Evaluating Clustering Techniques on Non-elliptical Data

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1 Background and Objective

Latent Class Analysis and K-means are two successful clustering algorithms that partition the given data into distinct subgroups where observations in each group are very similar. They are popular choice of method in solving healthcare research problems such as identifying clusters on microscopic images (Amin et al. 2015), categorizing suicides by risk factors (Logan, Hall, and Karch 2011), and grouping elderly patients with their access to health care (Thorpe et al. 2011). One important assumption that both of these algorithms require is the normality of the given data.

In our project, we focus on the unsupervised learning scenario and we investigate how well these two algorithms perform when the normality assumption is violated. We designed 4 simulation settings as violation of the normality assumption: 1) skewed data, 2) data with heavy tail, 3) data with outliers, 4) multimodal data. In the end, we compare their performance with Rand Index in each settings with varying sample sizes.

2 Statistical Method

2.1 K Means

K-means clustering is a popular clustering algorithm that partitions data into a prespecified number of clusters. The goal for k-means is to find clusters such that the total within-cluster variation is minimized. Formally, the within-cluster variation is defined as follows:

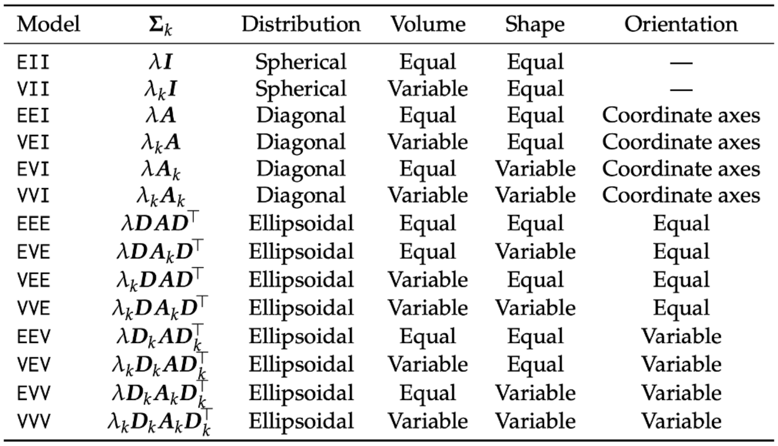
$$tot.withinss = \sum_{i=1}^{k} W(C_k) = \sum_{i=1}^{k} \sum_{x \in c_k} (x_i - \mu_k)^2$$

A general procedure of the k-means algorithm can be described as follows:
(1) Specify number of clusters k.
(2) Assign each observation to their closest centroid, minimizing $W(C_k)$.
(3) For each cluster, update the cluster centroid by calculating the new mean values of all the data points in the cluster. The centroid of a K_{th} cluster is a vector of length p containing the means of all variables.
(4) Iteratively minimize the total within sum of square. That is, iterate steps 3 and 4 until the cluster assignments stop changing or the maximum number of iterations is reached.

Specifying the number of clusters is a crucial step for the K means algorithms. There are multiple ways to determine the optimal number of clusters for k-means. In this project, we use the average silhouette method, which provides a measure of the similarity of an object is to its own cluster compared to other clusters. This method chooses the optimal number of clusters k that maximized the average silhouette.

2.2 Latent Class Analysis

In contrast to K means algorithm which uses a distance based criteria, LCA is a model-based clustering approach that derives clusters using a Gaussian finite mixture modeling that describes distribution the data. We use the R package **mclust** for this task which allows a wide range of parameterizations of the data as shown in figure 1(Scrucca et al. 2016).



Model	$\boldsymbol{\Sigma}_k$	Distribution	Volume	Shape	Orientation
EII	$\lambda \boldsymbol{I}$	Spherical	Equal	Equal	—
VII	$\lambda_k \boldsymbol{I}$	Spherical	Variable	Equal	—
EEI	$\lambda \boldsymbol{A}$	Diagonal	Equal	Equal	Coordinate axes
VEI	$\lambda_k \boldsymbol{A}$	Diagonal	Variable	Equal	Coordinate axes
EVI	$\lambda \boldsymbol{A}_k$	Diagonal	Equal	Variable	Coordinate axes
VVI	$\lambda_k \boldsymbol{A}_k$	Diagonal	Variable	Variable	Coordinate axes
EEE	$\lambda \boldsymbol{D}\boldsymbol{A}\boldsymbol{D}^{\top}$	Ellipsoidal	Equal	Equal	Equal
EVE	$\lambda \boldsymbol{D}\boldsymbol{A}_k\boldsymbol{D}^{\top}$	Ellipsoidal	Equal	Variable	Equal
VEE	$\lambda_k \boldsymbol{D}\boldsymbol{A}\boldsymbol{D}^{\top}$	Ellipsoidal	Variable	Equal	Equal
VVE	$\lambda_k \boldsymbol{D}\boldsymbol{A}_k\boldsymbol{D}^{\top}$	Ellipsoidal	Variable	Variable	Equal
EEV	$\lambda \boldsymbol{D}_k\boldsymbol{A}\boldsymbol{D}_k^{\top}$	Ellipsoidal	Equal	Equal	Variable
VEV	$\lambda_k \boldsymbol{D}_k\boldsymbol{A}\boldsymbol{D}_k^{\top}$	Ellipsoidal	Variable	Equal	Variable
EVV	$\lambda \boldsymbol{D}_k\boldsymbol{A}_k\boldsymbol{D}_k^{\top}$	Ellipsoidal	Equal	Variable	Variable
VVV	$\lambda_k \boldsymbol{D}_k\boldsymbol{A}_k\boldsymbol{D}_k^{\top}$	Ellipsoidal	Variable	Variable	Variable

Figure 1: Parameterisations of the within-group covariance matrix for multidimensional data available in the mclust package, and the corresponding geometric characteristics.

LCA uses finite mixture modeling for parameter estimation, which is crucial to determining the number of components. A variety of approaches can be used to estimate the component number and in this project, we utilize the Bayesian Information Criterion (BIC) for this task. BIC is one of the popular choice for model selection in the context of Gaussian Mixture Modeling. It takes on a penalized forms of the log-likelihood where a penalty term for the number of estimated parameters is subtracted from the log-likelihood. Formally,

$$BIC_{M,G} = 2l_{M,g}(X|\hat{\Psi}) - v\log(n)$$

where $l_{M,g}(X|\hat{\Psi})$ is the log-likelihood at the MLE $\hat{\Psi}$ for model M with G components, n is the sample size, and v is the number of estimated parameters The pair M, G which maximizes $BIC_{M,G}$ is selected as the final model.

3 Performance Metric

We use the Rand index as our performance metric in this study. It is used to compare the similarity of results between two different clustering methods. In our case, we compare our k-means or LCA clustering results to the true clustering that we have defined through our data generation.

Given a set of n elements $S = \{o_1, \ldots, o_n\}$ and two partitions of S to compare, $X = \{X_1, \ldots, X_r\}$, and $Y = \{Y_1, \ldots, Y_s\}$ we denote a as the number of times a pair of elements belongs to the same cluster across two clustering methods. And we denote b as the number of times a pair of elements belong to different clusters across the two methods. Finally, the Rand index is

$$R = \frac{a+b}{\binom{2}{n}},$$

which measures the proportion of agreement of two clustering methods in all unordered pairs.

4 Simulations Settings and Results

In simulations, we consider bivariate data with 2 true clusters. We generated data from different non-elliptical distributions in each setting.

For each simulation setting, we create 100 runs using randomly generated data sets in size of 500, 1000, 5000 and evaluate the Rand index for each method.

4.1 Skewed Data

4.1.1 Data Generation

In this setting, we want to test the performance of K-means and LCA when all features follow a skewed distribution. We assume the features X_1, X_2 are independent.

All data in the first feature $X_{11}, X_{12}, ..X_{1N}$ are random draws from a mixture model of Weibull distributions with density $0.5f_1(x|1,5) + 0.5f_2(x|12,14)$ where $f_1 \sim Weibull(1,5)$ and $f_2 \sim Weibull(12,14)$.

Similarly, all data in the second feature $X_{21}, X_{22}, ..X_{2N}$ are random draws from another mixture model of Weilbull distributions with density $0.5f_3(x|1,3) + 0.5f_4(x|1,4)$ where $f_3 \sim Weibull(1,3)$ and $f_4 \sim Weibull(1,4)$.

We generate 2 equal-sized clusters with total size being 500, 1000 and 5000. An example of a sample with size 5000 is shown below.

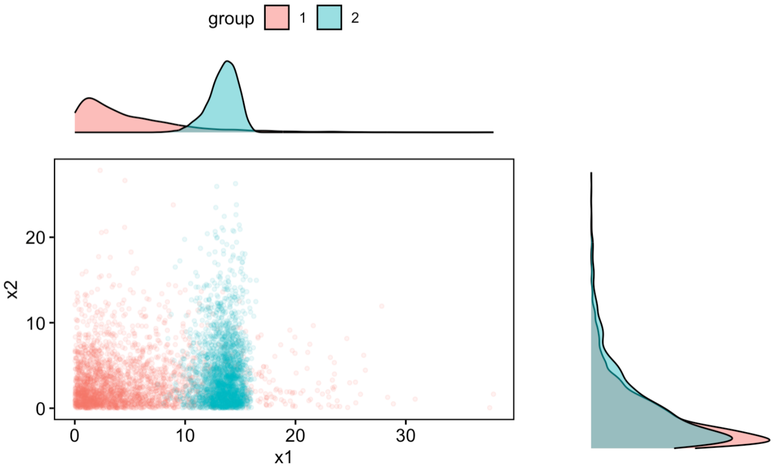


Figure 2: Skewed Data Sample

4.1.2 Results

We are interested in how well K-means and LCA perform when the input data already has two true clusters. We calculate Rand Index for sample data in each simulation run and conclude that after 100 simulations, K-means performs better than LCA across all sample sizes. As sample size increases, the variance of Rand Index decreases.

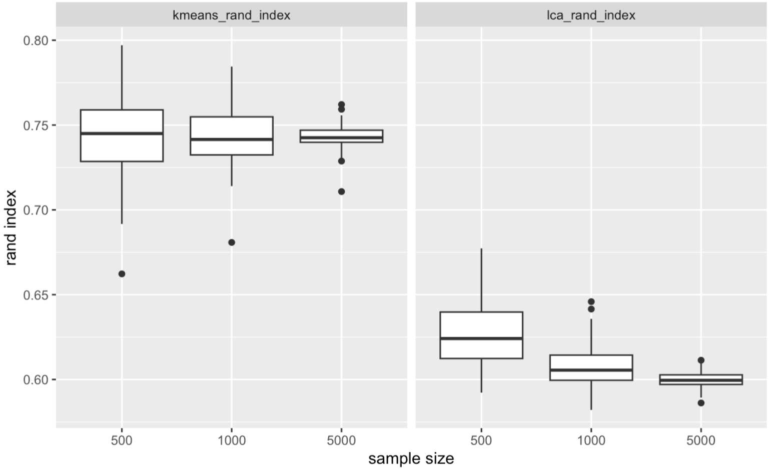


Figure 3: Skewed Data Comparison - Rand Index

To investigate some potential reasons behind this, we compare the optimal number of cluster number for each method in all simulations. Choosing the optimal cluster number is the first step for both methods. This number is crucial to our comparison because we predetermined the number of true clusters to be 2 and Rand Index uses the number of agreements in its calculation. Therefore, having a cluster number that is larger than 2 could hurt the performance.

In this figure, we compare the optimal number of clusters. Overall, K-means choose its optimal number of cluster around 3 which is much lower than that of LCA across all sample sizes. As sample size increases, the optimal number of cluster increases for LCA as well.

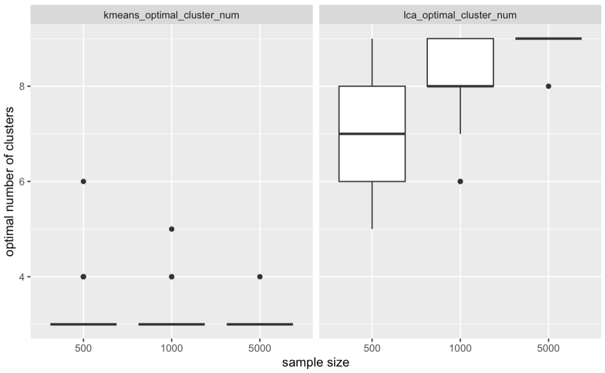


Figure 4: Skewed Data Comparison - Optimal Number of Clusters

4.2 Multimodal Data

4.2.1 Data Generation

In this setting, we have two independent variables X and Y, which both follow the same bimodal mixture distribution. Variables X and Y can each be partitioned into two parts, $\{X_1, X_2\}$ and $\{Y_1, Y_2\}$, where X_1, Y_1 are drawn from one bimodal distribution and X_2, Y_2 are drawn from a different bimodal distribution, as specified below.

$$X_1, Y_1 \sim \begin{cases} N(-3, \frac{3}{4}) & w/\ prob.\ 0.5 \\ N(0, \frac{3}{4}) & w/\ prob.\ 0.5 \end{cases}$$

$$X_2, Y_2 \sim \begin{cases} N(3, \frac{3}{4}) & w/\ prob.\ 0.5 \\ N(6, \frac{3}{4}) & w/\ prob.\ 0.5 \end{cases}$$

Since each bimodal distribution is a mixture of two Gaussian distributions, these data follow a Gaussian mixture distribution, leading to four distinct latent clusters. This can be seen in the figure below, which graphs an example dataset on X and Y axes and colors the data points by cluster.

Since this is a mixture Gaussian case, we should expect LCA to perform very well since it assumes mixture Gaussian data. K-mean should also perform well, since k-means is proven to identify cluster in normal data well.

4.2.2 Results

We found that the median Rand index for 100 runs using k-means with sample size $n = 500$ was 0.99 (IQR: 0.17) while for LCA it was 1 (IQR: 0). For sample size was $n = 1000$ the median Rand index for k-means was 0.99 (IQR: 0.25) and for LCA it was 1 (IQR: 0). For sample size $n = 5000$ the median Rand index for k-means was 1 (IQR: 0) and it was the same for LCA. These results are visualized below and show that k-means and LCA both perform almost perfectly in this case, with LCA performing better when the sample size is smaller. Variation from a Rand index of 1 (i.e., perfect classification) comes in only when k-means or LCA algorithms do not choose the correct number of clusters initially.

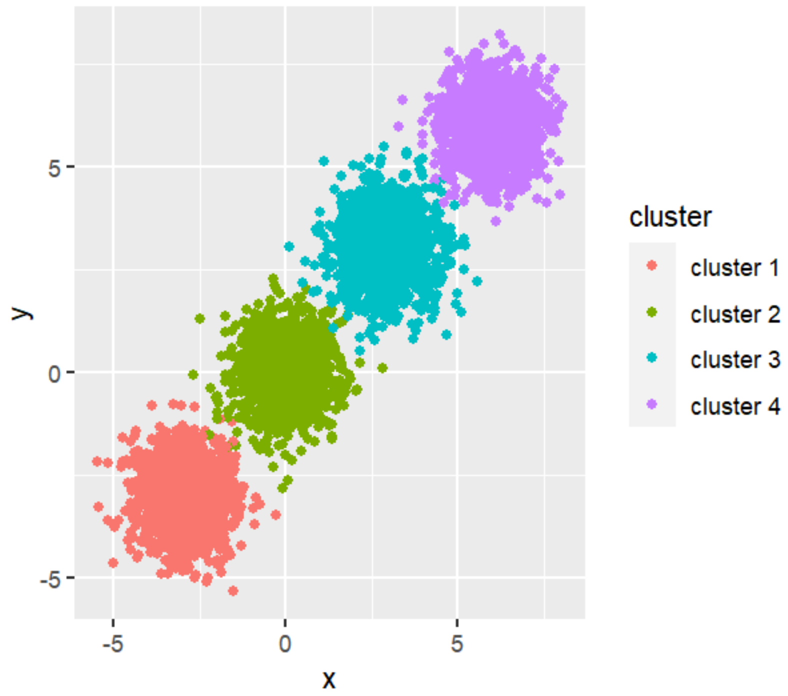


Figure 5: Mutlimodal Data - Latent Clusters

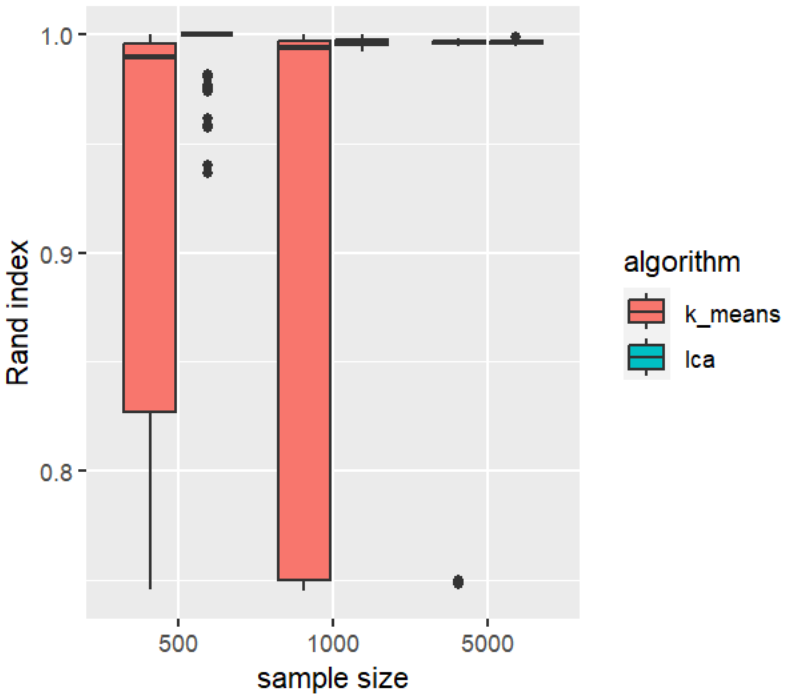


Figure 6: Mutlimodal Data - Results

4.3 Heavy Tails Data

4.3.1 Data Generation

To investigate the algorithm performance in the heavy tails data setting, we consider generating data from a mixture of the Cauchy distribution with two latent clusters. Specifically, we sample $X_{1i}, i = 1...N$ from a mixture of Cauchy distribution $\lambda_1 f_1 + \lambda_2 f_2$ where $f_1 \sim \text{Cauchy}(-3, 3), f_2 \sim \text{Cauchy}(3, 0.5)$ and we set the mixing weights $\lambda_1 = \lambda_2 = 0.5$ corresponding to the latent cluster $1, 2$. We further sample X_{2i} from an independent Gaussian distribution $\text{N}(0, 1)$.

We first examine the generated data via scatter plot and the density plot where the two colors denote two latent clusters. By a direct observation of these plots, we notice the two latent clusters are not easily separated.

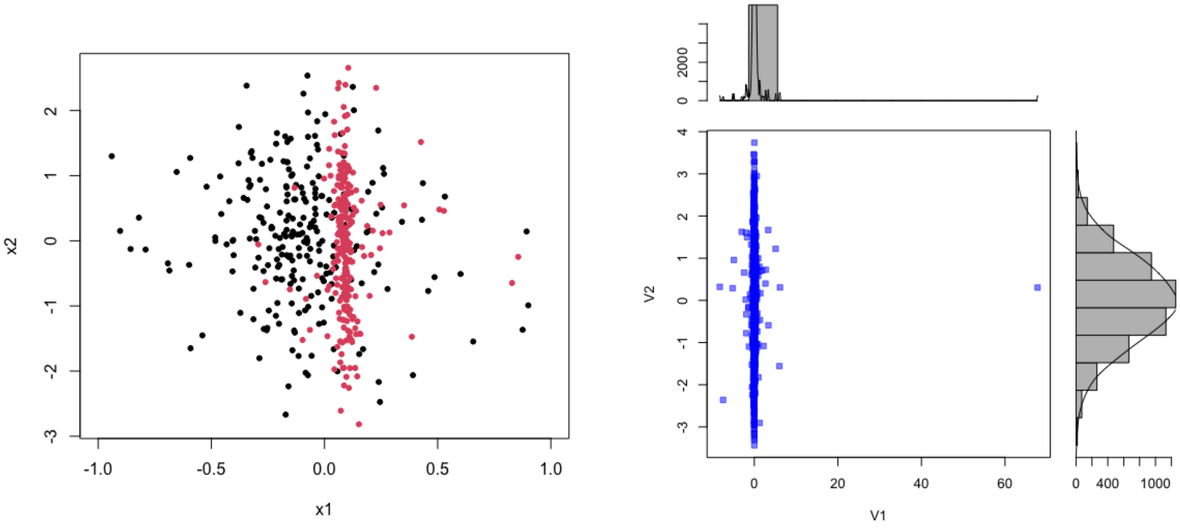


Figure 7: Scatter and density plot for the mixture of Cauchy distribution

4.3.2 Results

We examine the model performance of K means and LCA via 100 runs of simulation with sample sizes $N = 500, 1000, 5000$ using Rand index. We observe that in all our simulation settings, LCA performed better than K means in terms of Rand index. As sample size increases, LCA performed worse.

4.4 Prsence of Outliers

4.4.1 Data Generation

Finally, we investigate the scenario where there exits outliers in the data. We first generate $X_{1i}, i = 1, ..., N$ from a mixture of Gaussian distribution $\lambda_1 f_1 + \lambda_2 f_2$ where $f_1 \sim \text{N}(0, 1), f_2 \sim \text{N}(3, 1)$ and we set the mixing weights $\lambda_1 = \lambda_2 = 0.5$ corresponding to the latent cluster $1, 2$. We further sample X_{2i} from an independent Gaussian distribution $\text{N}(0, 1)$. We then generate outliers ϵ from $\text{N}(30, 1), \text{N}(-30, 1)$ and $\epsilon' s$ are added to X_1 with equal probabilities of 0.05 generated from $\text{bernouli}(0.05)$.

Similarly, we examine examine the generated data via scatter plot and the density plot where the two colors denote two latent clusters.

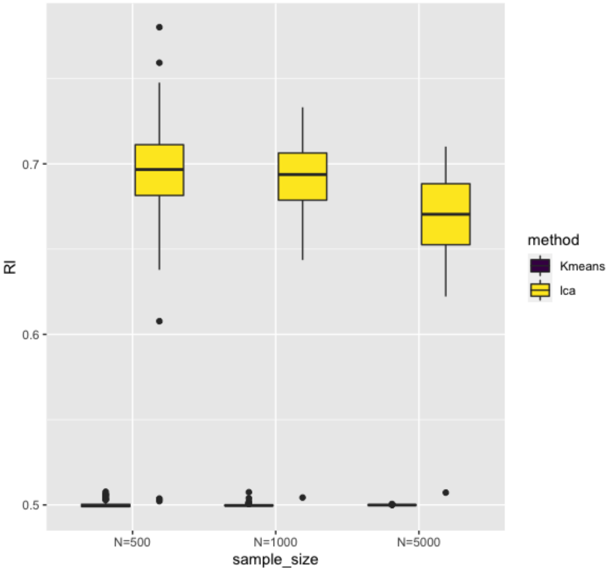


Figure 8: Boxplot of Rand Index for the mixture of Cauchy distribution

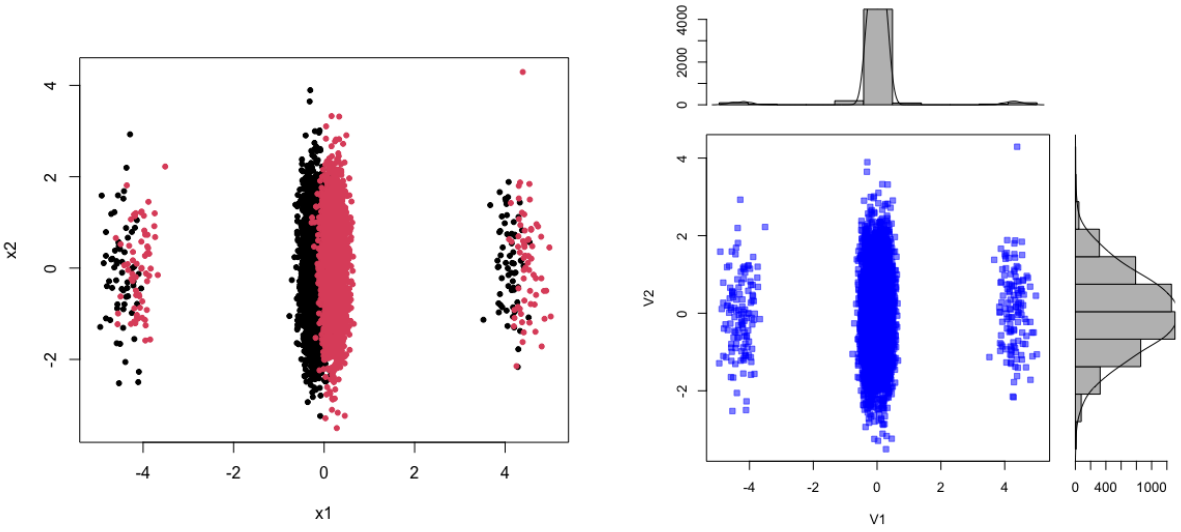


Figure 9: Scatter and density plot for data with Gaussian outlier

4.4.2 Results

Similarly, performance of K means and LCA via is examinined 100 runs of simulation with sample sizes $N = 500, 1000, 5000$ using Rand index. We observe that in all our simulation settings, LCA performed better than K means in terms of Rand index.

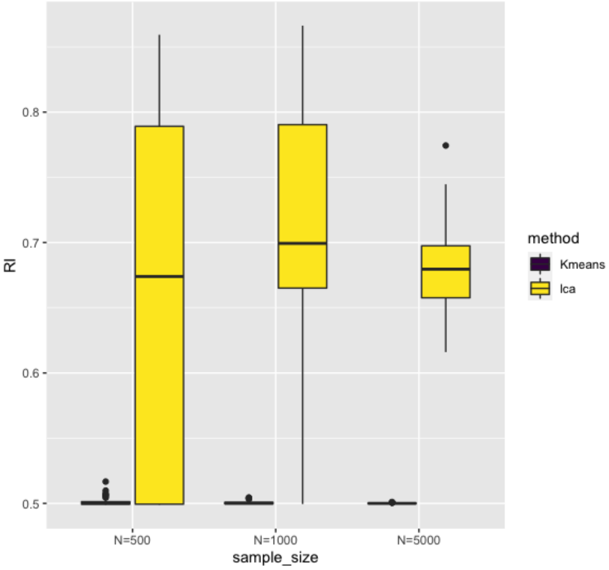


Figure 10: Boxplot of Rand Index for data with Gaussian outlier

5 Discussion

5.1 Conclusion

In conclusion, we found that for skewed data, k-means performs better than LCA. However, in all other cases, LCA outperformed k-means, except in the case where the data follows a Gaussian mixture distribution and the sample size of the dataset is very large, in which case k-means and LCA perform similarly.

5.2 Limitations

In this study, we found that there is no uniformly best algorithm for identifying latent clusters in data. This leads us to believe that knowing how the data is generated is important for deciding whether to use k-means or LCA. However, this information is rarely known.

We also found that variation in correct classification for both algorithms often comes from choosing the number of clusters. There are many ways to choose the number of clusters before actually performing the clustering algorithm. Varying these methods goes beyond the scope of this study, but future research should test k-means against LCA under different cluster number selection techniques.

In summation, we suggest that researchers make informed speculations about the shape and potential number of latent clusters in their data before running either k-means or LCA in order to get the best results.

6 References

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