An efficient clustering algorithm from the measure of local Gaussian distribution

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In this paper, I will introduce a fast and novel clustering algorithm based on Gaussian distribution and it can guarantee the separation of each cluster centroid as a given parameter, \( d_s \). The worst run time complexity of this algorithm is approximately \( \sim O(T \times N \times \log(N)) \) where \( T \) is the iteration steps and \( N \) is the number of features.

I. INTRODUCTION

Clustering algorithms have many applications\(^\text{12}\) to the unsupervised and semisupervised learning. They help classify data sets into clusters within few given parameters. Potentially, it can be applied to many different domains such as image analysis, object tracking, data compression, physical/chemical structure optimization problems, to name a few. Some cluster algorithms (e.g. K-means\(^\text{3}\) and Gaussian-Mixture\(^\text{4}\)) require the knowledge of number of clusters as input parameters, and some others (e.g. Dbscan\(^\text{5}\), Hdbscan\(^\text{6}\)) require a distance cut-off threshold to separate clusters. Each clustering algorithm has its own pros and cons and its own domain for different applications. My goal in this paper is to invent a new clustering algorithm which has the following properties:

- Require each cluster to be a Gaussian-like distribution.
- Free from the cluster number parameter.
- Able to deal with large number of data set efficiently.

Over all, this new clustering algorithm is able to automatically search for cluster numbers with a given separation threshold in a fast and robust way, which was difficult for K-means and Gaussian-Mixture. While, if all clusters are gaussian-like, it is also more efficient than Hdbscan in finding major clusters automatically. The reason for such efficient gain is based on the design of the new algorithm which is using local data information instead of compare each data pair in a global fashion. Nevertheless, this algorithm can be regarded as an efficient improvement between Gaussian-Mixture model and K-means, and an improvement of Hdbscan can be found in here\(^\text{7}\).

II. THE ALGORITHM

This section will walk through the concepts of this algorithm, and I will analyze more in-depth details in the next section. Over all, the entire algorithm is going through the following analysis pipeline:

a. Indexing all data points by the R-tree structure.

b. Seeding centroids across K-dimensional features.

c. Converge centroids and delete excessive ones to find the definitive cluster centroid.

d. Iteratively calculate co-variant matrix, \( \Sigma_c \), from weighted local data points.

e. Re-assign data points to each cluster id via the Gaussian distribution, \( P(x|\mu_c) \).

Where steps \( b. \) and \( c. \) are designed for finding the definitive centroid of each cluster. Once the definitive cluster centroid has been found, the next step is to calculate co variance matrix of the Gaussian distribution via a mean-field iterative calculation in step \( d. \). Finally, re-assign all the data points to the correspond cluster id in step \( e. \). The following paragraphs describe more details of the entire algorithm.

a. Indexing all data points by the R-tree structure.

The very first step is to construct the K-dimensional R-tree with all the data points, \( \vec{x}_i \), which generally gives average \( O(\log N) \) complexity of multi-dimensional range search. Here, the index \( i \) indicated the \( i-th \) data point. During the construction of R-tree, the minimum \( (x_{\text{min}}^a) \) and maximum \( (x_{\text{max}}^a) \) value of feature, \( a \), can also be found without loosing too much calculation resource.

b. Seeding centroids across K-dimensional features.

Now, the centroids, \( \vec{\mu}_{c=0} \), are seeded with a given separation distance, \( d_s \), across all features \( [x_{\text{min}}^a, x_{\text{max}}^a] \), where \( t = 0 \) means the zeroth iteration of the centroid. Fig. \( \text{I.a} \) shows the seeding of centroids, where \( \vec{\mu}_1 \) is the first centroid inside the red cube(square) and so on so forth.

During the seeding process, the algorithm also search for the data points in the K-dimensional cubic of volume, \( d_v^K \), around each centroid \( \vec{\mu}_c \), and thus find out the temporary local data sets, \( \vec{x}_{i\in c} \), to the correspond centroid. Note that, each \( \vec{\mu}_c \) possess a local count of data points, \( N_c \), inside each \( d_v^K \) volume. By this nature, several centroids can be excluded if they possess too few counts of data point by a given counting threshold, \( N_c < L \).

c. Converge centroids and delete excessive ones to find the definitive cluster centers. The previous step can be regarded as the zeroth iteration of the converge process. In order to find the best cluster centers, centroid need to be updated, \( \vec{\mu}_c \), by calculate the means of \( \vec{x}_{i\in c} \),

\[
\vec{\mu}_c^{t+1} = \frac{1}{N_c} \sum_{i \in c} \vec{x}_i.
\]  

(1)
After words, the iterations of each centroid can be stopped by the criterion,

$$|\mu_c^{t+1} - \mu_c^t| < \epsilon,$$

where $\cdots$ denotes the Euclidean distance under K-dimension and $\epsilon$ is the convergence threshold. In Fig. 1.a, the dotted lines show the iteration paths of each centroid, $\mu_c$.

During the iteration of centroids, two or more centroid seeds may end up in the same cluster center. According to this factor, the iteration process can be further speed up by delete the centroid $\mu_c$ with lower data point counting, $N_c$, within a collision detection. The collision detection is defined in a K-dimensional cubic box that spanned by the collision distance, $d_c \equiv 2d_s$. Fig. 1.b shows $\mu_1$ (red) and $\mu_3$ (orange) to be deleted as they possess less count ($N_c$) than $\mu_2$ (green) and $\mu_4$ (blue).

Note that, it is possible to set a different value of $d_c$ instead of using $d_c \equiv 2d_s$. However, it would be efficient and accurate by setting $d_c \equiv 2d_s$. In principal, there could be several different ways to implement the centroid deletion algorithm. However, I will not dive into too much details in here.

**d. Iteratively calculate co-variant matrix, $\Sigma_c$, from weighted local data points.** After finding all the definitive cluster centroid, $\mu_c$, the co-variant matrix $\Sigma_c$ of each cluster are ready to be calculated via the local data points, $x_{i \in c}$. Firstly, the Gaussian distribution is generally written,

$$P(\bar{x} | \mu_c) = \frac{1}{\sqrt{2\pi} |\Sigma_c|} \times e^{-(\bar{x} - \mu_c)^T \Sigma_c^{-1}(\bar{x} - \mu_c)},$$

where $\bar{x}$ and $\mu_c$ are column vectors and the $T$ operation is the transpose of them. The following formula is the usual way to calculate the co-variant matrix from a given data set,

$$\Sigma_{c}^{mn} = \frac{1}{N_c} \sum_{i \in c} (x_i^m - \mu_c^m)(x_i^n - \mu_c^n).$$

While, since $x_{i \in c}$ is not a complete data set from each cluster centroid $\mu_c$, it might induce inaccuracies. Therefore, Eq. 4 can be modified into the following equations,

$$\Sigma_{c}^{mn} \equiv \sum_{i \in c} w_{i,c}(x_i^m - \mu_c^m)(x_i^n - \mu_c^n),$$

$$w_{i,c} \equiv \frac{P(\bar{x}_i | \mu_c)}{\sum_{j \in c} P(\bar{x}_j | \mu_c)}.$$
co-variant matrix, $\Sigma_c$, that even it is only calculated via the local data set, $\tilde{x}_i \in c$. However, Eq. 5 also indicated a functional form, $P(\tilde{x}_i | \tilde{\mu}_c) \equiv P_i [\Sigma_c]$, and the following variational condition can be carried out to yield the optimization of $P[\Sigma_c]$, 

$$\delta \int d\tilde{x} P[\Sigma_c] = 0.$$  \hspace{1cm} (6)

A mathematical rigorous solution for Eq. 6 might be hard to get. While, Eq. 5 and 6 can be approximately solved by mean-field method, iteratively,

i. Calculate $\Sigma_c^1$ from Eq. 4, and set $\Sigma_c^1 = \Sigma_c^0$.

ii. Calculate $\Sigma_c^{t+1}$ from Eq. 5 with the input of the co-variant matrix for $P[\Sigma_c]$, where $\Sigma_c^t = \frac{1}{2}(\Sigma_c^{t-1} + \Sigma_c^t)$.

iii. Iterate process ii. until,

$$\text{max element}\{\mid \Sigma_c^{t+1,mn} - \Sigma_c^{\text{input.mn}} \mid \} < \epsilon,$$  \hspace{1cm} (7)

where $\epsilon$ is the convergence threshold. In above, the form of the second step is to ensure a smooth iteration process for the co-variant matrix. The entire process of the self-consistence loop calculation is shown in Fig. 2.

**e. Re-assign data points to each cluster center via the Gaussian distribution, $P(\tilde{x}_i | \tilde{\mu}_c)$**. Finally, after all of the co-variant matrix, $\Sigma_c$, for each centroid are calculated, the assignment of each data point, $\tilde{x}_i$, become very easy.

$$\tilde{x}_i \in \tilde{\mu}_{\text{max}}, \text{ where }$$

$$\tilde{\mu}_{\text{max}} \leftarrow \text{max P-value of } \{ P(\tilde{x}_1 | \tilde{\mu}_0), ..., P(\tilde{x}_n | \tilde{\mu}_n) \}.$$  \hspace{1cm} (8)

The entire process of the clustering algorithm ends here.

**III. DISCUSSIONS TO THE ALGORITHM**

This section is divided into three sub-sections, where I will discuss: A, how to set proper parameters for the clustering algorithm, B, analyze the run time complexities of the analysis pipeline, and C, establish some post clustering process to ensure the read out data quality.

**A. Parameter settings**

Three parameters was mentioned in ther previous section that describe the algorithm:

- The centroid separation distance, $d_s$.
- The local data counting threshold, $L$.
- The convergence threshold, $\epsilon$.

**B. Run time complexities**

It is complicate to establish a precise analysis for the run time complexity due to three inter-related variables: (a) number of features, (b) number of data points and (c) number of clusters. Therefore, I will focus on the special situation for “small number of feature” with “few clusters”. Here I list the worst run time complexity of each step for this situation,

a. Indexing all data points by the R-tree structure:

$$\sim O(N \times \log(N)),$$

b. Seeding centroids across K-dimensional features:

$$= \sum_{c=0}^{M} N_c \times \log(N) \sim O(N \times \log(N)),$$
where $N_T$ of centroid seeds, $\mu$ and it takes data. Iteratively calculate co-variant matrix, $\Sigma_c$, from weighted local data points: 
$\sim O(T_{\Sigma_c} \times N_c \times K^3)$,

e. Re-assign data points to each cluster id via the Gaussian distribution, $P(x|\mu_c)$:
$\sim O(N_c)$,

where $N$ is the total number of data points, $M$ is the number of centroid seeds, $T_{\mu_c}$ is the centroid iteration steps, $N_c$ is the number of local data points that belong to $\mu_c$, $T_{\Sigma_c}$ is the iteration steps in d., and $K$ is the dimension (feature) of the data.

Note that, a matrix-inversion operation is required for Eq.4 and it takes $O(K^3)$ run time complexity. If there are only few features (small number of K) to be considered, this operation could be regarded as constant run time complexity. Finally, it is easy to know the bottleneck of the entire algorithm is in either c. or d. which depends on the types of data sets. Therefore, the upper limit run time complexity could be roughly estimated, $\sim O(T_{\text{max}} \times N \times \log(N))$, where the maximum of iterations, $T_{\text{max}}$, is less then 20 in most of the cases.

C. Post clustering process

Clustering algorithms serve in many different purpose of usage. For example, in a cloth store, the salesmen can apply some clustering algorithms to suggest a customer to buy which size of cloth based on their hight and weight. In this situation, almost all data points (customers) should be considered, and thus to be assigned to the correspond cluster centroids (the size labels). However, it is not a good idea to include all data points in some other situations, where some falsely classified data points need to be avoid based on experimental facts. In this situation, it is more prefferable to take data points which are closer to the cluster centroid. If we are dealing with the second scenario, the benefit of the Gaussian distribution become obvious. Due to the nature of Gaussian distribution, the P-value can be easily traced with a good model fit, and Gaussian-Mixture model (GM) was invented to serve this purpose. However, GM is not able to deal with large number of data points due to its time complexity, $\sim O(T \times N^2)$, and this is one of the reasons for the creation of this paper.

Here, I define three cut-off threshold values to ensure the read out of data quality,

- P-value cut-off threshold, $L_p$:
  For any cluster of centroid-c, $\bar{x}_{i \in c}$, drop the data if $P(\bar{x}_i|\mu_c) < L_p$.

- Percentage cut-off threshold, $L_\%$:
  For any cluster of centroid-c, $x_{i \in c}$, sort the data points according to the P-value in ascending order, 
  $$\text{sort}\{P(\bar{x}_{i \in c}|\mu_c)\},$$
  and drop $L_\%$ of data from the begin of the sorted data list.

- Separation cut-off threshold, $L_s$:
  For any data point, $\bar{x}_i$, calculate first and second maximum value of $P(\bar{x}_i|\mu_c)$ denoted as $P(\bar{x}_i|1^{st})$ and $P(\bar{x}_i|2^{nd})$. Finally, drop data $\bar{x}_i$ if the following criterion matched,
  $$\frac{P(\bar{x}_i|1^{st})}{P(\bar{x}_i|1^{st}) + P(\bar{x}_i|2^{nd})} < L_s.$$  

In general, $L_p$ itself can ensure the data quality and exclude the false classified data points. However, the simple definition of $L_p$ may cause the imbalance loading of each cluster due to the variance of shapes of each cluster, $P(\bar{x}_i|\mu_c)$. Therefore, $L_\%$ can better ensure a balanced loading of data points in each cluster. After all, $L_s$ can ensure the separations of two clusters.

IV. CONCLUSION

In this paper, I introduced an efficient multi-dimensional clustering algorithm based on the multivariate Gaussian function. The run time complexity of this new algorithm is much better then the Gaussian mixture model due to the clusters are calculated with locally weighted data points. On the other hand, similar to Hdbscan algorithms, it automatically find out the locations of each cluster with a better run time complexity (the run time complexity for Hdbscan is roughly $O(N \log N)$). It would be worth to mention, since most of the operations of this new algorithm are just vector summations, which means it can be easily accelerated with a multi-thread parallel scheme.

While, one can perform a similar calculation by the mixture of Dbscan/Hdbscan and Gaussian mixture model.

1. run Dbscan/Hdbscan to find out the optimal cluster number and approximate locations of centroids,
2. run Gaussian Mixture model based on the input of cluster number and locations of centroids.

However, due to the run time complexity of Dbscan/Hdbscan and Gaussian mixture model and the difficulties of parallel the algorithm for minimal-spanning-tree, it is not practical to take this mixed “two step” algorithm rather then our new algorithm. I have tested some randomly generated cluster data with 150,000 features, over all, the run time is less than 20 seconds under a 2.5GHz single threaded CPU. The code is written in C++ with boost library for the need of R-tree data structure.

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