Exposition of Spatial Clustering Methods

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in
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Kaitlyn E. Haase

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Abstract

In recent years, the amount of geographic data has increased immensely with new technology (i.e. GPS and surveillance cameras). Additionally, the data has improved in accuracy and increased in complexity. This has provoked statisticians to create techniques to best analyze and draw conclusions from this new-found data. Earlier techniques of spatial data were not equipped to handle the complexity and quantity of the data. This project first explores how and why we analyze data based on geographic information. Next, I will explain some examples of spatial data algorithms, including PAM (Partitioning Around Medoids), CLARA (Clustering LARge Applications), and CLARANS (Clustering Large Applications based on RANdomized Search). The purpose of this exploration is to better analyze government health data from a previous STAT 495 project. I will then: use a sample of STAT 495 project data to demonstrate the CLARA algorithm, evaluate how CLARA performed, and develop a model to best predict cluster.

Introduction

Cassidy Mahar, Silvia Sotolongo, and I, for our STAT 495 project, used mapping techniques to visualize and analyze US Government data. The data contained spatial, demographic, and health status information. The only significant relationships we were able to find were between demographic information and health status; we were unable to relate health status with any spatial information. I am interested in analyzing the data through spatial clustering, to further analyze whether the location of an observation is related to one's health status. Since clustering utilizes spatial information, it may be helpful in finding patterns in the data.

0.1 Why Analyze Spatial Data?

We are interested in analyzing spatial data for many reasons, one being because there is so much of it available. Spatial data analysis is analyzing data based on topological, geometric, and geographic information. Spatial data may include latitude and longitude, zip code, or street address. Investigating spatial data can help us find dissimilarities and similarities among objects. This can aid in allocating resources to areas that need them most, discovering changes over time, and categorizing new objects.

0.2 Analyzing Spatial Data Algorithms

Many, many algorithms exist that analyze spatial data; most algorithms are focused around clustering. To get a glimpse of the number of algorithms and strategies to analyze spatial data, Figure 1 provides some examples (Wagaman, 2019).

As noted, the methods are aimed around clustering, which I will further explore in the next section.

Figure 1: Clustering Methods

0.2.1 Clustering

Clustering organizes a set of data items into groups so that items in the same group are similar to each other and different from those in other groups (Huo & Mennis, 2009). Clustering is helpful in finding patterns and similarities/differences between data points and groups; however it can be quite subjective. It is up to the statistician to determine how many clusters are appropriate for the data, as well as the cut off for what is considered "similar" or "dissimilar". Additionally, the statistician must choose which clustering algorithm is best to use.

Chapter 1

Clustering Basics

Since there are so many clustering algorithms, choosing the appropriate method becomes an important task. There are many factors to consider when choosing a clustering algorithm, such as the application of the problem (what do you want to find out about this data?), quality versus speed trade off (the size of the data plays a role), characteristics of the data (i.e. numeric distance measures), dimensionality (typically as dimension increases, the time it takes to run the method increases and quality of the data clusters decrease), and outliers (some methods are very sensitive to outliers) (Jiawei Han & Tung, n.d.). These were some of the considerations I had to think about in analyzing the data from my STAT 495 project.

1.1 Partitioning

There are four main types of clustering: hierarchical, partitioning, density-based, and methods-based. Next, I'll dive into the partitioning clustering technique.

Partitioning cluster methods divide a set of data items into a number of non-overlapping clusters. A data item is typically assigned to a cluster based on a proximity or dissimilarity measure (Jiawei Han & Tung, n.d.).

Usually, there is a data set with n observations and the goal is to divide the data points into k clusters so that an objective function is optimized.

The most common objective function is the sum of squared errors (SSE), where c_k is the centroid or medoid of the cluster C_k.

$$SSE(C) = \sum_{k=1}^{K} \sum_{x_i in C_k} ||x_i - c_k||^2$$

Note: the "element-of" symbol would not work in Latex, so I am using "in" to indicate

this instead.

Partitioning clustering algorithms classify the data into K groups by satisfying both that each group has at least one data point, and that each data point belongs to exactly one group (V & Surendran, 2013).

1.2 Methods to Create Clusters

There are many ways to create clusters. The most basic method is the K-means algorithm, which was developed by MacQueen in 1967 (V & Surendran, 2013). In response to K-means being very sensitive to outliers, the K-medoid algorithm was created in 1987 (V & Surendran, 2013). Both partitioning methods use iterative processes to find K clusters; however, they use different ways to represent these clusters.

1.2.1 *K*-Means

K-means algorithm represents its n observations in k groups, with the center of the groups being the mean/average observation. The goal of the algorithm is to find k centroids, one for each cluster. In order to do this, we must minimize an objective function, which is the squared error function for k means. The objective function is:

$$O = \sum_{j=1}^{k} \sum_{i=1}^{j} ||X_i^{(j)} - C_j||^2$$

Where $|X_i^{(j)} - C_j|$ is an indicator of the distance of the data points from their cluster centers.

The steps of the algorithm are as follows (V & Surendran, 2013):

1. Choose k points in the space to represent the centroids. This works best if they are chosen to be far apart from each other.

2. Assign each object in the data set to the cluster with the closest centroid.

3. When all of the clusters have been made, recalculate the positions of the k centroids.

4. Repeat steps 2 and 3 until the centroids no longer move.

This algorithm always terminates; however, it is sensitive both to outliers and to the initial randomly selected k cluster centers. Therefore, the algorithm should be run multiple times to reduce the effects from this sensitivity.

In order to determine how well K-means worked, we use the within cluster sum-of-squares, WSS, to determine the compactness/"goodness" of the clustering (and we want it as small as possible).

We calculate the WSS by the following equation:

$$WSS = \sum_{k=1}^{k} \sum_{x_i in C_k} (x_i - \mu_k)^2$$

Where x_i is a data point in cluster C_k and μ_k is the mean value assigned to the cluster C_k (Datanovia, n.d.).

1.2.2 *K*-Medoids

On the contrary, instead of taking the mean value of the objects in a cluster to be the center, the k-medoid method uses the most centrally located object in a cluster to be the cluster center (Jiawei Han & Tung, n.d.). This causes the method to be less sensitive to outliers, but also requires more time to run.

Steps for K-medoids (V & Surendran, 2013):

1. Initial guess for centers C_1, C_2,... C_k (i.e. randomly select k points from X_1, X_2,... X_n)

2. Minimize over C: for each i= 1, 2,... n, find the cluster center C_k closest to Xi and let C(i)=k.

3. Minimize over C_1, C_2,... C_k: for each k=1,... K, $C_k = X_k^*$, the medoid of points in cluster k. ie, the point Xi in the cluster k that minimizes

$$\sum_{c(j)=k} ||X_j - X_i||^2$$

Basically, K-means and K-medoids follow very similar algorithms; however, K-medoids uses the most centrally located object (medoid) in a cluster to be the cluster center. This causes there to only be at most one center changed for each iteration (makes the algorithm run slower).

1.3 How to Choose K

Now that we've discussed K-means and K-medoids partitioning methods, we know how to find k clusters of data points; but how do we determine what k is?

Well, there are many ways to choose k, which is why these methods are so subjective.

I will describe two of the many ways to determine k, both of which use visuals to determine what value of k is appropriate for the data. The elbow method and silhouette method are common ways to find k when using the K-means and K-medoids algorithms (Datanovia, n.d.).

1.3.1 Elbow Method

To start, the Elbow method looks at the total within-cluster sum of squares (WSS) and determines when there are enough clusters so that the next cluster does not improve the total WSS very much. This would be the appropriate k to choose.

The steps for this algorithm are as follows (Datanovia, n.d.):

1. Compute the clustering algorithm (i.e. k-medoids method) for different values of k (i.e. k from 1 to 10).

2. For each k, calculate the total WSS. WSS can be calculated as:

$$WSS = \sum_{i=1}^{k} \sum_{x_i in C_k} ||x_i - c_k||^2$$

Where x_i is a data point in cluster C_k and c_k is the medoid assigned to the cluster C_k. (Datanovia, n.d.).

3. Plot the curve of the total WSSs according to the number of clusters (k).

4. The location of the bend in the plot is generally considered an indicator for the appropriate number of clusters.

1.3.2 Silhouette Method

The Silhouette method focuses on the quality of clustering. A high average silhouette width indicates a good clustering (how well each object lies within its cluster).

The steps of the Silhouette Algorithm are (Datanovia, n.d.):

1. Compute clustering algorithm for different values of k (i.e. k from 1 to 10).

2. For each k, calculate the average silhouette of observations.

The silhouette of an object O_j, is a quantity varying between -1 and 1, that indicates how much O_j truly belongs to the cluster to which O_j is classified (Ng & Han, 2000).

There is a silhouette function in R that calculates the silhouette widths of the clusters.

3. Plot the curve of the average silhouettes according to the number of clusters (k).

4. The location of the maximum is considered the appropriate number of clusters.

Chapter 2

Clustering Methods Continued

2.1 PAM

Partitioning Around Medoids (PAM) is the most commonly used type of k-medoid clustering (Kaufmann & Rousseeuw, 1987).

As an overview, the algorithm iterates through all the k cluster centers and tries to replace the center with one of the other objects ($n - k$ possibilities) (Jiawei Han & Tung, 2002). For a replacement to occur, the squared error function must decrease. If it does not decrease, there is no replacement. The algorithm eventually terminates.

For the set up of this algorithm, let's let O_m be a current medoid that is to be replaced (i.e. A in Figure 2.1). Let's let O_p be a new medoid to replace O_m (i.e. M in Figure 2.1). O_j is an other non-medoid object that may or may not be moved (i.e. Y and Z in Figure 2.1). $O_{j,2}$ is a current medoid that is nearest to O_j without A and M (i.e. B in Figure 2.1).

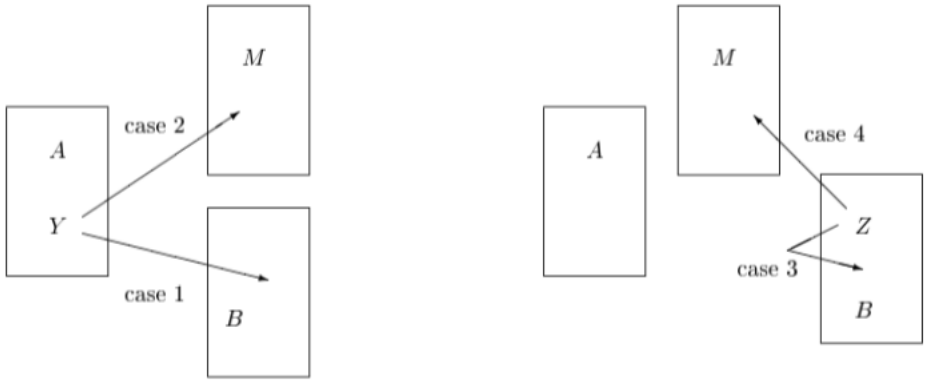


Figure 2.1: Four cases for Replacing A with M

Now that I have set us up, there are four different ways or "cases" in which PAM calculates the cost, C_{jmp}, for all of the non-medoid objects O_j (Jiawei Han & Tung, n.d.). For the sake of simplicity and in understanding the different cases in terms of Figure 2.1, I will denote O_m as A, O_p as M, O_j as Y or Z, $O_{j,2}$ as B.

Case 1:

Suppose Y currently belongs to the cluster represented by A. Additionally, Y is more similar to B than to M (i.e. $d(Y, M) \geq d(Y, B)$), where B is the second most similar medoid to Y. If A were to be replaced by M as a medoid, Y would belong to B (indicated by the Case 1 arrow in Figure 2.1). Therefore the cost of the switch is: $C_{jmp} = d(Y, B) - d(Y, A)$.

This equation will always give a non-negative C_{jmp}, indicating that there is a non-negative cost incurred in replacing A with M.

Case 2:

Suppose Y currently belongs to the cluster represented by A. But this time, A is less similar to B than to M ($d(Y, M) < d(Y, B)$). Then, if A is replaced by M, Y would belong to the cluster represented by M. The cost of this swap would be: $C_{jmp} = d(Y, M) - d(Y, A)$. The value of this C_{jmp} could be positive or negative, depending on whether Y is more similar to A or M.

Case 3:

Suppose Z currently belongs to the cluster other than the one represented by A. Also, let Z be more similar to B than to M. Then even if A is replaced by M, Z would stay in the cluster represented by B. The cost of this swap is: $C_{jmp} = 0$.

Case 4:

Suppose Z belongs to a cluster represented by B, but Z is less similar to B than to M. If we replaced A with M, Z would jump to the cluster of M, from that of B. The cost in this case would be: $C_{jmp} = d(Z, M) - d(Z, B)$. This cost would always be negative.

In combining all of the four cases described, the total cost of replacing A with M is:

$$TC_{mp} = \sum_j (C_{jmp})$$

.

The more formal steps of the algorithm are (Jiawei Han & Tung, n.d.):

1. Select k representative objects arbitrarily.
2. Compute TC_{mp} for all pairs of O_m, O_p where O_m is currently selected, and O_p is not.

3. Select the pair O_m, O_p which corresponds to $min_{O_m,O_p}TC_{mp}$. If the minimum TC_{mp} is negative, replace O_m with O_p and go back to Step 2.

4. Otherwise, for each non-selected object, find the most similar representative object.

The total complexity of PAM in one iteration is $O(k(n-k)^2)$ (O= each non-medoid data point, k= # of cluster centers, $(n-k)$ objects to compare to, and $(n-k)$ operations for calculating E). This makes for a costly computation when n is large. The algorithm works best when n= 100 and k=5.

2.2 CLARA

Because PAM does not scale well to large data sets, Clustering LARge Applications (CLARA) was developed (Kaufmann & Rousseeuw, 1990).

CLARA is a sampling based method, meaning a sample of the data is used to represent the entire data set. Medoids are chosen from this sample data using PAM and then the average dissimilarity is computed using the whole data set, not only the objects in the samples. If a new set of medoids gives a lower dissimilarity than a previous best solution, then the best solution is replaced with a new set of medoids (Jiawei Han & Tung, n.d.).

Experiments indicate that 5 samples of size 40+ $2k$ give satisfactory results (Ng & Han, 2000).

The steps for the algorithm are as follows (Jiawei Han & Tung, n.d.):

1. For i= 1 to 5, repeat the following steps:

2. Draw a sample of 40+ $2k$ objects from the entire data set, and use PAM to find k medoids of the sample.

3. For each object O_j in the entire data set, determine which of the k medoids are most similar to O_j.

4. Calculate the average dissimilarity of the clustering obtained in the previous step. If this value is less than the current minimum, use this value as the current minimum, and retain the k medoids found in Step 2 as the best medoids obtained so far.

5. Return to Step 1 to start the next iteration.

CLARA performs well on large data sets, i.e. around 1000 objects (n) in 10 clusters (k). CLARA can work on larger data sets because the complexity for each iteration is $Ok(40+k)^2 + k(n-k)$, which is much smaller than $O(k(n-k)^2)$ (which is the complexity for each iteration in PAM) (J. Han, n.d.).

2.3 CLARANS

CLARANS was created to handle even larger data sets than CLARA, and provides the highest quality clusters, in comparison to PAM and CLARA.

The easiest way to understand CLARANS, is through a graphic example involving both PAM and CLARA as well (Jiawei Han & Tung, n.d.).

The processes of finding k medoids can be described as searching through a graph of objects. This graph, denoted $G_{n,k}$ contains nodes represented by a set of k objects $\{O_{m1}, ..., O_{mk}\}$, indicating that the medoids of the objects are: $O_{m1}, ..., O_{mk}$. The set of nodes in the graph is the set $\{\{O_{m1}, ..., O_{mk}\} \mid O_{m1}, ..., O_{mk}$ are objects in the data set$\}$.

Two nodes are considered neighbors if their sets differ by only one object. Furthermore, two nodes, $S_1 = \{O_{m1}, ..., O_{mk}\}$ and $S_2 = \{O_{w1}, ..., O_{wk}\}$ are neighbors if the intersection of S_1, S_2 is k-1. Each node therefore has $k(n-k)$ neighbors. Each node is a cluster; each node can be assigned a cost that defines the total dissimilarity between every object and the medoid of its cluster.

PAM can be viewed as a search for a minimum on the graph $G_{n,k}$. At each iteration, the neighbors of the current node are examined, and the current node gets replaced by the neighbor with the greatest descent in costs. The search continues until a minimum is obtained. Examining $k(n-k)$ neighbors of a node is time consuming, which is why CLARA was created.

CLARA examines fewer neighbors and restricts the search in general on subgraphs of $G_{n,k}$. The subgraph, $G_{Sa,k}$, contains all the nodes that are subgraphs of Sa. CLARA searches through the nodes using PAM, however, the search is confined within $G_{Sa,k}$. This is problematic, because if M is the minimum node in the original graph $G_{n,k}$, but if M is not included in $G_{Sa,k}$, M will never be found. To make up for this deficiency, many, many samples would have to be collected and processed (Jiawei Han & Tung, 2002).

CLARANS was developed because of this deficiency. CLARANS does not restrict to a particular subgraph, instead it searches the entire graph $G_{n,k}$. CLARANS is unlike PAM in that it only checks a subgroup of the neighbors of a node (like CLARA). But

in contrast to CLARA, each sample is drawn in a way that no nodes corresponding to particular objects are outright eliminated.

CLARA draws a sample of *nodes* at the beginning of the search, while CLARANS draws a sample of *neighbors* in each step of a search. CLARANS provides higher quality clusters than CLARA and only requires few searches.

For the CLARANS algorithm, there are two parameters used: *maxneighbor* (the maximum numbers of neighbors examined) and *numlocal* (the number of local minima obtained). The higher the value of maxneighbor, the closer CLARANS is to PAM.

Steps for the CLARANS algorithm (Jiawei Han & Tung, 2002):

1. Input parameters *maxneighbor* and *numlocal*. Initialize i to 1, and mincost to a large number.
2. Set *current* to an arbitrary node in $G_{n,k}$.
3. Set j=1.
4. Consider a random neighbor of S of *current*. Calculate the cost differential of the two nodes, using:
$$TC_{mp} = \sum_j (C_{jmp})$$
5. If S has a lower cost, set *current* to S, and go to Step 3.
6. Otherwise, increment j by 1. If $j \leq maxneighbor$, go to Step 4.
7. Otherwise, when $j > maxneighbor$, compare the cost of *current* compared to *mincost*. If $current < mincost$, set *mincost* to the cost of *current*, and set *bestnode* to *current*.
8. Increment i by 1. If $i > numlocal$, output *bestnode* and stop. Otherwise, go to Step 2.

Since my data from my STAT 495 project has over 60,000 observations, I originally wanted to apply the CLARANS method. Unfortunately, the CLARANS function in R only works for SNP data (used in biology). Therefore, I had to take a representative sample my data, and apply the CLARA method instead.

Chapter 3

Application to Health Data

3.1 Exploring the Data

In this application, I will further explore the data from my STAT 495 final project. The data is from DataUSA, which uses public US Government data to analyze and visualize relationships (DataUSA, n.d.). In the previous project, we decided to use data from only 2016 because of size restrictions. The data contains spatial information, quantitative variables, and a few categorical variables.

The data contains demographic information, latitude and longitude, and variables that are indicators of health status. The health status variables include: poor to fair health (the percentage of adults reporting fair or poor health (age-adjusted)), poor physical health days (average number of physically unhealthy days reported in the past 30 days (age-adjusted)), physical inactivity (the percentage of adults aged 20 and over reporting no leisure-time physical inactivity), and adult obesity (the percentage of adults to report a BMI of greater than or equal to 30). In interpreting the health indicator variables, the higher the values for these variables, the less healthy a person is.

My research question is to see whether there are clusters of people with exceptionally good or exceptionally poor health. This information could lead to further insights into what environmental or other factors are impacting peoples' health.

I plan to use the CLARA method, since I have more than 100 observations (PAM works on data sets of n=100). The data set has over 60,000 observations, so I will need to sample about 1000 observations in order to produce the best results using CLARA.

I will first take a random sample of 1000 observations. I assume the sample is representative of the data set because n is so large ($n = 1000$).

```
set.seed(1)
#getting a sample of 1000 observations
mysample <- data_subset[sample(1:nrow(data_subset), 1000,
   replace=FALSE),]
```

The data set I imported has 64 variables, which are too many for this example. Since my research question is focused around peoples' health, I will include four health indicator variables and the latitude and longitude of the data (spatial information).

```
#only keeping the variables I want to look at
myvars <- c("Latitude_tri", "Longitude_tri", "poor_or_fair_health",
            "poor_physical_health_days", "physical_inactivity", "adult_obesity")
smallsample <- mysample[myvars]
new<- na.omit(smallsample) #getting rid of missing data
```

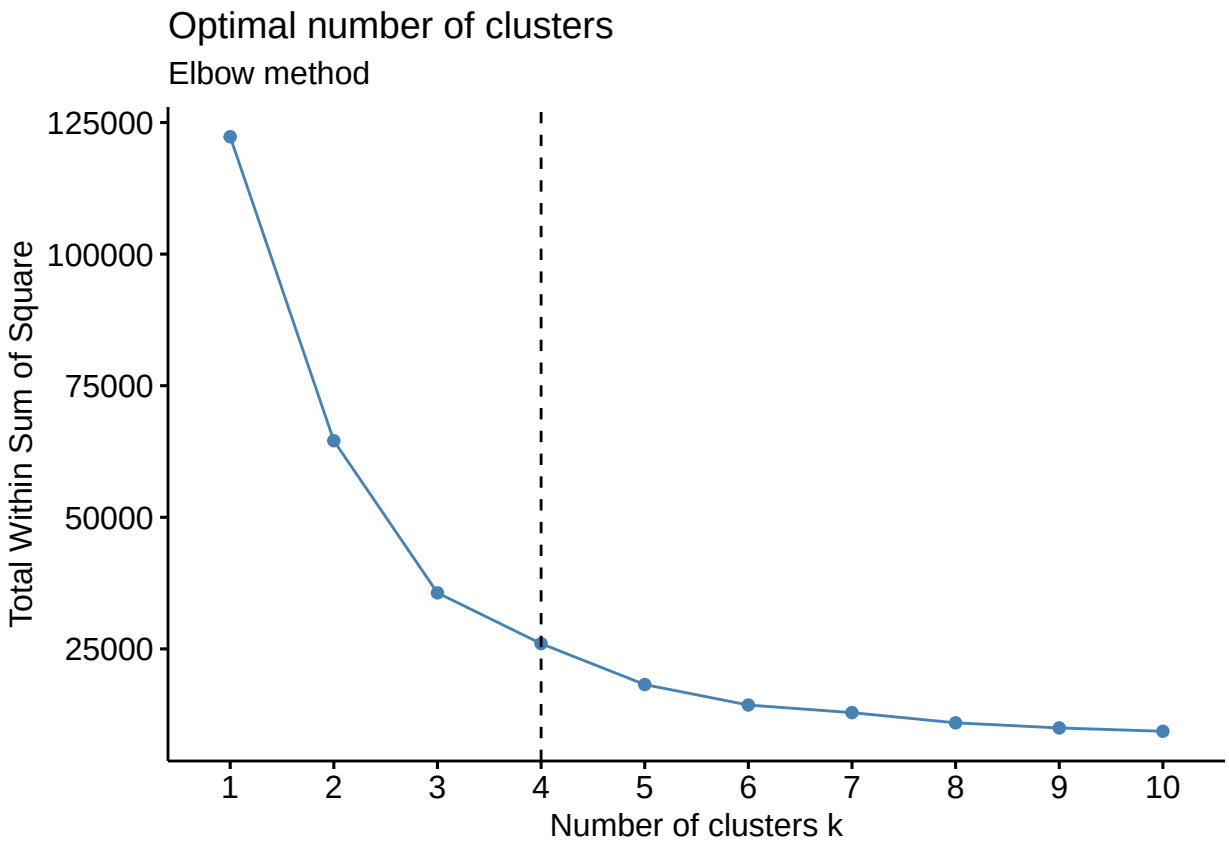
The data is now ready for the application of CLARA.

3.2 Applying CLARA

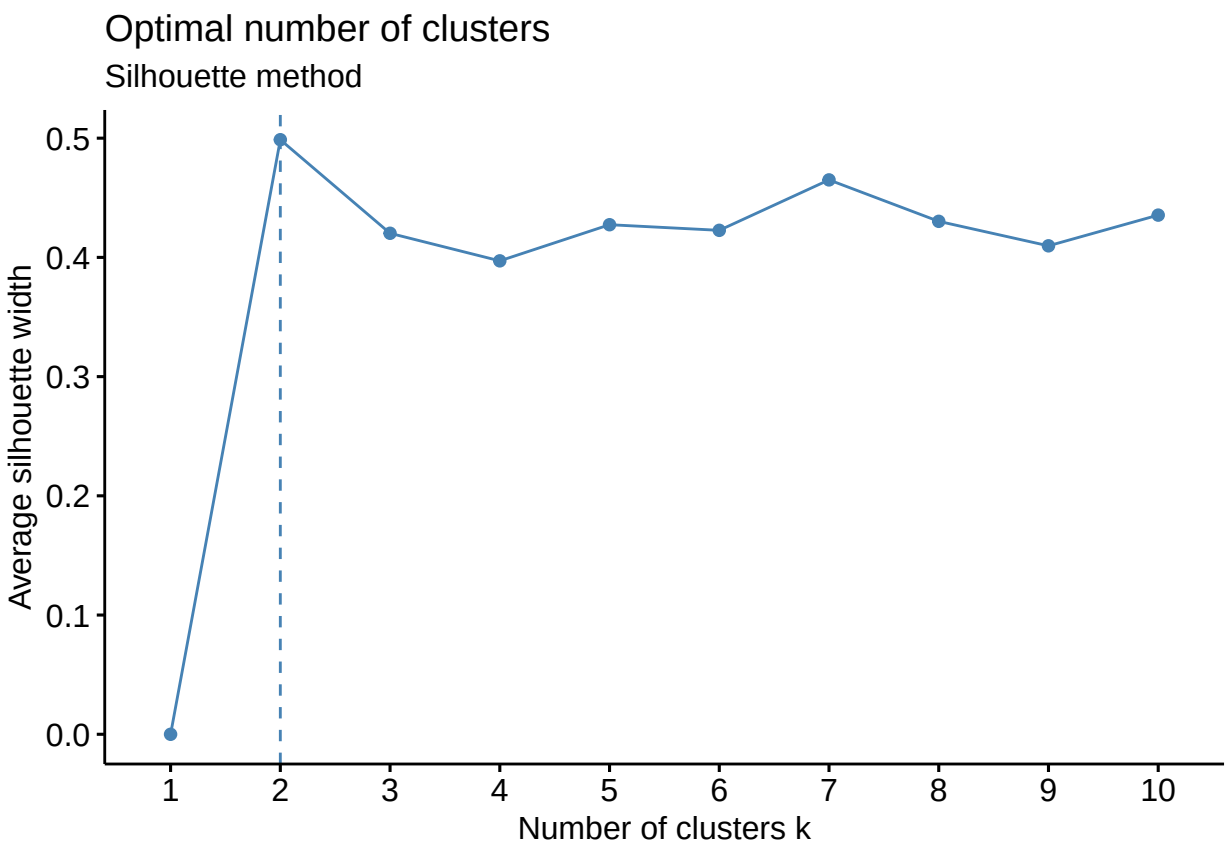
Step 1: Determining k.

One of the important steps in clustering algorithms is determining how many k clusters are appropriate. In Chapter 1, I explained the Elbow and Silhouette methods to determine k. I will perform both methods on this data to start.

```
#finding k using Elbow Method
fviz_nbclust(new, kmeans, method = "wss") +
    geom_vline(xintercept = 4, linetype = 2)+
  labs(subtitle = "Elbow method")
```




```
fviz_nbclust(new, kmeans, method = "silhouette") +
  labs(subtitle = "Silhouette method")
```



According to the Elbow method, k should be 4 (where the elbow is in the graph). According to the Silhouette method, k should be 2 (the maximum point in the graph). Since there is variation in values of k for these methods I will take the average of the two to determine k.

Step 2: Run CLARA function

Next, I will run the CLARA algorithm on the data, using the criteria of k=3.

```
## run CLARA
clarasamp <- clara(new[1:6], 3)
```

```
## print components of clara
print(clarasamp)
```

```
Call:     clara(x = new[1:6], k = 3)
Medoids:
     Latitude_tri Longitude_tri poor_or_fair_health
[1,]      39.3265      -84.4388               0.155
[2,]      40.3973      -75.9357               0.165
```

```
[3,]      36.1336      -96.1039               0.196
     poor_physical_health_days physical_inactivity adult_obesity
[1,]                       3.7               0.232         0.289
[2,]                       3.7               0.245         0.308
[3,]                       4.6               0.353         0.355
Objective function:  5.659219
Clustering vector:   int [1:925] 1 2 1 3 1 3 1 1 1 1 1 3 1 2 1 3 1 3 ...
Cluster sizes:           457 205 263
Best sample:
 [1]   5  24  86 139 149 175 177 192 208 224 242 285 306 316 333 353 361
[18] 370 389 400 404 410 429 468 471 489 502 506 567 593 679 691 703 719
[35] 726 741 780 800 811 815 818 877 882 883 902 918

Available components:
 [1] "sample"     "medoids"    "i.med"      "clustering" "objective"
 [6] "clusinfo"   "diss"       "call"       "silinfo"    "data"
```

This output tells us a lot about the results of the clustering. To start, the information from the Medoids section show that cluster 3 contains people with the worst health, in comparison to cluster 1 and 2. For example, cluster 1 and 2 average 3.7 *poor_physical_health_days*, while cluster 3 averages 4.6. This difference was seen in all four health indicator variables.

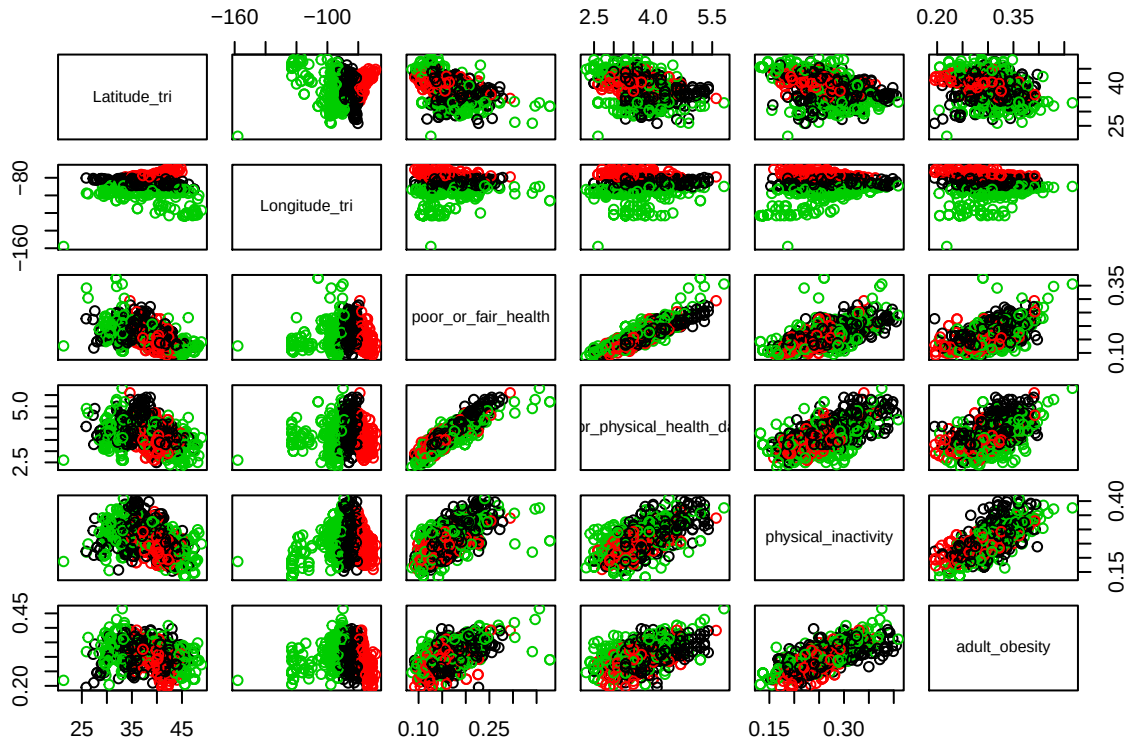
The cluster sizes are also noted. There are 457 observations in cluster 1, 205 in cluster 2, and 263 in cluster 3.

```
#cluster number for each observation
clarasamp$cluster
#silhouette width for each cluster
clarasamp$silinfo
```

This information tells us even more about the CLARA output. The first part gives us the categorizations of each data point to its cluster. The second part of information gives us the average silhouette width for each cluster. The silhouette widths were: 0.422183 for cluster 1, 0.634548 for cluster 2, and 0.172013 for cluster 3. The better the clustering is, the greater the silhouette width; so we can determine that cluster 2 was best compared to cluster 1 and 3.

Next, I will walk through some of the visualizations given this new clustering information.

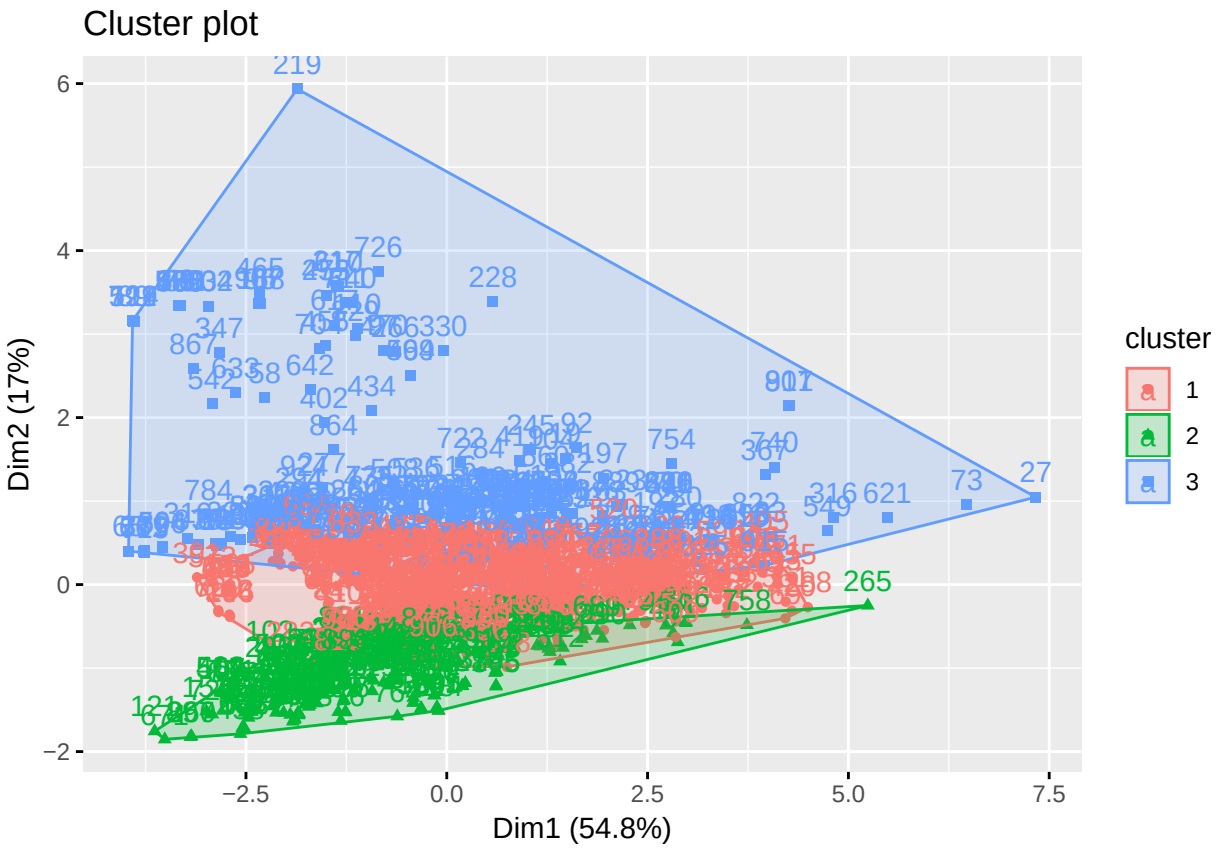
```
## plot clusters
plot(new, col = clarasamp$cluster)
## plot centers
points(clarasamp$centers, col = 1:2, pch = 8)
```



The plot of the clusters does not look great. Aside from comparing longitude with the other variables, the plots have entirely overlapping clusters. This indicates that the CLARA method was unable to find great patterns in the data.

Next, I will use a version of a ggplot to plot the clusters.

```
#plotting clara
factoextra::fviz_cluster(clarasamp)
```



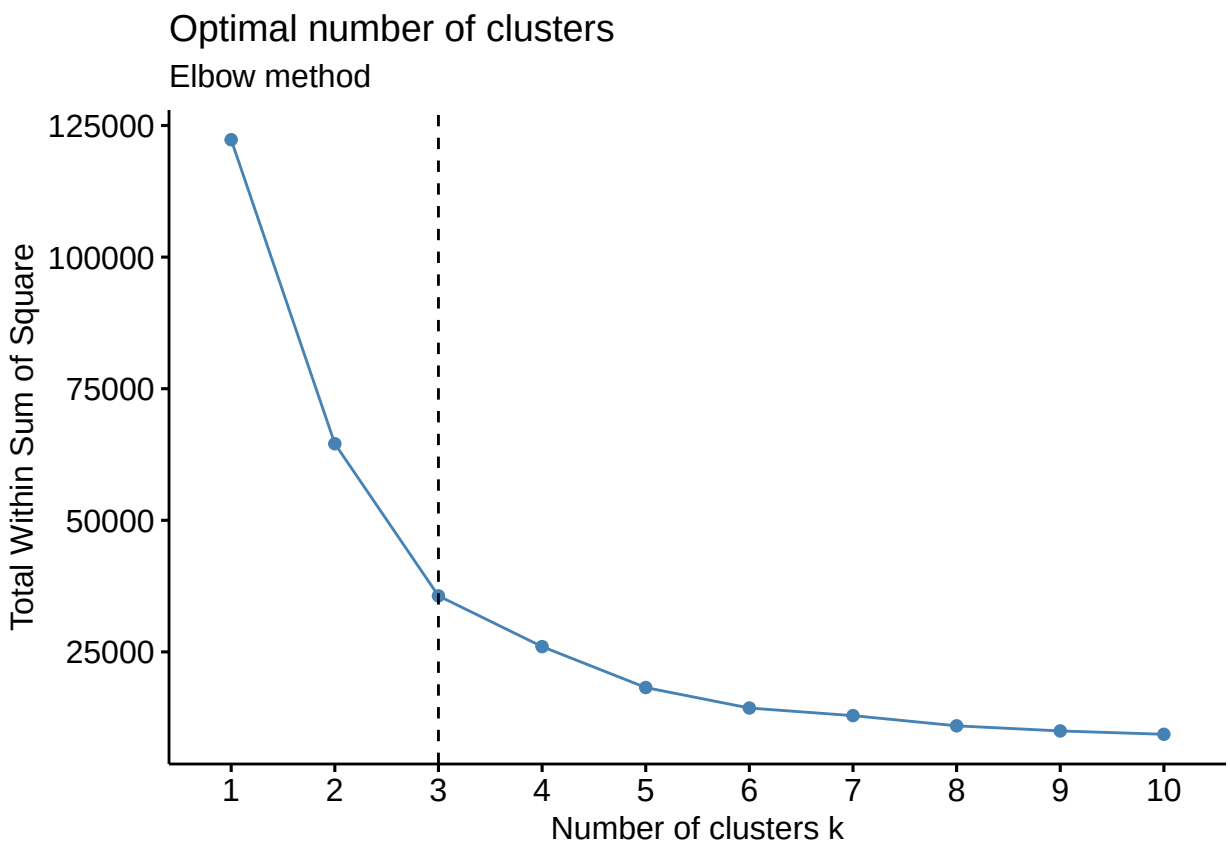
This plot shows the overlapping of the clusters as well.

3.3 Evaluation of CLARA

There are multiple ways to determine the effectiveness of CLARA and the quality of its clusters. One way to internally validate the method, is to look at its within-cluster sum of squares (WSS). If the WSS is high, it is likely the method did not work very well.

I plotted in the previous section in the Elbow method plot to determine the number of clusters to use. Since I decided to use k=3 clusters, I can now go back and calculate the WSS for the method.

```
fviz_nbclust(new, kmeans, method = "wss") +
    geom_vline(xintercept = 3, linetype = 2)+
  labs(subtitle = "Elbow method")
```



The Elbow method when k=3, shows a WSS to be about 35,000. This is very high, which is a concern when interpreting the cluster results.

Another method is to look at the silhouette widths of the clusters. As mentioned in Chapter 1, the Silhouette method helps us determine how many clusters best fits the data. The Silhouette widths of the clusters determine how well an object truly belongs to its assigned cluster.

Based on many experiments and research, a silhouette width of 0.71-1 indicates a strong cluster, 0.51-0.7 indicates a reasonable cluster, 0.26-0.5 indicates a weak or artificial cluster, and less than or equal to 0.25 indicates no cluster found (Ng & Han, 2000).

In this example, the silhouette widths were: 0.422183 for cluster 1, 0.634548 for cluster 2, and 0.172013 for cluster 3. In analyzing these values based on the criteria, cluster 1 is a weak or artificial cluster, cluster 2 is a reasonable cluster, and cluster 3 indicates no cluster found.

The overall evaluation of CLARA with this data is that the algorithm did not work well. The clusters were very weak, therefore, one should not draw conclusions based on the results from this analysis.

3.3.1 Model to Predict Cluster

The CLARA method found three clusters to group the health data. While the WSS value and silhouette widths of the clusters indicated the clustering may not be very accurate or useful, I still want to investigate if I can predict the cluster number (1, 2, or 3), given the health indicator variables. This would be helpful information, if I wanted to categorize a new observation, given its values for the health variables used.

To start this process, I first had to include a variable with cluster number (from the CLARA method) to the original sample of the data set.

```
#adding each data point's cluster #
cluster<- clarasamp$clustering
cluster_data<- cbind(new, cluster)
```

Next, I looked at possible relationships between the health indicator variables and cluster number. To start, I quickly looked at a multivariate linear regression model to predict cluster using all of the possible variables.

```
kitchen_sink<- lm(cluster~., data=cluster_data)
#summary(kitchen_sink)
```

	Estimate	Std. Error	t value	Pr(>|t|)
(Intercept)	0.3835	0.3762	1.02	0.3082
Latitude_tri	-0.0073	0.0065	-1.12	0.2614
Longitude_tri	-0.0393	0.0022	-17.91	0.0000
poor_or_fair_health	10.0890	1.4178	7.12	0.0000
poor_physical_health_days	-1.0820	0.0884	-12.25	0.0000
physical_inactivity	1.9868	0.7307	2.72	0.0067
adult_obesity	0.3328	0.8160	0.41	0.6835

Table 3.1: Kitchen Sink Model

According to this model, *longitude*, *poor_or_fair_health*, *poor_physical_health_days*, and *physical_inactivity* were strong predictors of cluster number. Overall, the model seemed to fit the data fairly well. The model had a high F-statistic and a low p-value of <2e-16. The adjusted R-squared value was 0.372.

In analyzing this model I realized that latitude and longitude were used as quantitative variables instead of categorical. Since multivariate regression predictive models do not use spatial information, I realized that the latitude and longitude would not be helpful.

```
#taking out latitude and longitude
vars <- names(cluster_data) %in% c("Latitude_tri", "Longitude_tri")
cluster_data_new <- cluster_data[!vars]
```

I ran another full multivariate regression model, an updated kitchen sink model, with only the health variables and cluster information.

```
new_kitchen_sink<- lm(cluster~., data=cluster_data_new)
#summary(new_kitchen_sink)
```

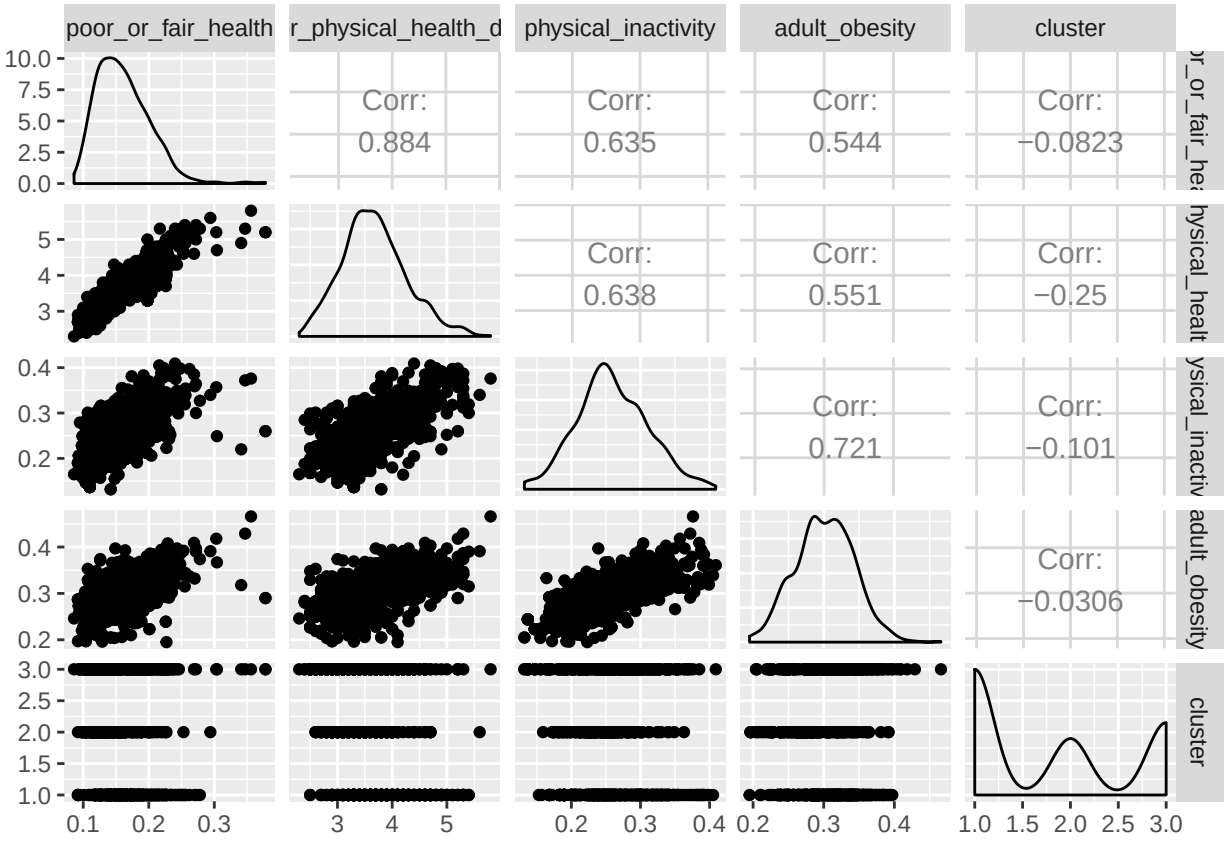
	Estimate	Std. Error	t value	Pr(>|t|)
(Intercept)	3.5366	0.2297	15.40	0.0000
poor_or_fair_health	13.0696	1.3988	9.34	0.0000
poor_physical_health_days	-1.2089	0.0964	-12.54	0.0000
physical_inactivity	-0.9774	0.8086	-1.21	0.2270
adult_obesity	2.8044	0.9247	3.03	0.0025

Table 3.2: Updated Kitchen Sink Model

This model had three significant predictors (*poor_or_fair_health*, *poor_physical_health_days*, and *adult_obesity*), a high F-statistic, and a low p-value of <2e-16. The model did not fit the data very well, and had an adjusted R-squared value of 0.155.

Next, I looked at the possible correlations between cluster number and the health indicator variables. I predicted the healthier people (lower scores on the health indicator variables) would be in cluster 1, while the least healthy people (higher scores on health indicator variables) would be in cluster 3. I also predicted the health indicator variables would be highly correlated with each other, considering they all are aiding in predicting one's health. My predictions were based on the CLARA output from the previous section.

```
ggpairs(cluster_data_new)
```



The correlation matrix shows strong positive correlations between *poor_or_fair_health*, *poor_physical_health_days*, *physical_inactivity*, and *adult_obesity*, as I had predicted. The highest correlation was 0.884, between *poor_physical_health_days* and *poor_to_fair_health*. All of the variables in general show bell-shaped curves with a relatively even shape.

The plots comparing the variables to the cluster number are hard to interpret at first. To start, the *poor_to_fair_health* versus cluster plot shows that the highest values of *poor_or_fair_health* are in cluster 3. These look to be possible outliers, but regardless, it confirms the prediction that the unhealthy people (high health variable scores) are in cluster 3.

The *poor_physical_health_days* versus cluster number and *adult_obesity* versus cluster number show a couple of observations with high health variable scores in cluster 3 as well. Again, it is unclear if these points are outliers or not.

In general, the plots show that cluster 2 has the smallest range of health scores, which further confirms that cluster 2 had the highest quality of clustering (the largest silhouette width). In terms of correlation values, cluster number was shows to be sightly negatively correlated with *poor_physical_health_days*, with a correlation value of -0.25.

I had predicted the correlation to be positive, because the CLARA output revealed cluster 3 to have the most unhealthy people. This would mean the higher the health variable value, the higher the cluster number. Since the correlations are in fact slightly negative, I believe the reason for the higher health value mean score from the CLARA output for cluster 3 was probably due to the outliers (shown in the plots).

All of correlations between the health variables and cluster number were negative, indicating there may be outliers impacting the original analysis of CLARA.

Nevertheless, I will continue to explore possible relationships between health variables and cluster number. Based on the correlation plot, I will explore *poor_or_fair_health* (because of the plot), *poor_physical_health_days* (because of the correlation value), and *adult_obesity* (because of the plot).

I tried numerous combinations of the variables as well as interaction terms, because the variables are so highly correlated. Some examples of the combinations I tried are found in Appendix A.

Most of the models had significant predictors; however, the R-squared values were small; indicating that the models did not fit the data very well.

In comparing adjusted R-squared values and the number of predictors used, the best model ended up being:

```
summary(best_model)
```

	Estimate	Std. Error	t value	Pr(>|t|)
(Intercept)	5.7368	0.3607	15.90	0.0000
poor_physical_health_days	-1.2465	0.0895	-13.92	0.0000
adult_obesity	-4.8119	1.0719	-4.49	0.0000
adult_obesity:poor_or_fair_health	42.1592	4.0394	10.44	0.0000

Table 3.3: Best Model to Predict Cluster

This model uses three predictors and has an R-squared value of 0.1736. The model has a high F-statistic and a low p-value of <2e-16. Ultimately, I chose this model because it has the highest R-squared value in comparison to the other models tested.

Conclusion

In conclusion, clustering methods are very useful for spatial data in determining patterns and in visualizing data sets. There are MANY algorithms out there that analyze spatial data, and these methods continue to grow year to year both in quantity and quality (handling more data and higher complexity data). The methods discussed in this paper are considered partitioning clustering methods. The most popular partitioning clustering method is K-means, which was discussed in comparison to K-medoids. To further dive into K-medoids algorithms, PAM (Partitioning Around Medoids), CLARA (Clustering LArge Applications), and CLARANS (Clustering Large Applications based on RANdomized Search) were explored. This fulfilled my first proposed task: Exposition of spatial clustering methods (describing and explaining), why they are useful, what they tell us, general information, exposition of PAM, CLARA, and CLARANS method.

Data from my STAT 495 project provided an explicit example of the CLARA algorithm. In my STAT 495 project, we were unable to draw conclusions about the health status and location of data observations through mapping visualizations. This lead to my interest in further analyzing the data using clustering algorithms, such as CLARA.

For the application, the Elbow and Silhouette methods were used to determine k clusters, and the CLARA algorithm then divided the objects into clusters. A brief evaluation of the clusters revealed a very high within-cluster sum of squares and low silhouette widths, indicating that the clusters were not of great quality. This section completed my second proposed task: Perform a CLARA analysis on my data or another data set.

In determining whether one could predict an observation's cluster based on a person's health status, multivariate linear regression models were performed. None of the models proved to be very useful; however, the best model ended up being able to predict 17.4% of the variation in the model. The data again didn't seem to have many patterns, which further confirmed the results from my STAT 495 project. This

completed the third and final item on my proposed task list: Perform a model where the cluster is the response variable to determine if we can predict the cluster of an observation based on other variables in the data.

Appendix A

The First Appendix

This first appendix includes all of the R chunks of code that were hidden throughout the document.

In Chapter 1:

```
if(!require(devtools))
  install.packages("devtools", repos = "http://cran.rstudio.com")
if(!require(dplyr))
    install.packages("dplyr", repos = "http://cran.rstudio.com")
if(!require(ggplot2))
    install.packages("ggplot2", repos = "http://cran.rstudio.com")
if(!require(acstats)){
  library(devtools)
  devtools::install_github("Amherst-Statistics/acstats")
}
```

In Chapter 3:

```
#loading in packages
library(readr)
library(factoextra)
library(NbClust)
library(ggplot2)
library(cluster)
library(GGally)
library(knitr)
library(xtable)
options(xtable.comment=FALSE)
```

```
#using data from final stat 495 project
data_subset <- read_csv("CopyOfdata_subset.csv")
```

```
set.seed(2)
#exploring possible relationships between health variables and cluster number

fun1<- lm(cluster~ poor_or_fair_health + poor_physical_health_days + adult_obesity, data
#low adjusted R-squared (0.155), but significant predictors

fun2<- lm(cluster~ poor_or_fair_health, data= cluster_data_new)
fun3<- lm(cluster~ poor_physical_health_days, data= cluster_data_new)
fun4<- lm(cluster~ adult_obesity, data= cluster_data_new)
#low adjusted R-squared, highest of the 3 functions was 0.06

fun5<- lm(cluster~ poor_or_fair_health + poor_physical_health_days + adult_obesity +
            poor_or_fair_health:poor_physical_health_days, data= cluster_data_new)
#added an interaction, raised the adjusted R-squared to 0.165

fun6<- lm(cluster~ poor_or_fair_health + poor_physical_health_days + adult_obesity +
            poor_physical_health_days:adult_obesity, data= cluster_data_new)
#tried a different interaction, about the same adjusted R-squared

fun7<- lm(cluster~ poor_or_fair_health + poor_physical_health_days + adult_obesity +
            poor_or_fair_health:adult_obesity, data= cluster_data_new)
#last combination of an interaction, highest adjusted R-squared yet (0.175)!
#only predictor not significant was poor_or_fair_health

best_model<- lm(cluster~  poor_physical_health_days + adult_obesity +
                  poor_or_fair_health:adult_obesity, data= cluster_data_new)
#dropped poor_or_fair_health, about the same adjusted R-squared (0.174)

fun9<- lm(cluster~ poor_physical_health_days + adult_obesity +
            poor_physical_health_days:adult_obesity, data= cluster_data_new)
#tried a different interaction, low adjusted R-squared (0.0958)

fun10<- lm(cluster~ poor_physical_health_days + adult_obesity +
             poor_or_fair_health:poor_physical_health_days, data= cluster_data_new)
#tried last combination of interaction, adjusted R-squared= 0.166
```

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