Careful seeding for the $k$-medoids algorithm with incremental $k^{++}$ cluster construction

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Abstract

The $k$-medoids algorithm is a popular variant of the $k$-means algorithm and widely used in pattern recognition and machine learning. A main drawback of the $k$-medoids algorithm is that it can be trapped in local optima. An improved $k$-medoids algorithm (INCKM) was recently proposed to overcome this drawback, based on constructing a candidate medoids subset with a parameter choosing procedure, but it may fail when dealing with imbalanced datasets. In this paper, we propose a novel incremental $k$-medoids algorithm (INCKPP) which dynamically increases the number of clusters from 2 to $k$ through a nonparametric and stochastic $k$-means++ search procedure. Our algorithm can overcome the parameter selection problem in the improved $k$-medoids algorithm, improve the clustering performance, and deal with imbalanced datasets very well. But our algorithm has a weakness in computation efficiency. To address this issue, we propose a fast INCKPP algorithm (called INCKPP$_{sample}$) which preserves the computational efficiency of the simple and fast $k$-medoids algorithm with an improved clustering performance. The proposed algorithm is compared with three state-of-the-art algorithms: the improved $k$-medoids algorithm (INCKM), the simple and fast $k$-medoids algorithm (FKM) and the $k$-means++ algorithm (KPP). Extensive experiments on both synthetic and real world datasets including

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imbalanced datasets illustrate the effectiveness of the proposed algorithm.

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1. Introduction

Clustering is an important class of unsupervised learning methods and has been widely used in many applications such as data mining \[4\], vector quantization \[8\], dimension reduction \[5\] and manifold learning \[7\]. The aim of a clustering task \[10\] is to partition a set of objects into clusters such that the objects within a cluster have a high degree of similarity but are dissimilar to objects in other clusters.

The \(k\)-means algorithm \[18\] is one of the most popular clustering algorithms, which minimizes the sum of the squared distance from each data point to its nearest center. It is popular for its easy implementation, linear time complexity and convergence guarantee \[17\]. Ball \(k\)-means was recently proposed in \[19\] to accelerate the \(k\)-means algorithm by using a ball to describe each cluster, which reduces the point-centroid distance computation. However, the \(k\)-means algorithm is very sensitive to both initialization and outliers. The \(k\)-medoids (or the Partition Around Medoids (PAM)) algorithm \[15\] is a variant of the \(k\)-means algorithm, which minimizes the sum of the dissimilarity between each data point and the center it belongs to. Compared with the \(k\)-means algorithm, the \(k\)-medoids algorithm is not only more accurate and more robust to outliers but is also more flexible in choosing dissimilarity measures to deal with diverse data distributions. But the \(k\)-medoids algorithm is still sensitive to both initialization and outliers. Further, it is inefficient for large-scale data sets due to its high computation complexity of \(O(n^2)\), where \(n\) is the number of data points. To address the second issue, a sampling-based method called CLARA was proposed in \[10\]. CLARA first draws multiple samples from the data set and then applies PAM on each sample to give the best clustering as the output. However, a good clustering based on samples does not necessarily represent a good clustering of the whole data set if the samples are biased. A Randomized CLARA (CLARANS) was then introduced in \[13\] which is scalable and more efficient than both PAM and CLARA. In 2009, a simple and fast algorithm (FKM) for \(k\)-medoids clustering was proposed in \[14\] to improve the clustering performance and computational efficiency of the \(k\)-medoids algorithm.

On the other hand, in order to improve the clustering performance of
$k$-means-like methods such as the $k$-means algorithm and the $k$-medoids algorithm, many initialization methods have been proposed. For example, the famous stochastic initialization method named $k$-means++ was introduced in [1] which achieves $O(\log(k))$-competitive results with optimal clustering. More initialization methods can be found in [16, 9, 23, 6, 20, 22]. Since 2003, several global $K$-means algorithms have been proposed to find a global minimizer of the $k$-means clustering problems, such as [12, 2, 11, 3]. A global $k$-means algorithm is an incremental approach to clustering that dynamically adds one cluster center at a time through a deterministic global search procedure consisting of $n$ executions of the $k$-means algorithm from suitable initial positions, where $n$ is the size of the data set. These methods improve the clustering performance significantly but introduce a much higher computation complexity, compared with the linear computation complexity in the traditional methods such as $k$-means++. The incremental approach can be introduced to the $k$-medoids algorithm, yielding an algorithm with a computation complexity of $O(n^2)$ which is competitive with the traditional $k$-medoids method. An improved $k$-medoids algorithm (INCKM) was proposed in [21] which has a better clustering performance than FKM in [14] and the density peaks clustering algorithm in [16] have. But INCKM needs to determine the candidate medoids subset with a parameter choosing procedure in the process of initialization. Though a range of choices for the parameter is given in [21] for INCKM, it often fails to deal with some complex data sets and, in particular, imbalanced data sets.

In this paper, we propose a novel incremental method (called INCKPP) which dynamically increases the number of clusters and centers from 2 to $k$ through a nonparametric, stochastic $k^{++}$ search procedure. INCKPP improves the clustering performance of INCKM without a hyper-parameter to choose and can also deal with imbalanced data sets very well, but INCKPP is inefficient computationally. To address this issue, we propose an improved INCKPP algorithm named INCKPP$_{sample}$ which is faster than INCKPP while keeping the clustering performance of INCKPP algorithm.

The remaining part of the paper is organized as follows. Section 2 introduces the related work. Section 3 gives details of the proposed algorithms. Extensive experimental results are conducted in Section 4 on synthetic and real-world data sets in comparison with INCKM, FKM and the $k$-means++ algorithm (KPP). Conclusions are given in 5.
2. Related work

2.1. Simple and fast k-medoids algorithm (FKM)

Given a data set $X = \{x_i \in \mathbb{R}^p | i = 1, 2, \ldots, n\}$, the simple and fast k-medoids (FKM) algorithm \[14\] aims to minimize the Sum of the Errors (SE) between $x_i \in X$ and the cluster center $c_j \in C = \{c_j \in X | j = 1, 2, \ldots, K\}$:

$$SE(C) = \sum_{i=1}^{n} \sum_{j=1}^{k} s_{ij} d(x_i, c_j), \quad (1)$$

where $S = \{s_{ij}| i = 1, 2, \ldots, m; j = 1, 2, \ldots, k\}$ is the assignment index set with $s_{ij} = 1$ indicating that $x_i$ is assigned to the $j$th cluster and $s_{ij} = 0$ otherwise, $d(x_i, c_j)$ is the distance between $x_i$ and $c_j$. FKM algorithm selects the cluster centers, which are called medoids, from the data set and updates the new medoids of each cluster which is the data point minimizing the sum of its distances to other data points in the cluster. The detailed description of FKM can be found in Algorithm 1 below.

\begin{algorithm}
\caption{FKM}
\begin{algorithmic}[1]
\Require Dissimilarity matrix $D$, data set $X$, cluster number $K$ and initial cluster centers $C = \{c_1, \ldots, c_K\}$
\Ensure Cluster centers $C^* = \{c_1^*, \ldots, c_K^*\}$
\State 1: Obtain the initial cluster results by assigning each data point to the nearest medoids.
\State 2: Calculate the sum of the distances from all data points to their medoids.
\State 3: Find a new medoid for each cluster, which is the data point minimizing the sum of its distances to other data points in the cluster. Update the current medoid in each cluster by replacing it with the new medoid.
\State 4: Assign each data point to the nearest medoids and obtain the cluster result.
\State 5: Calculate the sum of the distances from all data points to their medoids. If the sum is equal to the previous one, then stop the algorithm. Otherwise, go back to Step 3.
\State 6: \textbf{return} $C^*$
\end{algorithmic}
\end{algorithm}
2.2. $k$-means++

The $k$-means++ algorithm [1] is an augmented $k$-means algorithm which uses a simple, randomized seeding technique in the $k$-means algorithm. It chooses the first center randomly with equal probability and sequentially selects the rest ($k-1$) centers with the probability $d(x)^2/\sum_{x'} d(x')^2$, where $d(x)$ denotes the minimum distance from $x$ to the closest center that we have already chosen. The $k$-means++ algorithm can exclude the influence of the outliers.

2.3. The improved $k$-medoids algorithm

The improved $k$-medoids algorithm (INCKM) [21] is an incremental algorithm for solving the $j$-medoids problem from $j=2$ to $j=k$ in turn. It is easy to find the optimal solution of the 1-medoids problem, which is the data point minimizing the total distance from the data point to other data points in the data set. For solving the $(j+1)$-medoids problem, the solution of the $j$-medoids is used as the first $j$ initial cluster centers and one tries to find the $(j+1)$ initial cluster centers. The INCKM algorithm first computes the variances of the data set as follows:

\[
\sigma = \sqrt{\frac{1}{n-1} \sum_{i=1}^{n} \text{dist}(x_i, \bar{x})^2},
\]

\[
\sigma_i = \sqrt{\frac{1}{n-1} \sum_{j=1}^{n} \text{dist}(x_i, x_j)^2},
\]

where $\bar{x} = \sum_{i=1}^{n} x_i/n$ and $\text{dist}(x_i, x_j)$ is the distance between $x_i$ and $x_j$. It then constructs a candidate set $S = \{x_i|\sigma_i \leq \lambda \sigma, \ i = 1, \ldots, n\}$ with the $(j+1)$ initial centers given by

\[
c_j = \arg\max_{x_i \in S} \{d_i|i = 1, \ldots, n\},
\]

where $d_i$ is the distance between $x_i$ and the closest center we have already chosen and $\lambda$ is a stretch factor which needs to be given in advance. In [21] it was recommended that the parameter $\lambda$ can be taken to be between 1.5 and 2.5. However, this parameter range may certainly not be suitable for all types of data distributions and, in particular, for some imbalanced data distributions.
3. The proposed incremental \( K \)-medoids algorithm

In this section, we propose an incremental \( K \)-medoids algorithm, called INCKPP, which increases the number of clusters and centers from 2 to \( K \) through \( K \)-means++ searching. Being different from the INCKM algorithm, INCKPP has no parameter to be given in advance except for the cluster number \( K \) and can deal with complex and imbalanced data distributions very well, as demonstrated in experiments. Further, INCKPP has the ability to exclude the influence of the outliers in view of using \( K \)-means++ searching in execution. Details of the INCKPP algorithm is given in Algorithm 2 below.

**Algorithm 2 INCKPP**

**Require:** dissimilarity matrix \( D \), data set \( X \) and cluster number \( K \)

**Ensure:** cluster center \( C = \{c_1, \ldots, c_K\} \)

1: Initialize \( C = \{c_1\} \):

\[
c_1 = \arg \min_{x_i \in X} \sum_j d(x_i, x_j)
\]

2: for \( k=2, \ldots, K \) do
3: find \( c_k \) through \( K \)-means++ searching, that is, choosing \( c_k \) with the probability \( d(x)^2 / (\sum x' d(x')^2) \)
4: update \( C = C \cup c_k \)
5: update cluster center \( C \) by FKM (i.e., Algorithm 1)
6: end for
7: return \( C \)

The time complexity of the INCKPP algorithm is \( O(K^2 n^2) \), while most of the traditional \( K \)-medoids algorithms have the time complexity \( O(K n^2) \). To improve the time efficiency of INCKPP we further propose a sampled INCKPP algorithm called INCKPP\text{sample}. In INCKPP\text{sample}, INCKPP is executed first on randomly sampled \( p \) percent of each data set as a pre-search procedure. Then, by using the result of the pre-search procedure as the initial centers, INCKPP\text{sample} executes FKM on the whole dataset to find the final centers.

4. Experiments

In this section, we conduct a number of experiments to evaluate the clustering performance of the proposed INCKPP and INCKPP\text{sample} algorithms.
All the experiments are conducted on a single PC with Intel Core 2.6GHz i5 CPU (2 Cores) and 8G RAM.

4.1. The compared algorithms

In the experiments, we first compare INCKPP with INCKM [21] and then compare INCKPP\textit{sample} with KPP\textit{sample}, KPP, FKM [14] and FKM\textit{sample}, where

- KPP is the algorithm which chooses $K$ initial medoids through $K$-means++ searching and then uses FKM as a local search procedure,
- KPP\textit{sample} is the algorithm which first runs KPP on randomly sampled $p$ percent of each data set as a pre-search procedure and then runs FKM with the result in the pre-search procedure as initial centers to find the final result,
- FKM\textit{sample} is the algorithm which first runs FKM on randomly sampled $p$ of each data set ($p = 10$, i.e., 10 percent of the data points are used) as a pre-search procedure and then runs FKM with the result in the pre-search procedure as initial centers to find the final result.

4.2. The data sets

4.2.1. Overview of the data sets

The synthetic data sets can be downloaded from the clustering data set website\footnote{http://cs.joensuu.fi/sipu/datasets/}. The imbalanced data set contains 6500 two-dimensional data points. The experiments consider its three subsets that contain the classes \{6, 7\} (denoted as imbalance2), \{2, 6, 7, 8\} (denoted as imbalance4), \{1, 3, 4, 5, 6, 8\} (denoted as imbalance6) and the whole imbalance data set (denoted as imbalance). Dim-set contains 9 well separated Gaussian clusters with the dimension varying from 2 to 15. S-set contains 15 Gaussian clusters with different degrees of clusters overlapped. We choose two data sets from Shape-set which consist of hyper-spherical clusters. The real world data sets are from UCI Machine Learning Repository. Handwritten pendigits data set contains 7494 sixteen-dimensional data points. In the experiments, we consider three subsets that contain the class \{1, 3, 5\} (denoted as pendigits$_3$), \{0, 2, 4, 6, 7\} (denoted as pendigits$_5$), \{0, 1, 2, 3, 4, 5, 6, 7\} (denoted as pendigits$_8$) and the
whole handwritten digits data set (denoted as pendigits). In the several real
data sets we chosen, the class number varies from 2 to 10, the dimension
of the data points varies from 3 to 16 and the size of the data sets varies
from 215 to 7494. The Euclidean distance is used in both synthetic and real
data sets although other dissimilarity can also be used in the $k$-medoids type
algorithms.

Table 1: Overview of the synthetic datasets

| data set      | attribute | class | size  |
|---------------|-----------|-------|-------|
| Imbalanced-set| imbalance2| 2     | 2     |
|               | imbalance4| 2     | 4     |
|               | imbalance6| 2     | 6     |
|               | imbalance | 2     | 8     |
| Dim-set       | dim2      | 2     | 9     |
|               | dim6      | 6     | 9     |
|               | dim10     | 10    | 9     |
|               | dim15     | 15    | 9     |
| S-set         | S1        | 2     | 15    |
|               | S2        | 2     | 15    |
|               | S3        | 2     | 15    |
|               | S4        | 2     | 15    |
| Shape-set     | R15       | 2     | 15    |
|               | D31       | 2     | 31    |

Table 2: Overview of the real datasets

| dataset       | attribute | class | size  |
|---------------|-----------|-------|-------|
| newthyroid    | 5         | 3     | 215   |
| banknote      | 4         | 2     | 1372  |
| yeast         | 8         | 10    | 1484  |
| pendigits3    | 16        | 3     | 2218  |
| pendigits5    | 16        | 5     | 3838  |
| pendigits8    | 16        | 8     | 6056  |
| pendigits     | 16        | 10    | 7494  |
4.2.2. Attribute normalization

The normalization

\[ x_{\text{normalization}} = \frac{x - x_{\text{min}}}{x_{\text{max}} - x_{\text{min}}} \]  

is used to avoid the attributes with large values dominating the distance calculation and to get more accurate numerical computation results.

4.3. Performance criteria

In the experiments, four criteria are used to evaluate the performance of the algorithm: 1) the average of the sum of errors (aver-SE), 2) the minimum of the sum of errors (min-SE), 3) the number of iterations (#iter) and 4) the number of repeats (#repe) within the CPU time. In the experiments comparing INCKPP with INCKM, we take the stretch factor \( \lambda = 1.4 + 0.1k \) with \( k = 1, \ldots, 11 \) in the INCKM algorithm as in [21]. We regard the value of \( \lambda \) with the smallest sum of errors (SE) as the best parameter and record the corresponding SE which is denoted as min-SE*. We first run the INCKM algorithm to get an upper bound for the CPU time and record correspondingly the min-SE*, the best parameter \( \lambda \) and #iter of INCKM. We then run INCKPP repeatedly as many times as possible within the CPU time of INCKM. The min-SE, aver-SE, #iter and #repe of INCKPP were recorded when time is over. Similarly, in the experiments comparing INCKPP\_sample with the four stochastic algorithms, KPP, KPP\_sample, FKM and FKM\_sample, we first run the INCKPP\_sample algorithm \( N \) times to get an upper bound of the CPU time used by INCKPP\_sample and then run KPP, KPP\_sample, FKM and FKM\_sample repeatedly as many times as possible within the CPU time used by INCKPP\_sample. During this process, we recorded min-SE, aver-SE, #iter and #repe of the five comparing algorithms. The values of the CPU time, min-SE, aver-SE, #iter, #repe are the average of these criteria over 100 duplicate tests to reduce the randomness.

4.4. Experiments on the synthetic data sets

Table 3 presents the comparison results of INCKPP with INCKM on the synthetic data sets. From the results it is seen that the minimum of the sum of errors (min-SE) obtained by INCKPP is not bigger than the smallest sum of errors (i.e., the min-SE*) obtained by INCKM on 9 datasets; in particular, INCKPP achieves a much smaller min-SE than the min-SE* obtained by INCKM on the four imbalanced datasets with a much smaller number
of iterations. Figure 1 presents the clustering results obtained by INCKM and INCKPP on the imbalanced dataset, imbalance$_2$. For all recommended stretch factors $\lambda$, INCKM fails to correctly initialize the cluster center, that is, INCKM initializes two cluster centers in one class (Class 7) which has 20 times as many samples as another class (Class 6), so Class 7 was divided into two classes, as seen in Figure 1. However, INCKPP gets the correct clustering result, as shown in Figure 1. In fact, for the four imbalanced datasets, INCKM always gets an incorrect clustering result due to the wrong initialization of INKCM, but INCKPP gets the correct clustering result.

In what follows, we carry out extensive experiments to compare the fast version of INCKPP (i.e., INCKPP$_{sample}$) with KPP$_{sample}$, KPP and FKM, where we always denote by $p$ the randomly sampled percentage of the datasets in the pre-search procedure and by $N$ the running times of INCKPP$_{sample}$.

Table 3: Comparison between INCKM and INCKPP. The min-SE is the minimum of SE obtained within the CPU time used by INCKM in one run. The #repe is the number of repeats of INCKPP within the CPU time used by INCKM in one run. The #iter is the number of iterations when the local minimizer is attained.

| Data sets | INCKM | INCKPP |
|-----------|-------|--------|
|           | $\lambda$ | min-SE$^*$ | #iter | min-SE | #repe | #iter |
| imbalance$_2$ | 1.5 | 149.89 | 9.00 | 75.75 | 55.14 | 1.14 |
| imbalance$_4$ | 1.5 | 132.49 | 7.00 | 87.29 | 21.85 | 1.34 |
| imbalance$_6$ | 1.5 | 155.75 | 11.00 | 122.76 | 16.51 | 2.92 |
| imbalance | 2.5 | 140.72 | 12.45 | 126.92 | 18.13 | 3.02 |
| dim$_{15}$ | 1.5 | 702.09 | 1.00 | 702.09 | 11.85 | 1.03 |
| dim$_{10}$ | 1.5 | 304.78 | 1.09 | 304.78 | 13.14 | 1.03 |
| dim$_{6}$ | 1.5 | 131.10 | 1.00 | 131.10 | 11.81 | 1.03 |
| dim$_2$ | 1.6 | 12.62 | 1.55 | 12.62 | 14.34 | 1.04 |
| S$_1$ | 1.5 | 181.63 | 2.00 | 183.18 | 11.16 | 2.65 |
| S$_2$ | 2.0 | 219.09 | 2.82 | 221.54 | 11.38 | 3.41 |
| S$_3$ | 1.5 | 287.32 | 4.09 | 272.14 | 10.45 | 4.13 |
| S$_4$ | 1.5 | 253.35 | 5.36 | 255.69 | 11.71 | 5.63 |
| D$_{31}$ | 1.5 | 109.64 | 3.82 | 115.32 | 10.19 | 3.30 |
| R$_{15}$ | 1.5 | 16.46 | 2.00 | 16.62 | 10.83 | 2.14 |
Figure 1: The clustering result on the imbalanced data set, imbalance$_2$. INCKM gets an incorrect clustering result since it initializes two cluster centers in one class, leading to the fact that one original class is divided into two classes. Note that INCKPP gets the correct result.

4.4.1. Experiment on the imbalanced data sets

Tables 4, 5, 6 and 7 present the clustering results of INCKPP$_{sample}$, KPP$_{sample}$ and FKM$_{sample}$ on the four imbalanced datasets for different $p$ with $N = 3$. From these results it is seen that INCKPP$_{sample}$ gets the best clustering performance for all values of $p$ on all the four imbalanced datasets. Note that for the imbalanced dataset, imbalance$_2$, both INCKPP$_{sample}$ and KPP$_{sample}$ achieve the global minimum when $p = 13$.

We now compare INCKPP$_{sample}$, KPP$_{sample}$ and FKM$_{sample}$ with the conventional KPP and FKM algorithms for different $N$ when $p = 10$. In general, the minimum of sum of errors (Min-SE), which is obtained by each compared algorithm within the CPU time used by INCKPP$_{sample}$ running $N$ times, is
getting smaller as $N$ increases. Tables 8, 9, 10, 11 presents the Min-SE against $N$ for INCKPP\textsubscript{sample}, KPP\textsubscript{sample}, FKM\textsubscript{sample}, KPP and FKM on the four imbalanced datasets when $p = 10$. From Tables 9, 10, 11 it can be seen that for imbalance\textsubscript{2}, imbalance\textsubscript{4} and imbalance\textsubscript{6}, INCKPP\textsubscript{sample} gets a smaller Min-SE than the other compared algorithms and achieves the global minimum first before $N = 5, 3, 2$, respectively, for the three datasets. Table 8 illustrates that for imbalance, INCKPP\textsubscript{sample} and KPP both achieve the global minimum before $N = 20$, but INCKPP\textsubscript{sample} gets a smaller Min-SE for $N < 20$ compared with the other algorithms. Further, from Table 12 it is seen that the average of the sum of errors (aver-SE) and the number of iterations ($\#\text{iter}$) of INCKPP\textsubscript{sample} is generally much less than those of the other compared algorithms. In conclusion, INCKPP\textsubscript{sample} outperforms the other compared algorithms on the four imbalanced datasets in the experiments.

Table 4: The experiment results on the imbalanced dataset, imbalance, with different $p$, where $p$ is the randomly sampled percentage of the dataset in the pre-search procedure. The values in the table are the minimum of the sum of errors (min-SE) obtained by each compared algorithm within the CPU time used by INCKPP\textsubscript{sample} running $N$ times for different value of $p$.

| imbalance ($N = 3$) | INCKPP\textsubscript{sample} | KPP\textsubscript{sample} | FKM\textsubscript{sample} |
|---------------------|------------------------------|----------------------------|--------------------------|
| $p = 5$             | 128.20                       | 131.08                     | 224.92                   |
| $p = 6$             | 128.57                       | 130.24                     | 254.64                   |
| $p = 7$             | 128.81                       | 130.10                     | 262.40                   |
| $p = 8$             | 127.98                       | 131.71                     | 250.57                   |
| $p = 9$             | 128.11                       | 132.95                     | 261.99                   |
| $p = 10$            | 128.37                       | 130.61                     | 254.43                   |
| $p = 11$            | 127.97                       | 130.52                     | 243.42                   |
| $p = 12$            | 127.57                       | 133.35                     | 216.74                   |
| $p = 13$            | 128.03                       | 130.28                     | 239.80                   |
| $p = 14$            | 127.72                       | 130.99                     | 246.69                   |
| $p = 15$            | 128.01                       | 130.64                     | 247.27                   |

4.4.2. Experiments on the S-sets

Figure 2 presents the clustering results of INCKPP\textsubscript{sample}, KPP\textsubscript{sample} and FKM\textsubscript{sample} on the S-datasets for different $p$ with $N = 10$. Compared with KPP\textsubscript{sample} and FKM\textsubscript{sample}, INCKPP\textsubscript{sample} gets the smallest min-SE within the CPU time used by INCKPP\textsubscript{sample} running 10 times except for the $S_4$
Table 5: The experiment results on the imbalanced dataset, imbalance$_6$, for different $p$, where $p$ and the values in the table are the same as those in Table 4.

| imbalance$_6$ ($N = 3$) | INCKPP$_{sample}$ | KPP$_{sample}$ | FKM$_{sample}$ |
|-------------------------|-------------------|---------------|---------------|
| $p = 5$                 | **123.49**        | 125.19        | 233.88        |
| $p = 6$                 | **123.18**        | 126.00        | 227.17        |
| $p = 7$                 | **123.07**        | 125.73        | 241.53        |
| $p = 8$                 | **123.18**        | 131.49        | 250.72        |
| $p = 9$                 | **123.18**        | 125.21        | 256.16        |
| $p = 10$                | **122.97**        | 130.56        | 214.54        |
| $p = 11$                | **123.07**        | 128.06        | 237.77        |
| $p = 12$                | **123.07**        | 125.21        | 240.38        |
| $p = 13$                | **122.97**        | 127.96        | 246.10        |
| $p = 14$                | **123.49**        | 127.60        | 238.54        |
| $p = 15$                | **122.97**        | 125.01        | 230.73        |

Table 6: The experiment results on the imbalanced dataset, imbalance$_4$, for different $p$, where $p$ and the values in the table are the same as those in Table 4.

| imbalance$_4$ ($N = 3$) | INCKPP$_{sample}$ | KPP$_{sample}$ | FKM$_{sample}$ |
|-------------------------|-------------------|---------------|---------------|
| $p = 5$                 | **87.29**         | 93.15         | 209.86        |
| $p = 6$                 | **87.29**         | 94.87         | 206.51        |
| $p = 7$                 | **87.29**         | 90.44         | 214.53        |
| $p = 8$                 | **87.29**         | 90.44         | 216.79        |
| $p = 9$                 | **87.29**         | 90.89         | 215.68        |
| $p = 10$                | **87.29**         | 93.21         | 213.76        |
| $p = 11$                | **87.29**         | 88.63         | 209.55        |
| $p = 12$                | **87.29**         | 89.09         | 213.49        |
| $p = 13$                | **87.29**         | 93.52         | 210.30        |
| $p = 14$                | **87.29**         | 89.54         | 217.06        |
| $p = 15$                | **87.29**         | 93.52         | 208.15        |

dataset, for which KPP$_{sample}$ gets a smaller min-SE than INCKPP$_{sample}$ does when $p = 8$. Figure 3 presents the clustering results against $N$ of INCKPP$_{sample}$, KPP, KPP$_{sample}$, FKM and FKM$_{sample}$ on the S-datasets when $p = 10$. Figures 3 (a)-(b) illustrate that for the datasets $S_1$ and $S_2$, INCKPP$_{sample}$ achieves the global minimum before $N = 20$ and $N = 30$, respectively, and gets a smaller min-SE compared with the other compared algorithms. Figures 3 (c)-(d) show that for the datasets $S_3$ and $S_4$, non of the
Table 7: The experiment results on the imbalanced dataset, imbalance_2, for different $p$, where $p$ and the values in the table are the same as those in Table 4.

| Imbalance_2 ($N = 3$) | INCKPP_{sample} | KPP_{sample} | FKM_{sample} |
|-----------------------|-----------------|--------------|--------------|
| $p = 5$               | 75.75           | 78.71        | 138.00       |
| $p = 6$               | 75.75           | 81.67        | 137.25       |
| $p = 7$               | 75.75           | 78.71        | 138.74       |
| $p = 8$               | 75.75           | 79.45        | 137.26       |
| $p = 9$               | 75.75           | 77.23        | 138.74       |
| $p = 10$              | 75.75           | 79.45        | 139.48       |
| $p = 11$              | 75.75           | 80.93        | 138.00       |
| $p = 12$              | 75.75           | 77.23        | 137.25       |
| $p = 13$              | 75.75           | 75.75        | 140.96       |
| $p = 14$              | 75.75           | 78.71        | 139.47       |
| $p = 15$              | 75.75           | 79.45        | 141.70       |

Table 8: The experiment results on the imbalanced dataset, imbalance, with different $N$, where $N$ is the running times of INCKPP algorithm. The values in the table are the minimum of the sum of errors (min-SE) obtained by each compared algorithm within the CPU time used by INCKPP_{sample} running $N$ times, and $p = 10$.

| Imbalance ($p=10$) | INCKPP_{sample} | Kpp  | KPP_{sample} | FKM  | FKM_{sample} |
|---------------------|-----------------|------|--------------|------|--------------|
| $N = 1$             | 131.45          | 131.64 | 133.20       | 246.83 | 267.97       |
| $N = 2$             | 129.14          | 131.55 | 132.65       | 260.42 | 240.80       |
| $N = 3$             | 128.24          | 131.04 | 130.62       | 246.26 | 240.64       |
| $N = 5$             | 127.32          | 128.35 | 128.37       | 234.73 | 225.05       |
| $N = 10$            | 126.96          | 127.33 | 127.46       | 191.76 | 179.99       |
| $N = 20$            | 126.92          | 126.92 | 126.92       | 168.80 | 162.84       |
| $N = 40$            | 126.92          | 126.92 | 126.92       | 157.60 | 151.65       |

Compared algorithms achieve the global minimum before $N = 80$ but the min-SE value obtained by INCKPP_{sample} is getting smaller as $N$ increases. From Table 13 it is seen that INCKPP_{sample} obtains both the most number of repeats within the same time and the smallest aver-SE and #iter values. As seen from most of the experiments, more repeats and a smaller aver-SE value can yield a smaller min-SE value in the experiments. Based on this observation, it may be concluded that the clustering performance of INCKPP_{sample} is better than that of all the other compared algorithms on the S-sets.
Table 9: The experiment results on the imbalanced dataset, imbalance_6, for different N, where N and the values in the table are the same as those in Table 8.

| imbalance_6 (p=10) | Inckpp_{sample} | Kpp | Kpp_{sample} | FKM | FKM_{sample} |
|-------------------|------------------|-----|--------------|-----|--------------|
| N = 1             | 127.70           | 129.85 | 130.80      | 237.30 | 242.15       |
| N = 2             | 123.81           | 126.93 | 128.78      | 233.78 | 251.39       |
| N = 3             | 123.07           | 125.52 | 124.88      | 230.75 | 241.48       |
| N = 5             | 122.76           | 123.39 | 124.24      | 220.09 | 219.83       |
| N = 10            | 122.76           | 122.76 | 122.97      | 192.26 | 170.57       |
| N = 20            | 122.76           | 122.76 | 122.76      | 157.25 | 149.77       |

Table 10: The experiment results on the imbalanced dataset, imbalance_4, for different N, where N and the values in the table are the same as those in Table 8.

| imbalance_4 (p=10) | Inckpp_{sample} | Kpp | Kpp_{sample} | FKM | FKM_{sample} |
|-------------------|------------------|-----|--------------|-----|--------------|
| N = 1             | 89.54            | 93.98 | 95.77       | 217.27 | 212.90       |
| N = 2             | 87.74            | 93.07 | 94.88       | 216.26 | 219.37       |
| N = 3             | 87.29            | 89.99 | 90.00       | 217.38 | 206.99       |
| N = 5             | 87.29            | 87.29 | 87.29       | 213.76 | 196.18       |
| N = 10            | 87.29            | 87.29 | 87.29       | 188.41 | 169.96       |

Table 11: The experiment results on the imbalanced dataset, imbalance_2, for different N, where N and the values in the table are the same as those in Table 8.

| imbalance_2 (p=10) | Inckpp_{sample} | Kpp | Kpp_{sample} | FKM | FKM_{sample} |
|-------------------|------------------|-----|--------------|-----|--------------|
| N = 1             | 80.19            | 80.93 | 80.93       | 141.70 | 142.44       |
| N = 2             | 75.75            | 79.45 | 80.19       | 140.22 | 140.22       |
| N = 3             | 75.75            | 78.71 | 79.45       | 139.48 | 138.73       |
| N = 5             | 75.75            | 77.23 | 76.49       | 133.55 | 134.28       |
| N = 10            | 75.75            | 75.75 | 75.75       | 130.57 | 117.97       |

4.4.3. Experiments on the Dim data sets

Tables 14, 15, 16 and 17 show the clustering performance of INCKPP_{sample}, KPP_{sample} and FKM_{sample} on the Dim data sets for different p with N = 2. From these tables it is seen that INCKPP_{sample} gets the best clustering performance on almost all Dim data sets for different p except for the two datasets, dim_2 and dim_10, for which the min-SE value obtained by KPP_{sample} is slightly smaller than that obtained by INCKPP_{sample} when p = 14. Table 18, 19, 20, 21 presents the clustering results against N of INCKPP_{sample}, KPP, KPP_{sample}, FKM and FKM_{sample} on the Dim data sets when p = 10.
Table 12: The experiment results of INCKPP\textsubscript{sample}, KPP\textsubscript{sample}, FKM\textsubscript{sample}, KPP and FKM on the four imbalanced datasets when \( p = 10 \), where the aver-SE is the average of sum of errors, \#re (i.e., \#repe) is the number of repetitions within the CPU time used by INCKPP\textsubscript{sample} running 10 times, and \#it (i.e., \#iter) is the number of iterations when the local minimizer is achieved.

| Data set | INCKPP\textsubscript{sample} | KPP | KPP\textsubscript{sample} | FKM | FKM\textsubscript{sample} |
|----------|-------------------------------|-----|---------------------------|-----|---------------------------|
|          | \#re | \#it | aver-SE | \#re | \#it | aver-SE | \#re | \#it | aver-SE | \#re | \#it | aver-SE |
| imbalance | 10   | 2.44 | 132.11  | 9.98 | 4.11 | 132.84  | 7.03 | 4.15 | 133.05  | 3.55 | 3.78 | 245.72  |
| imbalance | 10   | 2.13 | 127.34  | 9.54 | 3.28 | 128.99  | 7.35 | 3.39 | 130.03  | 3.44 | 3.69 | 240.29  |
| imbalance | 10   | 1.11 | 90.83   | 9.30 | 1.33 | 92.59   | 6.86 | 0.39 | 92.76   | 2.05 | 1.35 | 212.08  |
| imbalance | 10   | 1.07 | 78.02   | 9.40 | 1.19 | 78.65   | 9.31 | 1.24 | 79.50   | 3.46 | 1.61 | 142.63  |

(a) S\textsubscript{1}  (b) S\textsubscript{2}  (c) S\textsubscript{3}  (d) S\textsubscript{4}

Figure 2: The clustering results of INCKPP\textsubscript{sample}, KPP\textsubscript{sample} and FKM\textsubscript{sample} on the S-datasets with different \( p \) for \( N = 10 \), where the meaning of the criteria is the same as in Table 4.
Table 13: The experiment results on the S-sets when \( p = 10 \), where the meaning of the criteria is the same as that in Table 12.

| Data set | INCKPP_{sample} | KPP | KPP_{sample} | FKM | FKM_{sample} |
|----------|-----------------|-----|--------------|-----|--------------|
|          | \#re | \#it | aver-SE   | \#re | \#it | aver-SE   | \#re | \#it | aver-SE   | \#re | \#it | aver-SE   |
| S_1      | 10   | 3.17 | 220.95    | 8.96 | 4.33 | 230.36    | 9.14 | 4.30 | 230.37    | 6.38 | 6.39 | 287.61    |
| S_2      | 10   | 4.53 | 252.35    | 8.38 | 6.50 | 258.92    | 5.28 | 9.09 | 290.76    | 7.88 | 6.68 | 287.63    |
| S_3      | 10   | 6.06 | 293.03    | 8.10 | 3.09 | 264.95    | 2.41 | 8.19 | 301.36    | 3.46 | 7.02 | 278.14    |
| S_4      | 10   | 8.21 | 272.25    | 8.06 | 10.44 | 273.21   | 8.64 | 10.48 | 273.43   | 7.18 | 12.74 | 275.70   |

Tables 18, 19 show that for dim_2 and dim_6, INCKPP_{sample} gets the smallest min-SE value compared with the other comparing algorithms and achieves the global minimum before \( N = 2 \). Table 21 shows that for dim_15, both
INCKPP\textsubscript{sample} and KPP attain the global minimizer before $N = 3$ but the former gets a smaller min-SE value than the latter does for $N < 3$. As seen in Table 20, both INCKPP\textsubscript{sample} and KPP\textsubscript{sample} attain the global minimizer before $N = 3$ but INCKPP\textsubscript{sample} gets a smaller min-SE value compared with the latter algorithm. Further, Table 22 illustrates that the aver-SE value and the number $\#\text{iter}$ of iterations of INCKPP\textsubscript{sample} are both smaller than those of the other comparing methods. As a result, INCKPP\textsubscript{sample} outperforms the other comparing algorithms for all the criteria on the Dim data sets.

| dim\textsubscript{2} ($N = 2$) | INCKPP\textsubscript{sample} | KPP\textsubscript{sample} | FKM\textsubscript{sample} |
|--------------------------------|-------------------------------|---------------------------|--------------------------|
| $p = 5$                        | 12.95                         | 13.99                     | 73.94                    |
| $p = 6$                        | 12.62                         | 14.76                     | 73.56                    |
| $p = 7$                        | 12.98                         | 14.60                     | 69.67                    |
| $p = 8$                        | 12.95                         | 14.75                     | 75.91                    |
| $p = 9$                        | 12.62                         | 13.70                     | 72.96                    |
| $p = 10$                       | 12.62                         | 12.95                     | 73.09                    |
| $p = 11$                       | 12.62                         | 12.62                     | 74.57                    |
| $p = 12$                       | 12.62                         | 12.62                     | 68.93                    |
| $p = 13$                       | 12.62                         | 13.28                     | 74.47                    |
| $p = 14$                       | 12.96                         | 12.95                     | 65.42                    |
| $p = 15$                       | 12.62                         | 12.62                     | 74.07                    |

4.4.4. Experiments on the Shape data sets

Figure 4 shows the clustering performance of INCKPP\textsubscript{sample}, KPP\textsubscript{sample} and FKM\textsubscript{sample} on the Shape data sets, $R_{15}$ and $D_{31}$, for different $p$ with $N = 10$. As seen from the results in Figure 4, the performance of both INCKPP\textsubscript{sample} and KPP\textsubscript{sample} is much better than that of FKM\textsubscript{sample} on the Shape data sets, but INCKPP\textsubscript{sample} has a slightly better performance in comparison with KPP\textsubscript{sample}.

Figure 5 shows the clustering results against $N$ of INCKPP\textsubscript{sample}, KPP, KPP\textsubscript{sample}, FKM and FKM\textsubscript{sample} on the Shape data sets for $p = 10$. From the results in Figure 5 it is found that INCKPP\textsubscript{sample}, KPP and KPP\textsubscript{sample} have a much better performance than FKM and FKM\textsubscript{sample} on both Shape data sets. Figure 5(a) illustrates that for the $R_{15}$ data set, INCKPP\textsubscript{sample}, KPP\textsubscript{sample} and KPP all achieve the global minimum at $N = 20$, but INCKPP\textsubscript{sample} and
Table 15: The experiment results on the dim6 dataset for different $p$, where the meaning of the values is the same as that in Table 4.

|    | INCKPP$_{sample}$ | KPP$_{sample}$ | FKM$_{sample}$ |
|----|-------------------|----------------|----------------|
| $p = 5$ | 131.10           | 143.30         | 634.84         |
| $p = 6$ | 133.30           | 137.44         | 591.15         |
| $p = 7$ | 131.10           | 137.95         | 647.89         |
| $p = 8$ | 135.25           | 135.86         | 605.90         |
| $p = 9$ | 131.10           | 142.22         | 626.31         |
| $p = 10$ | 131.10           | 137.32         | 665.15         |
| $p = 11$ | 131.10           | 137.95         | 609.20         |
| $p = 12$ | 133.29           | 133.79         | 560.37         |
| $p = 13$ | 131.10           | 137.93         | 643.55         |
| $p = 14$ | 131.10           | 135.37         | 559.72         |
| $p = 15$ | 131.10           | 131.10         | 628.63         |

KPP$_{sample}$ obtained almost the same min-SE value before $N < 20$ which is smaller than that obtained by KPP. Figure 3(b) shows that for the D$_{31}$ data set, none of the compared algorithms achieve the global minimum before $N = 40$. However, INCKPP$_{sample}$ gets a smaller min-SE value for all $N$ compared with other four algorithms. From Table 23 it is seen that INCKPP$_{sample}$ obtains the smallest value of $\#iter$ on both Shape data sets, D$_{31}$ and R$_{15}$. INCKPP$_{sample}$ gets the smallest aver-SE value on D$_{31}$ and a slightly bigger
Table 17: The experiment results on the dim\textsubscript{15} dataset for different \( p \), where the meaning of the values is the same as that in Table 4.

| \( \text{dim}_{15} (N = 2) \) | \( \text{INCKPP}_{\text{sample}} \) | \( \text{KPP}_{\text{sample}} \) | \( \text{FKM}_{\text{sample}} \) |
|-----------------------------|----------------|----------------|----------------|
| \( p = 5 \)                | 710.39         | 798.00         | 2560.88        |
| \( p = 6 \)                | 710.42         | 813.30         | 2464.89        |
| \( p = 7 \)                | 702.09         | 797.82         | 2409.37        |
| \( p = 8 \)                | 702.09         | 723.13         | 2439.26        |
| \( p = 9 \)                | 702.09         | 750.05         | 2578.53        |
| \( p = 10 \)               | 720.68         | 745.61         | 2337.29        |
| \( p = 11 \)               | 710.41         | 720.65         | 2526.35        |
| \( p = 12 \)               | 710.37         | 754.38         | 2522.34        |
| \( p = 13 \)               | 712.37         | 740.11         | 2587.71        |
| \( p = 14 \)               | 702.09         | 710.39         | 2457.90        |
| \( p = 15 \)               | 718.72         | 727.02         | 2594.46        |

Table 18: The experiment results on the dim\textsubscript{2} dataset for different \( N \), where the meaning of the values is the same as that in Table 8.

| \( \text{dim}_{2} (p=10) \) | \( \text{INCKPP}_{\text{sample}} \) | \( \text{KPP} \) | \( \text{KPP}_{\text{sample}} \) | \( \text{FKM} \) | \( \text{FKM}_{\text{sample}} \) |
|-----------------------------|----------------|----------------|----------------|----------------|----------------|
| \( N = 1 \)                | 14.05          | 14.74          | 13.95          | 73.57          | 75.71          |
| \( N = 2 \)                | 12.62          | 14.71          | 12.95          | 66.73          | 69.38          |
| \( N = 3 \)                | 12.62          | 13.61          | 12.62          | 64.06          | 66.10          |
| \( N = 5 \)                | 12.62          | 12.62          | 12.62          | 61.78          | 59.62          |

Table 19: The experiment results on the dim\textsubscript{6} dataset for different \( N \), where the meaning of the values is the same as that in Table 8.

| \( \text{dim}_{6} (p=10) \) | \( \text{INCKPP}_{\text{sample}} \) | \( \text{KPP} \) | \( \text{KPP}_{\text{sample}} \) | \( \text{FKM} \) | \( \text{FKM}_{\text{sample}} \) |
|-----------------------------|----------------|----------------|----------------|----------------|----------------|
| \( N = 1 \)                | 156.13         | 153.58         | 162.74         | 674.91         | 627.56         |
| \( N = 2 \)                | 131.10         | 140.13         | 140.00         | 650.18         | 625.60         |
| \( N = 3 \)                | 131.10         | 135.86         | 131.10         | 564.67         | 621.05         |
| \( N = 5 \)                | 131.10         | 131.10         | 131.10         | 467.92         | 478.57         |

Aver-SE value than the smallest aver-SE value obtained by KPP on \text{R}_{15}. Thus we may conclude that INCKPP\text{sample} outperforms the other four algorithms on \text{D}_{31} and has a similar performance on \text{R}_{15} with KPP_{sample}.
Table 20: The experiment results on the dim$_{10}$ dataset for different $N$, where the meaning of the values is the same as that in Table 8.

| $N$  | Inckpp$_{sample}$ | Kpp | Kpp$_{sample}$ | FKM | FKM$_{sample}$ |
|------|------------------|-----|----------------|-----|----------------|
| 1    | 363.51           | 324.00 | 339.65 | 1305.50 | 1217.07       |
| 2    | 309.42           | 323.34 | 333.06 | 1208.80 | 1174.50       |
| 3    | 304.78           | 314.29 | 304.78 | 1130.92 | 1130.72       |
| 5    | 304.78           | 304.78 | 304.78 | 1018.94 | 1001.97       |

Table 21: The experiment results on the dim$_{15}$ dataset for different $N$, where the meaning of the values is the same as that in Table 8.

| $N$  | Inckpp$_{sample}$ | Kpp | Kpp$_{sample}$ | FKM | FKM$_{sample}$ |
|------|------------------|-----|----------------|-----|----------------|
| 1    | 764.72           | 805.11 | 844.30 | 2515.94 | 2516.30       |
| 2    | 710.40           | 762.54 | 762.28 | 2465.36 | 2425.54       |
| 3    | 702.09           | 702.09 | 710.38 | 2394.93 | 2348.65       |
| 5    | 702.09           | 702.09 | 702.09 | 1867.72 | 2228.30       |

Table 22: The experiment results on the Dim-sets with $p = 10$, where the meaning of the criteria is the same as that in Table 12.

| Data set | Inckpp$_{sample}$ | KPP | KPP$_{sample}$ | FKM | FKM$_{sample}$ |
|----------|------------------|-----|----------------|-----|----------------|
| dim$_2$  |                  |     |                |     |                |
| $10$     | 1.07             | 15.65 | 10.84 | 15.44 | 11.68 | 11.14 | 15.41 | 3.84 | 4.50 | 7.39 | 4.87 | 3.62 | 7.24 |
| dim$_6$  |                  |     |                |     |                |
| $10$     | 1.02             | 144.38 | 11.01 | 11.03 | 15.55 | 11.10 | 11.05 | 15.24 | 5.36 | 2.42 | 642.25 | 7.09 | 1.53 | 611.86 |
| dim$_{10}$ |                 |     |                |     |                |
| $10$    | 1.04             | 337.71 | 10.83 | 1.09 | 348.93 | 10.79 | 1.10 | 351.33 | 5.08 | 2.81 | 1258.89 | 6.73 | 1.84 | 1215.27 |
| dim$_{15}$ |                |     |                |     |                |
| $10$    | 1.03             | 781.53 | 11.10 | 1.07 | 814.81 | 11.06 | 1.07 | 810.90 | 5.64 | 2.22 | 2485.81 | 7.47 | 1.98 | 244.56 |

Table 23: The experiment results on the Shape-sets with $p = 10$, where the meaning of the criteria is the same as that in Table 12.

| Data set | Inckpp$_{sample}$ | KPP | KPP$_{sample}$ | FKM | FKM$_{sample}$ |
|----------|------------------|-----|----------------|-----|----------------|
| R$_5$    |                  |     |                |     |                |
| $10$     | 3.09             | 19.92 | 9.32 | 21.24 | 19.84 | 11.38 | 11.36 | 20.16 | 7.81 | 4.31 | 28.95 | 8.51 | 4.08 | 28.53 |
| D$_5$    |                  |     |                |     |                |
| $10$     | 5.43             | 124.58 | 10.40 | 7.36 | 125.55 | 11.11 | 7.42 | 126.26 | 7.61 | 5.52 | 128.34 | 10.06 | 5.14 | 138.45 |

4.5. Experiments on real world data sets

In this subsection, we conduct experiments on seven real-world data sets to compare our algorithms INCKPP and INCKPP$_{sample}$ with INCKM, KPP, KPP$_{sample}$, FKM and FKM$_{sample}$.

We now compare INCKPP with INCKM. Table 24 presents the experiment results of INCKPP and INCKM on the real world data sets: pendigits$_3$, pendigits$_5$, pendigits$_8$, pendigits, yeast, banknote, newthyroid. The results illustrate that INCKPP achieves the smallest min-SE value (min-SE*) within
Figure 4: The the min-SE value against $p$ of INCKPP$_{sample}$, KPP$_{sample}$ and FKM$_{sample}$ on the Shape data sets when $N = 10$, where the meaning of the criteria is the same as in Table 4.

Figure 5: The the min-SE value against $N$ of INCKPP$_{sample}$, KPP, KPP$_{sample}$, FKM and FKM$_{sample}$ on the Shape data sets when $p = 10$, where the meaning of the criteria is the same as in Table 8.

the CPU time used by INCKM on the seven data sets.

4.5.1. Experiments on the Handwritten digits data sets

We first compare the clustering performance of the three sampled algorithms, INCKPP$_{sample}$, KPP$_{sample}$ and FKM$_{sample}$ on the handwritten digits data sets for different $p$ with $N = 10$. Figure 6 presents the experimental results obtained by INCKPP$_{sample}$, KPP$_{sample}$ and FKM$_{sample}$ on the four
Table 24: Comparison between INCKM and INCKPP, where the meaning of the criteria is the same as in Table 3

| Data sets | λ  | min-SE | #it | min-SE | #repe | #it |
|-----------|----|--------|-----|--------|-------|-----|
| pendigits 3 | 1.5 | 1673.30 | 2.00 | 1466.98 | 13.58 | 2.20 |
| pendigits 5 | 1.8 | 2492.06 | 5.64 | 2428.09 | 17.06 | 3.22 |
| pendigits 8 | 1.9 | 3664.18 | 4.09 | 3619.82 | 14.18 | 2.86 |
| pendigits 1.7 | 5125.03 | 1.45 | 4968.93 | 14.35 | 2.64 |
| yeast 1.7 | 293.22 | 1.64 | 282.42 | 11.85 | 1.57 |
| banknote 1.5 | 406.68 | 3.64 | 406.68 | 13.14 | 3.38 |
| newthyroid 2.2 | 41.30 | 1.27 | 41.30 | 11.81 | 2.06 |

handwritten digits data sets, pendigits, pendigits8, pendigits5, pendigits3, within the same CPU time used by INCKPPsample running 5, 10, 10, 10 times, respectively, on the four data sets. The results in Figure 6 shows that INCKPPsample gets the best clustering performance with the smallest min-SE on the handwritten digits data sets except for the pendigits5 dataset, for which FKMsample gets a smaller min-SE than INCKPPsample does when p = 11 and 13.

We now compare INCKPPsample, KPPsample and FKMsample with the conventional KPP and FKM algorithms on the four handwritten digits data sets for different N with p = 10. Figure 7 presents the clustering results against N of INCKPPsample, KPP, KPPsample, FKM and FKMsample on the four handwritten digits data sets when p = 10. Figures 7 (b)-(d) illustrate that for pendigits8, pendigits5 and pendigits3, INCKPPsample gets a smaller min-SE value compared with the other four algorithms and first achieves the global minimum at N = 20, 10, 5, respectively, on the three data sets. Figure 3 (a) illustrates that for pendigits, all five compared algorithms do not achieve the global minimum before N = 40 but INCKPPsample gets a much smaller min-SE value for each N compared with the other four algorithms. Table 25 shows that INCKPPsample obtains the smallest aver-SE value on pendigits, pendigits8 and pendigits3 and a slightly larger aver-SE value than that obtained by KPPsample on pendigits5. In addition, FKMsample obtains the smallest #repe value on pendigits, pendigits5 and pendigits3 and a lightly larger #repe value than that obtained by INCKPPsample on pendigits8. In conclusion, INCKPPsample has a better clustering performance compared with the other four compared algorithms on the four handwritten digits data sets.
Figure 6: The experiment results on the four handwritten digits data sets for different $p$ with $N = 10, 10, 10$ and $5$, respectively, where the meaning of the criteria is the same as in Table 4.

Table 25: The experiment results on the four handwritten digits data sets with $p = 10$, where the meaning of the criteria is the same as in Table 12.

| Data set | INCKPP sample | KPP sample | KPP sample | FKM sample | FKM sample |
|----------|---------------|------------|------------|------------|------------|
|          | $\#re$ | $\#it$ | aver-SE | $\#re$ | $\#it$ | aver-SE | $\#re$ | $\#it$ | aver-SE | $\#re$ | $\#it$ | aver-SE |
| pendigits | 10 | 2.79 | 5459.56 | 7.14 | 4.16 | 5199.83 | 7.14 | 4.14 | 5170.10 | 7.54 | 4.55 | 5220.36 |
| pendigits | 8 | 2.42 | 3854.31 | 7.05 | 3.96 | 3961.72 | 7.16 | 3.96 | 3865.13 | 6.14 | 4.46 | 3972.75 |
| pendigits | 10 | 10.16 | 1565.10 | 7.08 | 2.43 | 1574.32 | 7.08 | 2.43 | 1574.10 | 7.46 | 4.06 | 1649.26 |

4.5.2. Experiments on yeast, banknote and newthyroid data sets

We now compare the clustering performance of the three sampled algorithms, INCKPP sample, KPP sample and FKM sample, and the conventional
Figure 7: The experiment results on the four handwritten digits data sets for different \( N \) with \( p = 10 \), where the meaning of the criteria is the same as in Table 8.

KPP and FKM algorithms on the yeast, banknote and newthyroid data sets.

Figure 8 shows the min-SE value obtained by \( \text{INCKPP} \) sample, \( \text{KPP} \) sample and \( \text{FKM} \) sample on the yeast, banknote and newthyroid data sets for different \( p \) with \( N = 10 \), where the min-SE value was obtained by the three algorithms within the same CPU time as used by \( \text{INCKPP} \) sample running 10 times. From Fig 8(a) it is seen that \( \text{INCKPP} \) sample and \( \text{KPP} \) sample get a much smaller min-SE value than that obtained by \( \text{FKM} \) sample on the yeast dataset with \( \text{INCKPP} \) sample achieving the smallest min-SE value, from Fig 8(b) it is observed that \( \text{INCKPP} \) sample gets the the smallest min-SE value on the banknote dataset among the three algorithms except for \( p = 5 \) where both \( \text{KPP} \) sample and \( \text{FKM} \) sample achieve a smaller min-SE value than that obtained
by \text{INCKPP}_{\text{sample}} \text{ and for } p = 11 \text{ where INCKPP}_{\text{sample}} \text{ and FKM}_{\text{sample}} \text{ get the same min-SE value which is bigger than that got by KPP}_{\text{sample}}, \text{ whilst from Fig 8(b) it is found that, on the newthyroid dataset, KPP}_{\text{sample}} \text{ gets the smallest min-SE value and FKM}_{\text{sample}} \text{ gets the largest min-SE value among the three comparing algorithms for } p < 10, \text{ but for } p \geq 10 \text{ INCKPP}_{\text{sample}} \text{ and KPP}_{\text{sample}} \text{ almost get the same min-SE value which is much smaller than that obtained by FKM}_{\text{sample}}. \text{ It is then concluded from the above discussions that INCKPP}_{\text{sample}} \text{ achieves an overall better clustering performance than KPP}_{\text{sample}} \text{ and FKM}_{\text{sample}} \text{ have on the three data sets.}

We now compare \text{INCKPP}_{\text{sample}}, \text{KPP}_{\text{sample}} \text{ and FKM}_{\text{sample}} \text{ with the conventional KPP and FKM algorithms on the three data sets for different } N \text{ with } p = 10.

Figure 9 presents the clustering results against \( N \) of \text{INCKPP}_{\text{sample}}, \text{KPP}, \text{KPP}_{\text{sample}}, \text{FKM} \text{ and FKM}_{\text{sample}} \text{ on the three data sets for } p = 10. \text{ Figure 9 (a) shows that INCKPP}_{\text{sample}} \text{ gets the smallest min-SE value on the yeast dataset for all values of } N \text{ among the five comparing algorithms. It is seen from Figure 9 (b) that for the banknote dataset INCKPP}_{\text{sample}} \text{ and FKM}_{\text{sample}} \text{ achieve the global minimum at } N = 5 \text{ and } N = 7, \text{ respectively. From Figure 9 (c) it is seen that for the newthyroid dataset KPP}_{\text{sample}} \text{ has the best performance among the five comparing algorithms and is the only one which achieves the global minimum at } N = 5 \text{ with the smallest min-SE value among those obtained by the five comparing algorithms, whilst the min-SE value obtained by INCKPP}_{\text{sample}} \text{ decreases faster than those obtained by KPP, FKM and FKM}_{\text{sample}} \text{ do with } N \text{ increasing and is the second smallest at } N = 5. \text{ As a result, the clustering performance of INCKPP}_{\text{sample}} \text{ is better than that of the other four comparing algorithms on the yeast and banknote datasets, but KPP}_{\text{sample}} \text{ outperforms the other four comparing algorithms on the newthyroid dataset.}

Table 26: Experiment results of \text{INCKPP}_{\text{sample}}, \text{KPP}_{\text{sample}}, \text{FKM}_{\text{sample}}, \text{KPP} \text{ and FKM} \text{ on the yeast, banknote and newthyroid data sets when } p = 10, \text{ where the meaning of the criteria is the same as in Table 12.}

| Data set      | \( \#\text{re} \) | \( \#\text{it} \) | aver-SE | \( \#\text{re} \) | \( \#\text{it} \) | aver-SE | \( \#\text{re} \) | \( \#\text{it} \) | aver-SE | \( \#\text{re} \) | \( \#\text{it} \) | aver-SE | \( \#\text{re} \) | \( \#\text{it} \) | aver-SE |
|---------------|----------------|----------------|---------|----------------|----------------|---------|----------------|----------------|---------|----------------|----------------|---------|----------------|----------------|---------|
| yeast         | 10             | 2.59           | 292.80  | 2.94           | 292.74         | 9.48     | 2.68           | 292.74         | 9.80     | 2.96           | 290.05         | 10.84   | 3.02           | 296.26         | 11.78   | 2.44           | 295.48         |
| banknote      | 10             | 1.99           | 410.14  | 2.26           | 410.58         | 3.26     | 2.66           | 411.08         | 3.44     | 2.79           | 411.25         | 3.91    | 2.95           | 411.85         | 10.63   | 1.88           | 411.77         |
| newthyroid    | 10             | 2.18           | 42.94   | 2.96           | 42.84          | 13.16    | 2.31           | 42.95          | 12.91    | 2.61           | 43.58          | 14.06   | 2.23           | 43.34          | 26      |
Figure 8: The min-SE value obtained by INCKPP\textsubscript{sample}, KPP\textsubscript{sample} and FKM\textsubscript{sample} on the yeast, banknote and newthyroid sets for different $p$ with $N = 10$, where the meaning of the criteria is the same as in Table 4.

5. Conclusions

In this paper, we proposed a novel incremental $k$-medoids algorithm (named INCKPP). INCKPP addressed the parameter selection issue in the improved $k$-medoids algorithm and thus can dynamically increase the number of clusters from 2 to $k$ through a nonparametric and stochastic $k$-means++ search procedure. INCKPP can also deal with imbalanced datasets very well. We further proposed a modified INCKPP algorithm (named INCKPP\textsubscript{sample}) which is fast and improves the computational efficiency of INCKPP without affecting its clustering performance. Extensive experiments results on synthetic and real-world data sets including imbalanced data sets have been con-
Figure 9: The min-SE value obtained by INCKPP sample, KPP sample, FKM sample, KPP and FKM on the yeast, banknote and newthyroid sets for different $N$ with $p = 10$, where the meaning of the criteria is the same as in Table 8.

ducted in comparison with three state-of-the-art algorithms: the improved $k$-medoids algorithm (INCKM), the simple and fast $k$-medoids algorithm (FKM) and the $k$-means++ algorithm (KPP) and illustrated the effectiveness of our algorithm.

References

References

[1] Arthur, D. and Vassilvitskii, S. (2007). $k$-means++: The advantages of careful seeding. In Proc. 8th ann. ACM-SIAM Symposium on Discrete
Algorithms, pages 1027–1035. SIAM.

[2] Bagirov, A. M. (2008). Modified global k-means algorithm for minimum sum-of-squares clustering problems. *Pattern Recognition*, 41(10):3192–3199.

[3] Bai, L., Liang, J., Sui, C., and Dang, C. (2013). Fast global k-means clustering based on local geometrical information. *Information Sciences*, 245:168–180.

[4] Berkhin, P. (2006). A survey of clustering data mining techniques. In *Group. Multidimens. Data*, pages 25–71. Springer.

[5] Boutsidis, C., Zouzias, A., Mahoney, M. W., and Drineas, P. (2015). Randomized dimensionality reduction for k-means clustering. *IEEE Transactions on Information Theory*, 61(2):1045–1062.

[6] Broin, P. Ó., Smith, T. J., and Golden, A. A. (2015). Alignment-free clustering of transcription factor binding motifs using a genetic-k-medoids approach. *BMC Bioinformatics*, 16(1):1–12.

[7] Canas, G., Poggio, T., and Rosasco, L. (2012). Learning manifolds with k-means and k-flats. In *Proc. NIPS*, pages 2465–2473.

[8] Coates, A. and Ng, A. Y. (2011). The importance of encoding versus training with sparse coding and vector quantization. In *Proc. 28th ICML*, pages 921–928.

[9] Erisoglu, M., Calis, N., and Sakallioglu, S. (2011). A new algorithm for initial cluster centers in k-means algorithm. *Pattern Recognition Letters*, 32(14):1701–1705.

[10] Kaufman, L. and Rousseeuw, P. J. (2009). *Finding Groups in Data: an introduction to Cluster Analysis*, volume 344. John Wiley.

[11] Lai, J. Z. and Huang, T.-J. (2010). Fast global k-means clustering using cluster membership and inequality. *Pattern Recognition*, 43(5):1954–1963.

[12] Likas, A., Vlassis, N., and Verbeek, J. J. (2003). The global k-means clustering algorithm. *Pattern Recognition*, 36(2):451–461.
[13] Ng, R. T. and Han, J. (2002). Clarans: A method for clustering objects for spatial data mining. *IEEE Transactions on Knowledge and Data Engineering*, (5):1003–1016.

[14] Park, H.-S. and Jun, C.-H. (2009). A simple and fast algorithm for k-medoids clustering. *Expert Systems with Applications*, 36(2):3336–3341.

[15] RDUSSEEUN, L. K. P. J. (1987). Clustering by means of medoids.

[16] Rodriguez, A. and Laio, A. (2014). Clustering by fast search and find of density peaks. *Science*, 344(6191):1492–1496.

[17] Selim, S. Z. and Ismail, M. A. (1984). K-means-type algorithms: a generalized convergence theorem and characterization of local optimality. *IEEE Transactions on Pattern Analysis and Machine Intelligence*, (1):81–87.

[18] Wu, X., Kumar, V., Quinlan, J. R., et al. (2008). Top 10 algorithms in data mining. *Knowledge and Information Systems*, 14(1):1–37.

[19] Xia, S., Peng, D., Meng, D., Zhang, C., Wang, G., Giem, E., Wei, W., and Chen, Z. (2022). Ball k-means: fast adaptive clustering with no bounds. *IEEE Transactions on Pattern Analysis and Machine Intelligence*, 44(1):87–99.

[20] Xie, J. and Qu, Y. (2016). K-medoids clustering algorithms with optimized initial seeds by density peaks. *Journal of Frontiers of Computer Science and Technology*, 10(02):230–247.

[21] Yu, D., Liu, G., Guo, M., and Liu, X. (2018). An improved k-medoids algorithm based on step increasing and optimizing medoids. *Expert Systems with Applications*, 92:464–473.

[22] Zadegan, S. M. R., Mirzaie, M., and Sadoughi, F. (2013). Ranked k-medoids: A fast and accurate rank-based partitioning algorithm for clustering large datasets. *Knowledge-Based Systems*, 39:133–143.

[23] Žalik, K. R. (2008). An efficient k’-means clustering algorithm. *Pattern Recognition Letters*, 29(9):1385–1391.