Comparison of K-Means, K-Medoids and K-Means++ algorithms based on the Calinski-Harabasz index for COVID-19 epidemic in China

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Abstract. The novel coronavirus spreads from person to person through close contact and respiratory droplets such as coughing or sneezing. Various studies have been conducted globally to deal with COVID-19. However, no cure for the virus has been found, and efficient data processing methods for sudden outbreaks have not yet been identified. This study compares three algorithms for data sets to analyze clustering patterns to determine the best data processing method. The data of this study comes from the Chinese Center for Disease Control and Prevention, including two attributes of confirmed cases and death cases. We selected the data from the initial stage of the outbreak until October 31, 2021. We compared the data analysis and processing results of the clustering of the spread of the new coronavirus in China by the K-Means, K-Medoids and K-Means++ algorithms. By comparing the Calinski-Harabasz index values from K=2 to K=10, the results show that the K-Means, K-Medoids and K-Means++ algorithms have almost the same clustering effect when K does not exceed 6, but when the K value is greater than 6. When the K-Medoids clustering effect is significantly better, therefore, from the three clustering algorithms used, it can be concluded that the best method for clustering the spread of the novel coronavirus outbreak in China is the K-Medoids method. The results of this study provides ideas for future researchers to choose an appropriate cluster analysis method to effectively process the data in the early stages of the epidemic.

Keywords: COVID-19, Calinski-Harabasz, K-Means, K-Medoids, K-Means++.

1. Introduction

1.1. Background

COVID-19 is a disease that causes severe acute respiratory symptoms, which first emerged in Wuhan, China, at the end of 2019 [1] - [2]. From that point forward, travelers facilitated the transmission of the illness to virtually all nations globally, leading the WHO to announce it as a pandemic on March 22nd, 2020. The virus poses a significant risk due to its capability to incite severe symptoms such as respiratory distress, chest discomfort, speech impairment and breathing complications, which can even result in fatalities. Individuals possessing compromised immunity and the aged population are particularly susceptible to this viral contagion and its consequences. The virus propagates swiftly through direct

human interaction and via respiratory particles produced during coughing or sneezing. Numerous research initiatives have been undertaken to combat COVID-19, yet a definitive cure still needs to be discovered.

Various studies have been carried out by both local and foreign researchers, including K-Means Clustering COVID-19 Data [3], Hierarchical Clustering Analysis of COVID-19 Transmission in Wuhan, China[4], Identifying Links Between SARS-CoV-2 Transmission and Clustered Environments[5], Epithelial Cells lining Salivary Gland Ducts are Early Target Cells of Severe Acute Respiratory Syndrome Coronavirus Infection in The Upper Respiratory Tracts of Rhesus Macaques[6], Therapeutic and Triaging Strategies for 2019 Novel Coronavirus Disease in Fever Clinics[7]. This study distinctively utilizes three comparative methods - the K-Means, K-Medoids and K-Means++ algorithms - for clustering the spread of COVID-19 in China, differentiating it from the methodologies employed in prior research.

1.2. Materials and data

According to the data updated on the Netease News Epidemic Report [8] page as of December 28, 2022, the total number of confirmed cases worldwide is 624,398,550, and the death toll is 6,618,427, accounting for 10.6% of the confirmed cases. The total number of confirmed cases in China is 9,006,774, and the death toll is 31,509, accounting for 0.350% of the number of confirmed cases. The data from the Chinese Center for Disease Control and Prevention page[9] retrieved on October 31st, 2021, from 34 provinces, municipalities, and autonomous regions in China is chosen in this research, including confirmed and death cases. This research conducts a head-to-head comparison of three algorithms using a dataset to investigate grouping patterns and identify the most effective algorithms for data manipulation. The results of this study provide insights for future researchers on effectively utilizing cluster analysis to handle early-stage data of epidemic spread.

In this examination, we utilized MATLAB. Additionally, the Calinski-Harabasz index value was employed for reference in clustering. The resultant clustering pattern allowed for data analysis, transforming it into fresh information. This can assist those in decision-making roles (stakeholders) in curtailing the proliferation of the coronavirus and reducing the count of individuals confirmed as COVID-19 positive. Furthermore, this method may yield the optimal algorithm from the validity testing on K-Means, K-Medoids and K-Means++.

2. Method

Clustering analysis is a highly active research field in data mining, with numerous algorithms proposed. These algorithms can be categorized into partitioning algorithms, hierarchical, density-based, network-based, and model-based methods[10].

The method applied to analyze the spread of the coronavirus in China using K-Means, K-Medoids and K-Means++ algorithms, as portrayed in **Figure 1**, involves numerous steps during its execution.

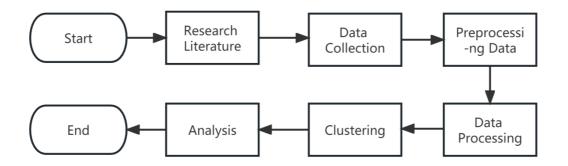


Figure 1. Research Methodology

2.1. Data mining

Data mining is extracting valuable patterns and knowledge from large datasets. As described by Witten and Frank [11], it involves various techniques such as clustering, classification, and association rule mining. These techniques are used to discover hidden patterns and relationships in the data, which can be used for decision-making and prediction. Data mining has applications in various fields like marketing, healthcare, and finance, where it helps identify trends, customer behavior, and fraud detection [11].

2.2. K-Means algorithm

The K-Means algorithm is a popular unsupervised machine learning method for clustering data. It aims to partition a given dataset into K distinct clusters, where each data point belongs to the cluster with the closest mean value. The algorithm iteratively updates the centroids of the clusters until convergence. According to Mitchell, T. M. (1997)[12], K-Means is based on minimising the within-cluster variance. On the other hand, Lloyd, S. P. (1982)[13] introduced the original algorithm that iteratively assigns data points to their closest cluster centroid.

The K-Means algorithm is a commonly used clustering technique. It aims to partition a dataset into K clusters, where each data point belongs to the cluster with the nearest mean. The algorithm follows a simple formula:

1. Initialize K cluster centroids randomly.

2. Assign each data point to the cluster with the closest centroid based on Euclidean distance.

3. Update the centroids by computing the mean of all data points in each cluster.

4. Repeat steps 2 and 3 until convergence when the cluster assignments no longer change significantly.

The K-Means algorithm process is shown in the Figure 2.

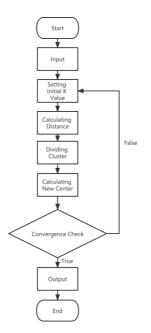


Figure 2. K-Means Algorithm Process

2.3. K-Medoids algorithm

The K-Medoids algorithm is a popular data mining and pattern recognition clustering technique. It is a variation of the K-Means algorithm that uses medoids (representative objects) instead of means to determine the cluster centroids. According to [14], the K-Medoids algorithm was first introduced by Kaufman and Rousseeuw in 1987. They proposed a method to find robust medoids, data points that

minimize the sum of dissimilarities within a cluster. The algorithm iteratively replaces a medoid with a non-medoid point in order to reduce the total dissimilarity in the cluster. In a more recent study by Park et al. [15], an improved version of the K-Medoids algorithm was proposed, known as the Partitioning Around Medoids (PAM) algorithm. This variant utilizes a more efficient pairwise update approach, which reduces the computational complexity while maintaining the accuracy of the clustering results.

The K-Medoids algorithm is a clustering technique that aims to partition a given dataset into k clusters. Unlike the K-Means algorithm, which uses the mean of a cluster as its centroid, the K-Medoids algorithm employs the medoid. The medoid is the data point that minimizes the sum of distances to all other points within the cluster. By iteratively updating the medoids and reassigning data points to clusters, the algorithm converges to a solution that optimizes the overall clustering objective.

Overall, the K-Medoids algorithm and its variants have been widely applied in various fields such as image analysis, bioinformatics, and recommendation systems due to their ability to handle non-numeric data and outliers effectively.

2.4. *K*-Means++ algorithm

The K-Means++ algorithm is an improved version of the K-Means clustering algorithm, widely used in data mining and machine learning. It was introduced by David Arthur and Sergei Vassilvitskii in their research paper titled "K-Means++: The Advantages of Careful Seeding"[16], published in 2007. The algorithm addresses the issue of initialization bias in the original K-Means algorithm by introducing a more thoughtful and deliberate method to select initial cluster centroids. According to the paper, the algorithm improves the convergence speed and achieves better clustering results. Another critical research paper that references the K-Means++ algorithm is "Scalable K-Means++" by Bahman Bahmani, Benjamin Moseley, Andrea Vattani, Ravi Kumar, and Sergei Vassilvitskii[17] published in 2012. This paper explores scalable implementations of the K-Means++ algorithm, making it applicable to large-scale datasets and improving efficiency.

The algorithm consists of the following steps:

1. Randomly select the first centroid from the given data points.

2. For each remaining data point, calculate the shortest distance (D) to the nearest centroid from the current set of centroids.

- 3. Choose a new centroid with a probability proportional to D^2 .
- 4. Repeat steps 2 and 3 until k centroids are selected.
- 5. Perform the standard K-Means algorithm using the initialized centroids.

2.5. Calinski-Harabasz index

Calinski-Harabasz is a popular index used for evaluating the quality and effectiveness of clustering algorithms. It measures the degree of separation between different clusters and the compactness within each cluster. The index is calculated by taking the between-cluster dispersion to within-cluster dispersion ratio.

In a study by Calinski and Harabasz (1974)[18], they introduced this index as an alternative to other clustering validity indices. They highlighted that the strength of Calinski-Harabasz lies in its ability to handle datasets with varying cluster sizes and densities. Another research conducted by Nguyen et al. (2017)[19] demonstrated the usefulness of Calinski-Harabasz in the field of image segmentation. By applying this index to evaluate different clustering algorithms, they were able to identify the most effective one for accurately segmenting images.

3. Data processing and analysis

3.1. Steps in data pre-processing

This study utilized data obtained from the Chinese Center for Disease Control and Prevention page on October 31, 2021. The data set includes confirmed and fatal cases across 34 provinces, municipalities,

and autonomous regions in China. Then the data pre-processing stage is carried out before running the clustering process of some of the attributes used. The data is shown in **Table 1**.

	Cumulative	Cumulative	Population	Millions of	Million	Infection
Region	Infection	Death	(Ten Thousand)	People Infected	Deaths	Lethality
Hong Kong	12346	213	743	1661.64	28.668	1.73%
Hubei Province	68309	4512	5902	1157.39	76.449	6.61%
Taiwan Province	16412	847	2369	692.78	35.753	5.16%
Aomen	77	0	63	122.22	0.000	0.00%
Shanghai	2726	7	2418	112.74	0.289	0.26%
Beijing	1162	9	2171	53.52	0.415	0.77%
Heilongjiang Province	1768	13	3789	46.66	0.343	0.74%
Xinjiang Province	981	3	2445	40.12	0.123	0.31%
Fujian Province	1303	1	3911	33.32	0.026	0.08%
Yunnan Province	1563	2	4801	32.56	0.042	0.13%
Tianjin	504	3	1557	32.37	0.193	0.60%
Guangdong Province	3224	8	11169	28.87	0.072	0.25%
Zhejiang Province	1484	1	5657	26.23	0.018	0.07%
Nei Monggol province	594	1	2529	23.49	0.040	0.17%
Jilin Province	577	3	2717	21.24	0.110	0.52%
Hainan Province	190	6	926	20.52	0.648	3.16%
Jiangxi Province	939	1	4622	20.32	0.022	0.11%
Jiangsu Province	1600	0	8029	19.93	0.000	0.00%
Chongqing	604	6	3048	19.82	0.197	0.99%
Shaanxi Province	697	3	3835	18.17	0.078	0.43%
Hebei Province	1323	7	7520	17.59	0.093	0.53%
Hunan Province	1197	4	6860	17.45	0.058	0.33%
Henan Province	1559	22	9559	16.31	0.230	1.41%
Anhui Province	1008	6	6255	16.12	0.096	0.60%

Table 1. Dataset for the spread of COVID-19 in China

Ningxia Province	107	0	682	15.69	0.000	0.00%
Sichuan Province	1222	3	8302	14.72	0.036	0.25%
Gansu Province	295	2	2626	11.23	0.076	0.68%
Liaoning Province	466	2	4369	10.67	0.046	0.43%
Shandong Province	978	7	10006	9.77	0.070	0.72%
Shanxi Province	260	0	3702	7.02	0.000	0.00%
Guangxi Province	338	2	4885	6.92	0.041	0.59%
Guizhou Province	158	2	3580	4.41	0.056	1.27%
Qinghai Province	22	0	598	3.68	0.000	0.00%
Xizang Province	1	0	337	0.30	0.000	0.00%

Table 1. (continued).

3.2. Steps of data processing

The purpose of this research is to compare which algorithms are best among K-Means, K-Medoids and K-Means++ in clustering data on the spread of the COVID-19 disease in China in clusters 1 to cluster 10. There is the clustering process using these three algorithms, which in the next stage of this research is to determine the best number of clusters with MATLAB as presented on the Calinski-Harabasz index. This processing can be done to find the Calinski-Harabasz index value of each algorithm in each group. Then the test process is carried out from clusters k = 2 to k = 10. To mitigate the error caused by randomness, this study relies on repeated runs and statistical analysis. Each run records the optimal clustering result and its corresponding evaluation metric, and then the average is taken as the final evaluation metric. Generally, this approach yields more stable results and better reflects the true performance of the algorithm. Furthermore, the results of the Calinski-Harabasz index comparison can be shown in **Figure 3**.

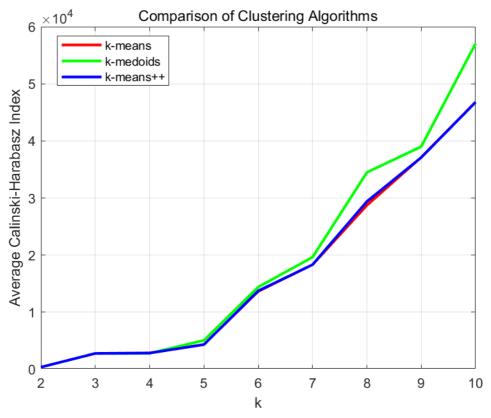


Figure 3. Comparison of K-Means, K-Medoids and K-Means++ algorithm

Furthermore, it can be seen that the test results in each cluster using K-Means, K-Medoids and K-Means++ algorithm methods can be seen in **Table 2**.

K	K-Means	K-Medoids	K-Means++
2	0.03775	0.03775	0.03775
3	0.27823	0.27823	0.27823
4	0.28533	0.27841	0.28452
5	0.40452	0.506504	0.43211
6	1.36308	1.44018	1.37944
7	1.83770	1.96425	1.84381
8	2.92399	3.45595	2.94865
9	3.73776	3.90274	3.71083
10	4.73572	5.74596	4.72021

Table 2. Results of the Calinski-Harabasz index comparison

3.3. Analysis

After previously making comparisons through the Calinski-Harabasz index using the K-Means, K-Medoids and K-Means++ algorithm methods, We can clearly see that when the value of K does not exceed 6, the clustering results of the three algorithms are not significantly different. Therefore, it can be concluded that they have similar capabilities in processing data from the initial stage of the COVID-19 outbreak in China. However, as the value of K increases, the superiority of the K-Medoids algorithm becomes evident. It can be considered that the K-Medoids algorithm is superior to K-Means and K-Means++ when K is large. Similarly, to reduce the error caused by randomness, the statistical average

of multiple runs is still taken as the conclusion. Based on the analysis results, the best cluster then interprets the data clustering of the spread of COVID-19, and the results can be obtained in **Table 3**.

Cluster	Number	Region
1	0	itegion
1	0	Ush si Dessie sa
2	1	Hubei Province
3	0	
4	2	Hong Kong, Taiwan Province
5	0	
6	22	Aomen,Shanghai, Heilongjiang Province, Yunnan Province, Tianjin, Guangdong Province, Zhejiang
7	9	Beijing, Xinjiang Province, Fujian Province, Jiangxi Province, Hebei Province, Hunan Province, Anhui Province, Sichuan Province, Shandong Province
8	0	
9	0	
10	0	

Table 3. The best cluster results based on K-Medoids algorithm

4. Conclusion and Discussion

In conclusion, the K-Means, K-Medoids, and K-Means⁺⁺ algorithms have emerged as important clustering algorithms in data mining and have proven to be valuable tools in solving practical problems. This study focused on the initial stage of the COVID-19 outbreak in 34 provinces, autonomous regions, and municipalities in China, and compared the performance of these algorithms in clustering analysis. The analysis results indicated that these three algorithms produced similar clustering results when the value of K is not large. However, when K becomes large, the K-Medoids algorithm outperformed the other two algorithms by yielding more effective clustering. This finding implies that the K-Medoids algorithm is well-suited for large-scale data analysis, particularly in situations where the number of clusters needs to be relatively high.

The significance of this conclusion lies in its potential contribution to future researchers who may be analyzing similar data. By identifying the most effective algorithm for clustering analysis during the initial stage of the COVID-19 outbreak, researchers can adopt the K-Medoids algorithm to obtain more accurate and meaningful insights. This can lead to better decision-making and resource allocation in managing the pandemic.

However, it is important to acknowledge the limitations of this study. Firstly, the analysis was restricted to the number of confirmed cases and deaths, which may not capture the full complexity of the COVID-19 outbreak. Future research should consider incorporating additional variables, such as demographic factors, economic indicators, and healthcare infrastructure, to gain a more comprehensive understanding of the outbreak. Secondly, this study focused solely on the initial stage of the COVID-19 outbreak in China. The findings may not be directly applicable to other countries or different stages of the pandemic. Therefore, it is crucial for future research to replicate and expand upon this study in diverse contexts to validate the generalizability of the conclusions. Thirdly, while the three algorithms were evaluated based on their clustering performance, there are other aspects that could be considered for comparison, such as computational efficiency and scalability. Future studies could explore these dimensions to provide a more comprehensive assessment of the algorithms. In light of these limitations, future research should aim to address these gaps and address the broader implications of clustering analysis in understanding and managing public health crises like COVID-19. By incorporating a wider range of variables, examining different stages of the outbreak, and evaluating various aspects of the algorithms, researchers can strengthen the knowledge base and provide more robust insights for decision-makers. Hopefully, in future research, we can focus on solving the above problems.

To summarize the above, the K-Means, K-Medoids, and K-Means++ algorithms have demonstrated their significance in clustering analysis during the initial stage of the COVID-19 outbreak. The K-Medoids algorithm has shown superior performance when the number of clusters is large. However, further research is needed to overcome the limitations of this study and explore the broader implications of clustering analysis in public health crises. This study serves as a foundation for future researchers and highlights the potential for using clustering algorithms to inform decision-making and resource allocation in managing pandemics.

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