Course: Exploratory Data Analysis 2 Lesson: K Means Clustering 3 4 - Class: text 5 Output: "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.)" 6 7 8 - Class: text Output: 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. 10 11 - Class: text 12 Output: 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." 13 14 - Class: text 15 Output: Since clustering organizes data points that are close into groups we'll assume we've decided on a measure of distance, e.g., Euclidean. 16 17 - Class: figure 18 Output: 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. 19 Figure: ranPoints.R 20 FigureType: new 21 2.2 - Class: text 23 Output: 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. 24 25 - Class: text 26 Output: 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. 27 28 - Class: mult question 29 Output: As described, what does this process require? 30 AnswerChoices: A defined distance metric; A number of clusters; An initial guess as to cluster centroids; All of the others 31 CorrectAnswer: All of the others 32 AnswerTests: omnitest(correctVal='All of the others') 33 Hint: Which choice includes all the others. 34 35 - Class: mult question 36 Output: 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? AnswerChoices: A final estimate of cluster centroids; An assignment of each point to 37 a cluster; All of the others 38 CorrectAnswer: All of the others 39 AnswerTests: omnitest(correctVal='All of the others') 40 Hint: Which choice includes all the others. 41 42 - Class: text

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Output: When it's finished k-means clustering returns a final position of each
43
       cluster's centroid as well as the assignment of each data point or observation to a
       cluster.
44
45
     - Class: text
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       Output: 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.
47
     - Class: cmd question
48
       Output: We've created two 3-long vectors for you, cx and cy. These respectively hold
49
       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.
50
       CorrectAnswer: cmat
       AnswerTests: omnitest(correctExpr='cmat')
51
52
       Hint: Type cmat at the command prompt.
53
54
     - Class: cmd question
55
       Output: 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.
       CorrectAnswer: points(cx,cy,col=c("red","orange","purple"),pch=3,cex=2,lwd=2)
56
57
       AnswerTests:
       omnitest(correctExpr='points(cx,cy,col=c("red","orange","purple"),pch=3,cex=2,lwd=2)')
       Hint: Type points(cx,cy,col=c("red","orange","purple"),pch=3,cex=2,lwd=2) at the
58
       command prompt.
59
60
     - Class: text
61
       Output: 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.
62
63
     - Class: mult question
64
       Output: 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?
6.5
      AnswerChoices: 15; 36; 9; 108
66
      CorrectAnswer: 36
67
      AnswerTests: omnitest(correctVal='36')
68
       Hint: The distance between each point and one centroid means 12 distances have to be
       calculated for each centroid. This has to be done for all 3 centroids.
69
70
     - Class: cmd question
71
       Output: 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.
72
       CorrectAnswer: mdist(x,y,cx,cy)
73
       AnswerTests: omnitest(correctExpr='mdist(x,y,cx,cy)')
74
       Hint: Type mdist(x,y,cx,cy) at the command prompt.
75
76
77
     - Class: mult question
78
       Output: We've stored these distances in the matrix distImp for you. Now we have to
       assign a cluster to each point. To do that we'll look at each column and ?
79
       AnswerChoices: pick the minimum entry; pick the maximum entry; add up the 3 entries.
80
       CorrectAnswer: pick the minimum entry
81
       AnswerTests: omnitest(correctVal='pick the minimum entry')
82
       Hint: We assign each point to the centroid closest to it. Recall that the matrix
      holds distances.
83
84
     - Class: mult question
85
       Output: From the distTmp entries, which cluster would point 6 be assigned to?
86
       AnswerChoices: 1; 2; 3; none of the above
87
       CorrectAnswer:
88
      AnswerTests: omnitest(correctVal='3')
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89 **Hint:** Which row in column 6 has the lowest value? 90 91 92 - Class: cmd question 93 Output: 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 distImp. Try this now. 94 CorrectAnswer: apply(distTmp, 2, which.min) 95 **AnswerTests:** omnitest(correctExpr='apply(distTmp,2,which.min)') 96 Hint: Type apply(distTmp, 2, which.min) at the command prompt. 97 98 - Class: text 99 Output: 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. 100 101 - Class: cmd question 102 Output: 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]. 103 CorrectAnswer: points(x,y,pch=19,cex=2,col=cols1[newClust]) 104 AnswerTests: omnitest(correctExpr='points(x,y,pch=19,cex=2,col=cols1[newClust])') 105 **Hint:** Type points(x,y,pch=19,cex=2,col=cols1[newClust]) at the command prompt. 106 107 - Class: text 108 Output: 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. 109 - Class: cmd question 110 111 Output: 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). 112 CorrectAnswer: tapply(x,newClust,mean) 113 AnswerTests: omnitest(correctExpr='tapply(x,newClust,mean)') 114 **Hint:** Type tapply(x,newClust,mean) at the command prompt. 115 116 - Class: cmd question 117 Output: Repeat the call, except now apply it to the vector y instead of x. 118 CorrectAnswer: tapply(y,newClust,mean) 119 AnswerTests: omnitest(correctExpr='tapply(y,newClust,mean)') 120 Hint: Type tapply(y,newClust,mean) at the command prompt. 121 122 123 - Class: cmd question 124 Output: 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. 125 CorrectAnswer: points(newCx, newCy, col=cols1, pch=8, cex=2, lwd=2) 126 AnswerTests: omnitest(correctExpr='points(newCx,newCy,col=cols1,pch=8,cex=2,lwd=2)') 127 Hint: Type points(newCx,newCy,col=cols1,pch=8,cex=2,lwd=2) at the command prompt. 128 129 - Class: cmd question 130 Output: 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. 131 CorrectAnswer: mdist(x,y,newCx,newCy) 132 AnswerTests: omnitest(correctExpr='mdist(x,y,newCx,newCy)') 133 Hint: Type mdist(x,y,newCx,newCy) at the command prompt. 134

- 135 Class: mult question
- Output: 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?

 AnswerChoices: Nothing; They will both change to cluster 2; They will both change
- clusters; They're the only points that won't change clusters

 CorrectAnswer: They will both change clusters
- AnswerTests: omnitest(correctVal='They will both change clusters')
- Hint: Two of the choices are obviously wrong. That leaves two possibilities which are similar. Look carefully at the numbers in columns 4 and 7 to see where the minimum values are.
- 142 Class: cmd question

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- Output: Now call apply with 3 arguments, distTmp2, 2, and which.min to find the new cluster assignments for the points.
- 144 **CorrectAnswer**: apply(distTmp2,2,which.min)
- AnswerTests: omnitest(correctExpr='apply(distTmp2,2,which.min)')
- 146 **Hint:** Type apply(distTmp2,2,which.min) at the command prompt.
- 148 Class: cmd question
- Output: 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].
- 150 **CorrectAnswer:** points(x,y,pch=19,cex=2,col=cols1[newClust2])
- AnswerTests: omnitest(correctExpr='points(x,y,pch=19,cex=2,col=cols1[newClust2])')
- Hint: Type points(x,y,pch=19,cex=2,col=cols1[newClust2]) at the command prompt.
- 154 Class: text
- Output: 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).
- 157 Class: cmd question
- Output: Now use tapply to find the x coordinate of the new centroid. Recall there are 3 arguments, x, newClust2, and mean.
- 159 **CorrectAnswer:** tapply(x,newClust2,mean)
- 160 **AnswerTests:** omnitest(correctExpr='tapply(x,newClust2,mean)')
- 161 **Hint:** Type tapply(x,newClust2,mean) at the command prompt.
- 163 Class: cmd question
- Output: Do the same to find the new y coordinate.
- 165 **CorrectAnswer:** tapply(y,newClust2,mean)
- AnswerTests: omnitest(correctExpr='tapply(y,newClust2,mean)')
- 167 **Hint:** Type tapply(y,newClust2,mean) at the command prompt.
- 169 Class: cmd question
- Output: 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.
- 171 **CorrectAnswer:** points(finalCx,finalCy,col=cols1,pch=9,cex=2,lwd=2)
- 172 **AnswerTests:**
 - omnitest(correctExpr='points(finalCx, finalCy, col=cols1, pch=9, cex=2, lwd=2)')
- Hint: Type points (finalCx, finalCy, col=cols1, pch=9, cex=2, lwd=2) at the command prompt.
- 175 Class: text
- Output: 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.
- 178 Class: text
- Output: 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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181
      - Class: cmd question
182
        Output: Call kmeans now with 2 arguments, dataFrame (which holds the x and y
        coordinates of our 12 points) and centers set equal to 3.
183
        CorrectAnswer: kmeans (dataFrame, centers=3)
184
        AnswerTests: omnitest(correctExpr='kmeans(dataFrame,centers=3)')
        Hint: Type kmeans(dataFrame, centers=3) at the command prompt.
185
186
187
      - Class: cmd question
188
        Output: 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$iter to see how many iterations the algorithm went through.
        CorrectAnswer: kmObj$iter
189
190
        AnswerTests: omnitest(correctExpr='kmObj$iter')
191
        Hint: Type kmObj$iter at the command prompt.
192
193
      - Class: cmd question
194
        Output: 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.
195
        CorrectAnswer: plot(x,y,col=kmObj$cluster,pch=19,cex=2)
196
        AnswerTests: omnitest(correctExpr='plot(x,y,col=kmObj$cluster,pch=19,cex=2)')
197
        Hint: Type plot(x,y,col=km0bj$cluster,pch=19,cex=2) at the command prompt.
198
199
      - Class: cmd question
200
        Output: Now add the centroids which are stored in kmObj$centers. Use the points
        function with 5 arguments. The first two are kmObj$centers and
        col=c("black", "red", "green"). The last three, pch, cex, and lwd, should all equal 3.
201
        CorrectAnswer: points(kmObj$centers,col=c("black","red","green"),pch=3,cex=3,lwd=3)
202
        AnswerTests:
        omnitest(correctExpr='points(kmObj$centers,col=c("black","red","green"),pch=3,cex=3,lwd
        =3)')
203
        Hint: Type points(kmObj$centers,col=c("black","red","green"),pch=3,cex=3,lwd=3) at
        the command prompt.
204
205
206
      - Class: text
207
        Output: 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.
208
209
210
      - Class: cmd question
211
        Output: 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) $cluster. The last two (pch and cex) are set to 19 and
        2 respectively.
212
        CorrectAnswer: plot(x,y,col=kmeans(dataFrame,6)$cluster,pch=19,cex=2)
213
        AnswerTests:
        omnitest(correctExpr='plot(x,y,col=kmeans(dataFrame,6)$cluster,pch=19,cex=2)')
214
        Hint: Type plot(x,y,col=kmeans(dataFrame,6)$cluster,pch=19,cex=2) at the command
        prompt.
215
216
      - Class: cmd question
217
        Output: See how the points cluster? Now recall your last command and rerun it.
218
        CorrectAnswer: plot(x,y,col=kmeans(dataFrame,6)$cluster,pch=19,cex=2)
219
        omnitest(correctExpr='plot(x,y,col=kmeans(dataFrame,6)$cluster,pch=19,cex=2)')
220
        Hint: Type plot(x,y,col=kmeans(dataFrame,6)$cluster,pch=19,cex=2) at the command
        prompt.
221
222
      - Class: cmd question
```

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223
        Output: See how the clustering has changed? As the Teletubbies would say, "Again!
        Again!"
224
        CorrectAnswer: plot(x,y,col=kmeans(dataFrame,6)$cluster,pch=19,cex=2)
225
        AnswerTests:
        omnitest(correctExpr='plot(x,y,col=kmeans(dataFrame,6)$cluster,pch=19,cex=2)')
226
        Hint: Type plot(x,y,col=kmeans(dataFrame,6)$cluster,pch=19,cex=2) at the command
        prompt.
227
228
      - Class: text
229
        Output: So the clustering changes with different starts. Perhaps 6 is too many
        clusters? Let's review!
230
231
      - Class: mult question
232
        Output: True or False? K-means clustering requires you to specify a number of
        clusters before you begin.
        AnswerChoices: True; False
233
234
                       True
        CorrectAnswer:
235
        AnswerTests: omnitest(correctVal='True')
236
        Hint: What did you provide when you called the R function?
237
238
      - Class: mult question
239
        Output: True or False? K-means clustering requires you to specify a number of
        iterations before you begin.
240
       AnswerChoices: True; False
        CorrectAnswer: False
241
242
        AnswerTests: omnitest(correctVal='False')
243
        Hint: What did you provide when you called the R function?
244
245
     - Class: mult question
        Output: True or False? Every data set has a single fixed number of clusters.
246
247
        AnswerChoices: True; False
248
        CorrectAnswer: False
249
        AnswerTests: omnitest(correctVal='False')
250
       Hint: The number of clusters depends on your eye.
251
252
      - Class: mult question
253
        Output: True or False? K-means clustering will always stop in 3 iterations
254
        AnswerChoices: True; False
255
        CorrectAnswer: False
256
        AnswerTests: omnitest(correctVal='False')
257
        Hint: The number of iterations depends on your data.
258
259
260
      - Class: mult question
261
        Output: True or False? When starting kmeans with random centroids, you'll always end
        up with the same final clustering.
262
       AnswerChoices: True; False
        CorrectAnswer: False
263
264
        AnswerTests: omnitest(correctVal='False')
265
        Hint: Recall the last experiment we did in the lesson, rerunning the same routine.
266
267
     - Class: text
268
        Output: Congratulations! We hope this means you found this lesson oK.
269
270
      - Class: mult question
271
        Output: "Would you like to receive credit for completing this course on
272
          Coursera.org?"
273
        CorrectAnswer: NULL
274
        AnswerChoices: Yes; No
275
        AnswerTests: coursera on demand()
276
        Hint: ""
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