K Means Clustering

> library(swirl)

| Hi! Type swirl() when you are ready to begin.

> swirl()

| Welcome to swirl! Please sign in. If you've been here before, use the same name as you did then. If you are new,

| call yourself something unique.

What shall I call you? Stephen

| Please choose a course, or type 0 to exit swirl.

1: Data Analysis

2: Exploratory Data Analysis

3: Getting and Cleaning Data

4: Mathematical Biostatistics Boot Camp

5: Open Intro

6: R Programming

7: Regression Models

8: Statistical Inference

9: Take me to the swirl course repository!

Selection: 2

| Please choose a lesson, or type 0 to return to course menu.

1: Principles of Analytic Graphs 2: Exploratory Graphs 3: Graphics Devices in R

4: Plotting Systems 5: Base Plotting System 6: Lattice Plotting System

7: Working with Colors 8: GGPlot2 Part1 9: GGPlot2 Part2

10: GGPlot2 Extras 11: Hierarchical Clustering 12: K Means Clustering

13: Dimension Reduction 14: Clustering Example 15: CaseStudy

Selection: 12

| Attempting to load lesson dependencies...

| Package ‘ggplot2’ loaded correctly!

| Package ‘fields’ loaded correctly!

| Package ‘jpeg’ loaded correctly!

| Package ‘datasets’ loaded correctly!

| | 0%

| K_Means_Clustering. (Slides for this and other Data Science courses may be found at github

| https://github.com/DataScienceSpecialization/courses/. If you care to use them, they must be downloaded as a zip

| file and viewed locally. This lesson corresponds to 04_ExploratoryAnalysis/kmeansClustering.)

...

|== | 2%

| In this lesson we'll learn about k-means clustering, another simple way of examining and organizing

| multi-dimensional data. As with hierarchical clustering, this technique is most useful in the early stages of

| analysis when you're trying to get an understanding of the data, e.g., finding some pattern or relationship

| between different factors or variables.

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|==== | 4%

| R documentation tells us that the k-means method "aims to partition the points into k groups such that the sum of

| squares from points to the assigned cluster centres is minimized."

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|====== | 6%

| Since clustering organizes data points that are close into groups we'll assume we've decided on a measure of

| distance, e.g., Euclidean.

...

|========= | 8%

| To illustrate the method, we'll use these random points we generated, familiar to you if you've already gone

| through the hierarchical clustering lesson. We'll demonstrate k-means clustering in several steps, but first we'll

| explain the general idea.

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  |=========== | 10%

| As we said, k-means is a partioning approach which requires that you first guess how many clusters you have (or

| want). Once you fix this number, you randomly create a "centroid" (a phantom point) for each cluster and assign

| each point or observation in your dataset to the centroid to which it is closest. Once each point is assigned a

| centroid, you readjust the centroid's position by making it the average of the points assigned to it.

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  |============= | 12%

| Once you have repositioned the centroids, you must recalculate the distance of the observations to the centroids

| and reassign any, if necessary, to the centroid closest to them. Again, once the reassignments are done, readjust

| the positions of the centroids based on the new cluster membership. The process stops once you reach an iteration

| in which no adjustments are made or when you've reached some predetermined maximum number of iterations.

...

  |============== | 14%

| As described, what does this process require?

1: A number of clusters

2: An initial guess as to cluster centroids

3: All of the others

4: A defined distance metric

Selection: 3

| Great job!

|================= | 16%

| So k-means clustering requires some distance metric (say Euclidean), a hypothesized fixed number of clusters, and

| an initial guess as to cluster centroids. As described, what does this process produce?

1: An assignment of each point to a cluster

2: All of the others

3: A final estimate of cluster centroids

Selection: 2

| All that practice is paying off!

|=================== | 18%

| When it's finished k-means clustering returns a final position of each cluster's centroid as well as the

| assignment of each data point or observation to a cluster.

...

  |====================== | 20%

| Now we'll step through this process using our random points as our data. The coordinates of these are stored in 2

| vectors, x and y. We eyeball the display and guess that there are 3 clusters. We'll pick 3 positions of centroids,

| one for each cluster.

...

  |======================== | 22%

| We've created two 3-long vectors for you, cx and cy. These respectively hold the x- and y- coordinates for 3

| proposed centroids. For convenience, we've also stored them in a 2 by 3 matrix cmat. The x coordinates are in the

| first row and the y coordinates in the second. Look at cmat now.

> cmat

     [,1] [,2] [,3]

[1,]   1 1.8 2.5

[2,]   2 1.0 1.5

| Excellent work!

  |========================= | 24%

| The coordinates of these points are (1,2), (1.8,1) and (2.5,1.5). We'll add these centroids to the plot of our

| points. Do this by calling the R command points with 6 arguments. The first 2 are cx and cy, and the third is col

| set equal to the concatenation of 3 colors, "red", "orange", and "purple". The fourth argument is pch set equal to

| 3 (a plus sign), the fifth is cex set equal to 2 (expansion of character), and the final is lwd (line width) also

| set equal to 2.

> points(cx,cy,col=c("red", "orange", and "purple"), pch=3, cex=2, lwd=2)

Error: unexpected string constant in "points(cx,cy,col=c("red", "orange", and "purple""

> points(cx,cy,col=c("red", "orange", "purple"), pch=3, cex=2, lwd=2)

| You got it!

  |============================ | 26%

| We see the first centroid (1,2) is in red. The second (1.8,1), to the right and below the first, is orange, and

| the final centroid (2.5,1.5), the furthest to the right, is purple.

...

  |============================== | 28%

| Now we have to calculate distances between each point and every centroid. There are 12 data points and 3

| centroids. How many distances do we have to calculate?

1: 36

2: 15

3: 9

4: 108

Selection: 1

| You're the best!

|================================ | 30%

| We've written a function for you called mdist which takes 4 arguments. The vectors of data points (x and y) are

| the first two and the two vectors of centroid coordinates (cx and cy) are the last two. Call mdist now with these

| arguments.

> View(mdist)

| Keep trying! Or, type info() for more options.

| Type mdist(x,y,cx,cy) at the command prompt.

> mdist(x,y,cx,cy)

[,1] [,2] [,3] [,4] [,5] [,6] [,7] [,8] [,9] [,10]

[1,] 1.392885 0.9774614 0.7000680 1.264693 1.1894610 1.2458771 0.8113513 1.026750 4.5082665 4.5255617

[2,] 1.108644 0.5544675 0.3768445 1.611202 0.8877373 0.7594611 0.7003994 2.208006 1.1825265 1.0540994

[3,] 3.461873 2.3238956 1.7413021 4.150054 0.3297843 0.2600045 0.4887610 1.337896 0.3737554 0.4614472

[,11] [,12]

[1,] 4.8113368 4.0657750

[2,] 1.2278193 1.0090944

[3,] 0.5095428 0.2567247

| Nice work!

|================================== | 32%

| We've stored these distances in the matrix distTmp for you. Now we have to assign a cluster to each

| point. To do that we'll look at each column and ?

1: pick the maximum entry

2: pick the minimum entry

3: add up the 3 entries.

Selection: 2

| You got it!

|=================================== | 34%

| From the distTmp entries, which cluster would point 6 be assigned to?

1: none of the above

2: 1

3: 2

4: 3

Selection: 4

| Nice work!

  |===================================== | 36%

| R has a handy function which.min which you can apply to ALL the columns of distTmp with one call.
| Simply call the R function apply with 3 arguments. The first is distTmp, the second is 2 meaning
| the columns of distTmp, and the third is which.min, the function you want to apply to the columns
| of distTmp. Try this now.

> apply(distTmp, 2, which.min)
 [1] 2 2 2 1 3 3 3 1 3 3 3 3

| You're the best!

  |====================================== | 38%

| You can see that you were right and the 6th entry is indeed 3 as you answered before. We see the
| first 3 entries were assigned to the second (orange) cluster and only 2 points (4 and 8) were
| assigned to the first (red) cluster.

...

  |======================================= | 40%

| We've stored the vector of cluster colors ("red","orange","purple") in the array cols1 for you and

| we've also stored the cluster assignments in the array newClust. Let's color the 12 data points
| according to their assignments. Again, use the command points with 5 arguments. The first 2 are x
| and y. The third is pch set to 19, the fourth is cex set to 2, and the last, col is set to
| cols1[newClust].

```
> points(x,y,pch=19, cex=2, col=cols1[newClust])
```

| That's correct!

```
  |=========================================                                  |  42%
```

| Now we have to recalculate our centroids so they are the average (center of gravity) of the cluster
| of points assigned to them. We have to do the x and y coordinates separately. We'll do the x
| coordinate first. Recall that the vectors x and y hold the respective coordinates of our 12 data
| points.

...

```
  |=============================================                              |  44%
```

| We can use the R function tapply which applies "a function over a ragged array". This means that
| every element of the array is assigned a factor and the function is applied to subsets of the array
| (identified by the factor vector). This allows us to take advantage of the factor vector newClust
| we calculated. Call tapply now with 3 arguments, x (the data), newClust (the factor array), and
| mean (the function to apply).

```
> tapply(x, newClust, mean)
      1       2       3
1.210767 1.010320 2.498011
```

| That's a job well done!

  |== | 46%

| Repeat the call, except now apply it to the vector y instead of x.

> tapply(y, newClust, mean)

      1   2   3

1.730555 1.016513 1.354373

| Perseverance, that's the answer.

  |== | 48%

| Now that we have new x and new y coordinates for the 3 centroids we can plot them. We've stored off
| the coordinates for you in variables newCx and newCy. Use the R command points with these as the
| first 2 arguments. In addition, use the arguments col set equal to cols1, pch equal to 8, cex equal
| to 2 and lwd also equal to 2.

> points(newCx,newCy,pch=8, cex=2, col=2, lwd=2)

| You almost had it, but not quite. Try again. Or, type info() for more options.

| Type points(newCx,newCy,col=cols1,pch=8,cex=2,lwd=2) at the command prompt.

> points(newCx,newCy,col=cols1,pch=8,cex=2,lwd=2)

| You are quite good my friend!

|== | 50%

| We see how the centroids have moved closer to their respective clusters. This is especially true of
| the second (orange) cluster. Now call the distance function mdist with the 4 arguments x, y, newCx,
| and newCy. This will allow us to reassign the data points to new clusters if necessary.

> mdist(x,y,newCx,newCy)

[,1] [,2] [,3] [,4] [,5] [,6] [,7] [,8] [,9]

[1,] 0.98911875 0.539152725 0.2901879 1.0286979 0.7936966 0.8004956 0.4650664 1.028698 3.3053706

[2,] 0.09287262 0.002053041 0.0734304 0.2313694 1.9333732 1.8320407 1.4310971 2.926095 3.5224442

[3,] 3.28531180 2.197487387 1.6676725 4.0113796 0.4652075 0.3721778 0.6043861 1.643033 0.2586908

[,10] [,11] [,12]

[1,] 3.282778 3.5391512 2.9345445

[2,] 3.295301 3.5990955 3.2097944

[3,] 0.309730 0.3610747 0.1602755

| All that hard work is paying off!

|== |
52%

| We've stored off this new matrix of distances in the matrix distTmp2 for you. Recall that the first
| cluster is red, the second orange and the third purple. Look closely at columns 4 and 7 of
| distTmp2. What will happen to points 4 and 7?

1: They're the only points that won't change clusters

2: They will both change to cluster 2

3: Nothing

4: They will both change clusters

Selection: 4

| Excellent work!

  |=== |
54%

| Now call apply with 3 arguments, distTmp2, 2, and which.min to find the new cluster assignments for
| the points.

> apply(distTmp2, 2, which.min)
 [1] 2 2 2 2 3 3 1 1 3 3 3 3

| You are doing so well!

  |=== |
56%

| We've stored off the new cluster assignments in a vector of factors called newClust2. Use the R
| function points to recolor the points with their new assignments. Again, there are 5 arguments, x
| and y are first, followed by pch set to 19, cex to 2, and col to cols1[newClust2].

> points(x,y,pch=19, cex=2, col=cols1[newClust2])

| Excellent work!

|== |
58%

| Notice that points 4 and 7 both changed clusters, 4 moved from 1 to 2 (red to orange), and point 7
| switched from 3 to 2 (purple to red).

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|===
| 60%

| Now use tapply to find the x coordinate of the new centroid. Recall there are 3 arguments, x,
| newClust2, and mean.

```
> tapply(x, newClust2, mean)
      1       2       3
1.8878628 0.8904553 2.6001704
```

| Keep up the great work!

|===
| 62%

| Do the same to find the new y coordinate.

```
> tapply(y, newClust2, mean)
     1       2       3
2.157866 1.006871 1.274675
```

| Keep up the great work!

  |==
| 64%

| We've stored off these coordinates for you in the variables finalCx and finalCy. Plot these new
| centroids using the points function with 6 arguments. The first 2 are finalCx and finalCy. The
| argument col should equal cols1, pch should equal 9, cex 2 and lwd 2.

> points(finalCx,finalCy,col=cols1,pch=9,cex=2,lwd=2)

| Keep up the great work!

  |==
| 66%

| It should be obvious that if we continued this process points 5 through 8 would all turn red, while
| points 1 through 4 stay orange, and points 9 through 12 purple.

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  |==
| 68%

| Now that you've gone through an example step by step, you'll be relieved to hear that R provides a
| command to do all this work for you. Unsurprisingly it's called kmeans and, although it has several
| parameters, we'll just mention four. These are x, (the numeric matrix of data), centers, iter.max,
| and nstart. The second of these (centers) can be either a number of clusters or a set of initial
| centroids. The third, iter.max, specifies the maximum number of iterations to go through, and
| nstart is the number of random starts you want to try if you specify centers as a number.

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  |==
| 70%

| Call kmeans now with 2 arguments, dataFrame (which holds the x and y coordinates of our 12 points)

| and centers set equal to 3.

> kmeans(dataFrame, centers = 3)

K-means clustering with 3 clusters of sizes 8, 2, 2

Cluster means:

        x   y

1 2.4220935 1.4954726

2 0.6447237 0.9113461

3 1.1361870 1.1023953

Clustering vector:

 [1] 2 3 3 2 1 1 1 1 1 1 1 1

Within cluster sum of squares by cluster:

[1] 3.96919665 0.03479993 0.02904713

 (between_SS / total_SS = 64.0 %)

Available components:

[1] "cluster"   "centers"   "totss"   "withinss"   "tot.withinss" "betweenss"

[7] "size"   "iter"   "ifault"

| You're the best!

|===
| 72%

| The program returns the information that the data clustered into 3 clusters each of size 4. It also
| returns the coordinates of the 3 cluster means, a vector named cluster indicating how the 12 points
| were partitioned into the clusters, and the sum of squares within each cluster. It also shows all
| the available components returned by the function. We've stored off this data for you in a kmeans
| object called kmObj. Look at kmObj$iter to see how many iterations the algorithm went through.

```
> kmObj$iter
[1] 2
```

| You are really on a roll!

|===
| 74%

| Two iterations as we did before. We just want to emphasize how you can access the information
| available to you. Let's plot the data points color coded according to their cluster. This was
| stored in kmObj$cluster. Run plot with 5 arguments. The data, x and y, are the first two; the
| third, col is set equal to kmObj$cluster, and the last two are pch and cex. The first of these
| should be set to 19 and the last to 2.

```
> plot(x,y,col=kmObj$cluster, pch=19, cex=2)
```

| You got it!

|===
| 76%

| Now add the centroids which are stored in kmObj$centers. Use the points function with 5 arguments.
| The first two are kmObj$centers and col=c("black","red","green"). The last three, pch, cex, and
| lwd, should all equal 3.

> points(kmObj$centers, col=c("black","red","green"), pch=3, cex=3, lwd=3)

| You are quite good my friend!

|===
| 78%

| Now for some fun! We want to show you how the output of the kmeans function is affected by its
| random start (when you just ask for a number of clusters). With random starts you might want to run
| the function several times to get an idea of the relationships between your observations. We'll
| call kmeans with the same data points (stored in dataFrame), but ask for 6 clusters instead of 3.

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|===
== | 80%

| We'll plot our data points several times and each time we'll just change the argument col which
| will show us how the R function kmeans is clustering them. So, call plot now with 5 arguments. The
| first 2 are x and y. The third is col set equal to the call kmeans(dataFrame,6)$cluster. The last
| two (pch and cex) are set to 19 and 2 respectively.

> plot(x,y,col=kmeans(dataFrame,6)$cluster, pch=19, cex=2)

| Perseverance, that's the answer.

|===| 82%

| See how the points cluster? Now recall your last command and rerun it.

> plot(x,y,col=kmeans(dataFrame,6)$cluster, pch=19, cex=2)

| That's a job well done!

|===| 84%

| See how the clustering has changed? As the Teletubbies would say, "Again! Again!"

> plot(x,y,col=kmeans(dataFrame,6)$cluster, pch=19, cex=2)

| That's the answer I was looking for.

|===| 86%

| So the clustering changes with different starts. Perhaps 6 is too many clusters? Let's review!

...

|==========
========== | 88%

| True or False? K-means clustering requires you to specify a number of clusters before you begin.

1: False

2: True

Selection: 2

| You nailed it! Good job!

|==========
============ | 90%

| True or False? K-means clustering requires you to specify a number of iterations before you begin.

1: True

2: False

Selection: 2

| Great job!

|==========
============== | 92%

| True or False? Every data set has a single fixed number of clusters.

1: True

2: False

Selection: 2

| You got it right!

|==
================= | 94%

| True or False? K-means clustering will always stop in 3 iterations

1: True

2: False

Selection: 2

| That's a job well done!

|==
================== | 96%

| True or False? When starting kmeans with random centroids, you'll always end up with the same final

| clustering.

1: True

2: False

Selection: 2

| Your dedication is inspiring!

|==========
========== | 98%

| Congratulations! We hope this means you found this lesson oK.

...

|==========
==========| 100%

| Would you like to receive credit for completing this course on Coursera.org?

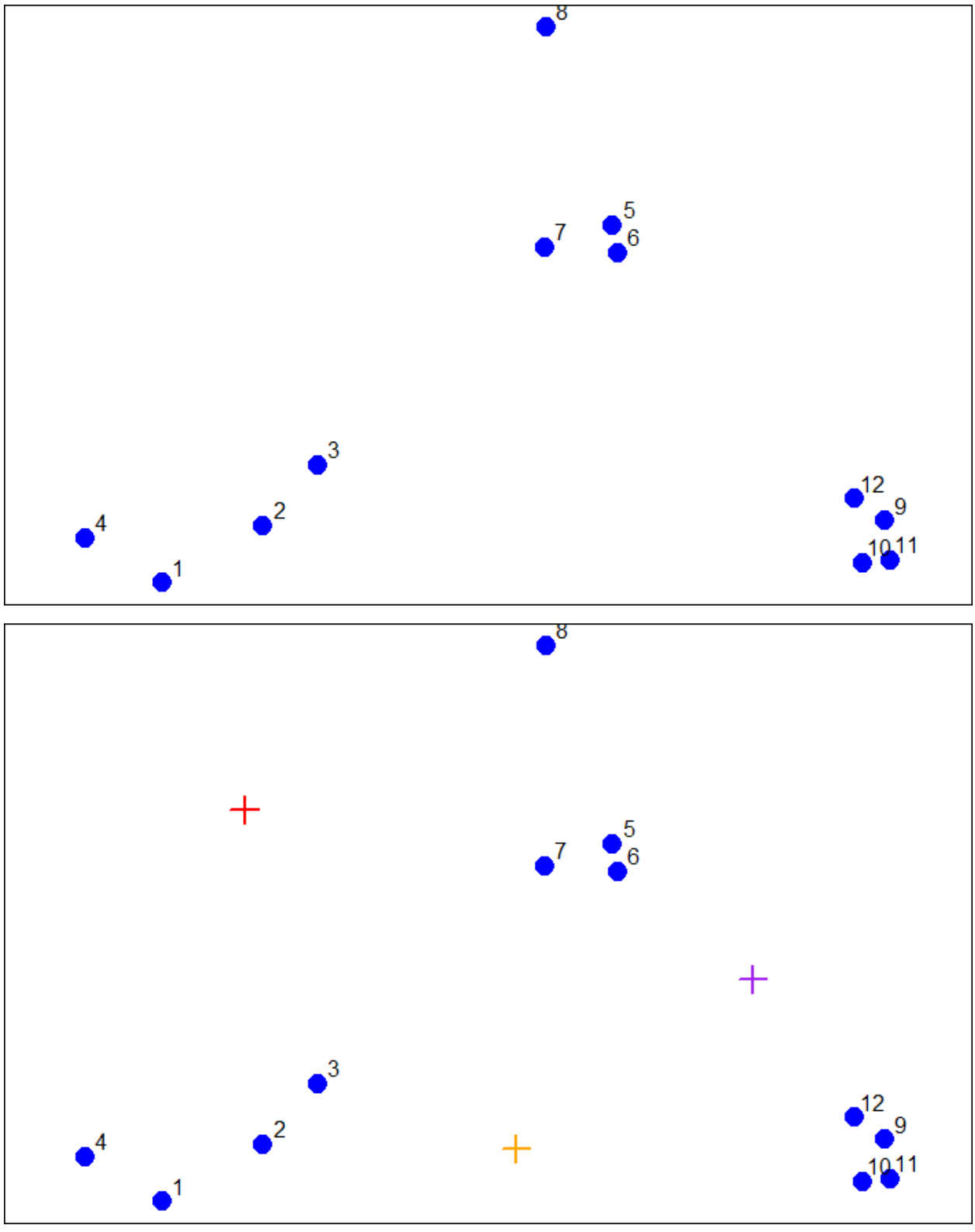
1: No

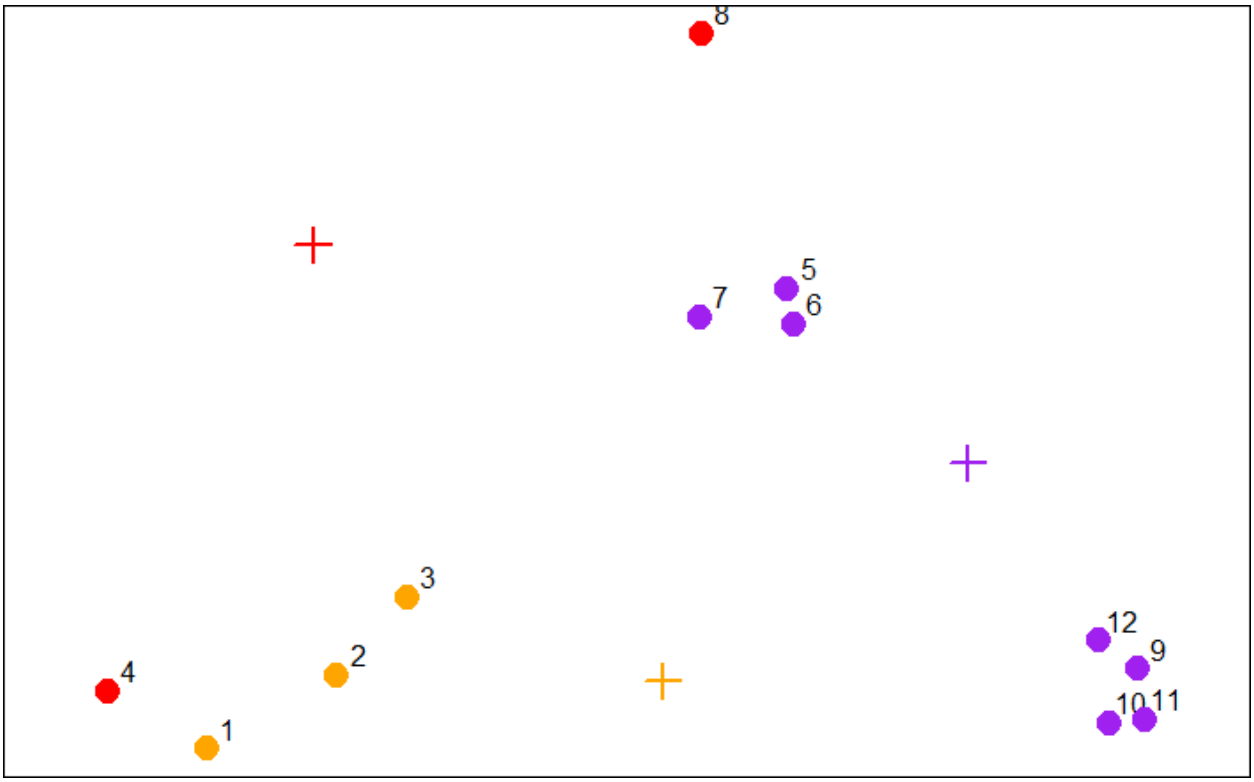
2: Yes

Functions

```
mdist <- function(x,y,cx,cy){
  distTmp <- matrix(NA,nrow=3,ncol=12)
  distTmp[1,] <- (x-cx[1])^2 + (y-cy[1])^2
  distTmp[2,] <- (x-cx[2])^2 + (y-cy[2])^2
  distTmp[3,] <- (x-cx[3])^2 + (y-cy[3])^2
  return(distTmp)
}
```

Plots

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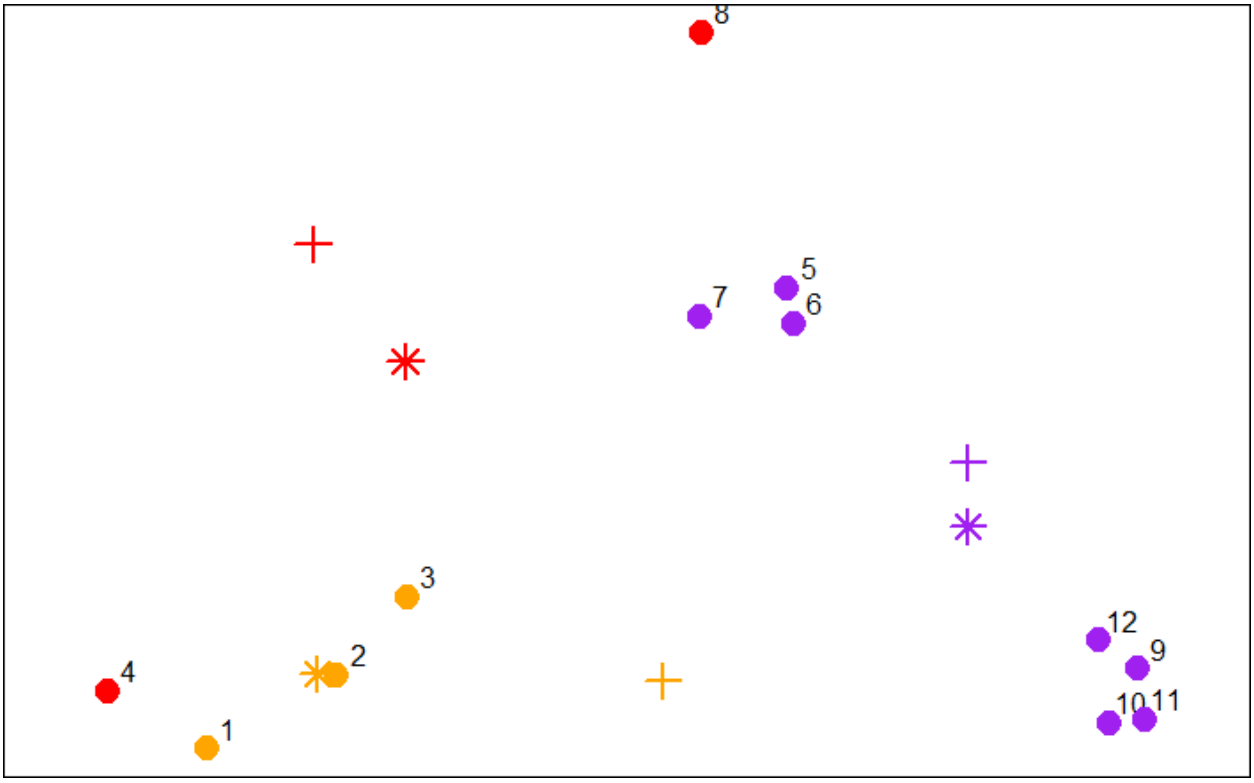
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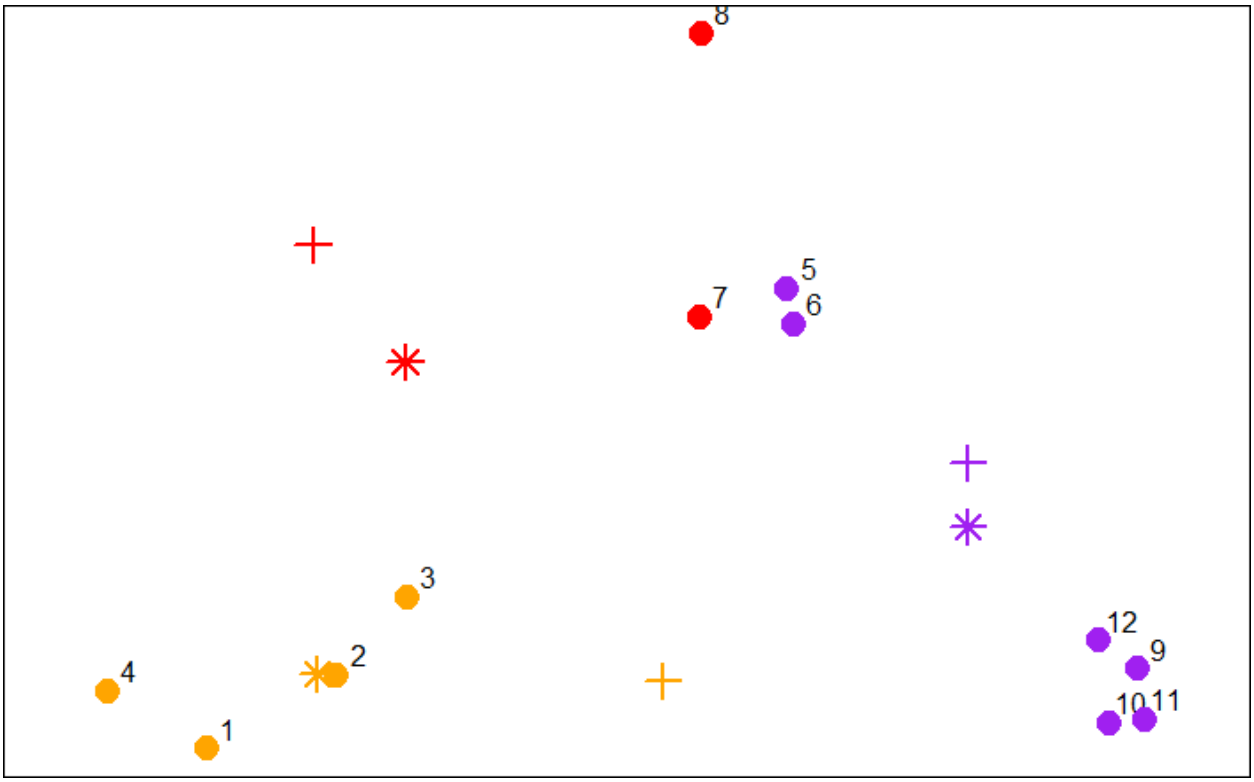
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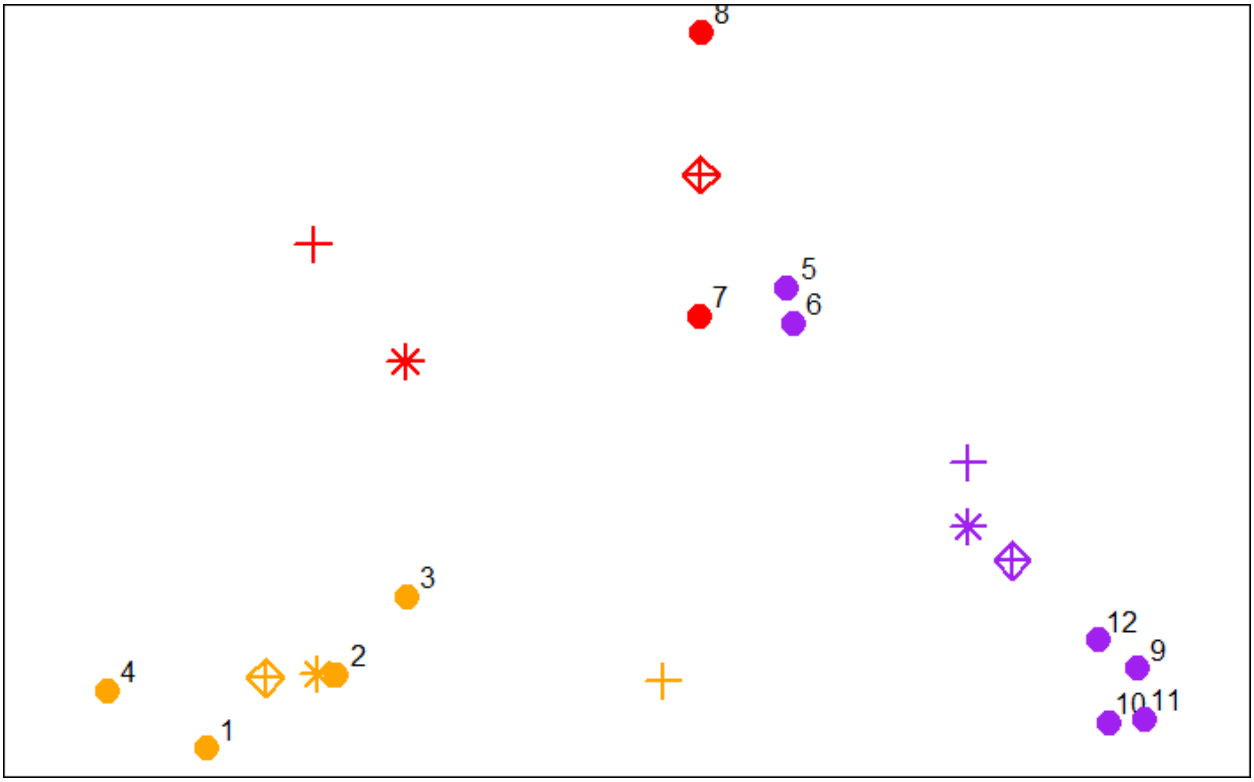
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