously wrote to the entire list of iris datasets and perform clustering analysis.
3. Visualize the assignments obtained from the K-means algorithm, and save your plots (6 in total) as 6 png files.

Coursework: Part III (15 points)

The following code saves a plot to the `points.png` file.

```
#create file
png("./points.png", width = 500, height = 500)
#create the plot
plot(c(-5,5),c(-5,5),type = "n")
points(rnorm(10), rnorm(10), cex = 2)
#close the file
dev.off()
```

Coursework: Part IV (20 points)

Part IV contains two slightly more difficult challenges. **For each challenge, you need to create a new file**.

Challenge 1:

1. You can use different distance functions in K means algorithm. Consider the following distance functions:
   - Taxi Cab distance: $\operatorname{dist}(\boldsymbol{a}, \boldsymbol{b}) := \sum_k |a_k - b_k|$.
   - Cosine distance: $\operatorname{dist}(\boldsymbol{a}, \boldsymbol{b}) := 1 - \frac{\langle \boldsymbol{a}, \boldsymbol{b} \rangle}{\|\boldsymbol{a}\| \|\boldsymbol{b}\|}$.
   - Chebyshev distance: $\operatorname{dist}(\boldsymbol{a}, \boldsymbol{b}) := \max_k |a_k - b_k|$.

Coursework: Part IV (20 points)

2. Load this dataset to your R environment and visualize it.
3. Which distance do you think works the best for this dataset (choose from Taxi cab, Cosine, and Chebyshev)?
4. Modify your K means code and replace the Euclidean distance with your choice. Test the new K means algorithm on this dataset and visualize the result.

Coursework: Part IV (20 points)

Challenge 2:

- In the previous examples, we tested K means algorithm for $K = 2$.
- Modify your K means algorithm, such that it can divide your dataset D into arbitary $K \geq 2$ subsets. Generate a toy dataset and test your modification.
    - K is provided to your algorithm as an input parameter.

Marking Criteria

- Part I: 15 points
- Part II: 30 points
- Part III: 15 points
- Part IV: 20 points
- Coding Style: 20 points.
  - Vectorization, Functional Programming, OOP.
  - Comments
  - Variable naming, Code formatting, etc.

DOs and DONTs

- You are encouraged to discuss this coursework with other students.
- All coursework questions should be addressed to the lecturer or TA during lab sessions or using the blackboard forum.
- You are only allowed to use the base R and `Rcpp`.
- You are not allowed to use external machine learning libraries without the permission from the lecturer.
- You are not allowed to copy other people's work.
    - You are not allowed to pass your work to other students.

Submission

- Deadline: 9th May.
- Submit a zip file containing all your R scripts (and C++ files if you use Rcpp).
    - You do not need to submit any data file.