New search strategies and a new derived inequality for efficient k-medoids-based algorithms

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Abstract

In this paper, a new inequality is derived which can be used for the problem of nearest neighbor searching. We also present a searching technique referred to as a previous medoid index to reduce the computation time particularly for the k-medoids-based algorithms. A novel method is also proposed to reduce the computational complexity by the utilization of memory. Four new search strategies for k-medoids-based algorithms based on the new inequality, previous medoid index, the utilization of memory, triangular inequality criteria and partial distance search are proposed. Experimental results demonstrate that the proposed algorithm applied to the *CLARANS* algorithm may reduce the computation time from 88.8% to 95.3% with the same average distance per object comparing with *CLALRANS*. The derived new inequality and proposed search strategies can also be applied to the nearest neighbor searching and the other clustering algorithms.

1 Introduction

The goal of clustering , in general, is to group sets of objects into classes such that homogeneous objects are placed in the same cluster while dissimilar objects are in separate clusters. Clustering (or classification) techniques are common forms

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of data mining [1] and have been studied extensively in image compression [2], texture segmentation [3], computer vision [4], vector quantization [5, 6], medicine and marketing. Recent works in the database community have been proposed including *CLARANS* [15], *BIRCH* [9], *CURE* [10], *CACTUS* [11], *CHAMELEON* [12] and *DBSCAN* [13]. No single algorithms is appropriate for all types of objects, nor are all algorithms suitable for all problems, however, the k-medoids algorithms [8] have been experimentally shown to be more robust and effective than k-means [7] in the presence of noise and outliers and are not generally influenced by the order of presentation of objects.

Partitioning Around Medoids (*PAM*) [8], Clustering LARge Applications (*CLARA*) [8] and Clustering Large Applications based on RANdomized Search (*CLARANS*) [14] are three well known k-medoids-based algorithms. To improve the performance of medoids generation, Clustering Large Applications based on Simulated Annealing (*CLASA*) algorithm applied the simulated annealing to select better medoids [16]. The fuzzy theory is also applied to develop fuzzy k-medoids algorithms [17] and genetic algorithm is applied to get genetic k-medoids algorithm [18]. In this paper, we derive a new inequality for the problem of nearest neighbor searching and present the technique of previous medoid index, the utilization of memory for efficient clustering algorithms.

2 Proposed algorithms

2.1 Literature review

The basic idea of k-medoids-based algorithms are designed for processing large data set, however, all existing k-medoids-based algorithms are exhaustive enumeration. The computational complexity of k-medoids-based algorithms can be reduced by applying the concept in VQ-based codeword search [19, 20, 21, 22, 23, 25, 26, 27, 28, 30, 31, 32]. In VQ-based signal compression, the efficient codeword searching algorithms have never been applied to k-medoids-based algorithms. The partial distance search (*PDS*) algorithm [19] is a simple and efficient codeword search algorithm which consists of a simple modification to the way that distances are calculated. During the computation of the distance measure, if the partial distance exceeds the distance to the nearest neighbor found so far, the computation is premature. Given the squared Euclidean distance measure, one object $x = x_1, x_2, \ldots, x_k$ and two medoids (i.e. representative objects) $o_p = o_{p1}, o_{p2}, \ldots, o_{pk}$ and $o_j = o_{j1}, o_{j2}, \ldots, o_{jk}$, assume the current minimum distance is

$$D(x, o_p) = \sum_{i=1}^{d} (x_i - o_{pi})^2 = D_{min}, \tag{1}$$

$$if \qquad \sum_{i=1}^{h} (x_i - o_{ji})^2 \geq D_{min}, \tag{2}$$

$$then \qquad D(x, o_j) \geq D(x, o_p), \tag{3}$$

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where $1 \leq h \leq k$. The efficiency of *PDS* is derived from the elimination of an unfinished distance computation if its partial accumulated distortion is larger than the current minimum distance. This will reduce $(k-h)$ multiplications and $2(k-h)$ additions at the expense of h comparisons.

Vidal proposed the approximating and elimination search algorithm (AESA) [20] whose computation time is approximately constant for a codeword search in a large codebook size. The high correlation characteristics between data vectors of adjacent speech frames and the triangular inequality elimination (TIE) criterion were utilized to VQ-based recognition of isolated words [21]. However, the TIE criterion requires considerable memory of size $\frac{(N-1)N}{2}$ to store the distance between any pair of codewords. The *equal-average nearest neighbor search* (ENNS) algorithm [22, 32] uses the mean of an input vector to eliminate the impossible codewords. This algorithm reduces a great deal of computation time compared with the conventional full-search algorithm with only k additional memory, where k is the number of codewords (or the number of medoids for k-medoids-based algorithms). The improved algorithm [23] uses the variance as well as the mean of an input vector. It can be referred to as the *equal-average equal-variance nearest neighbor search* (EENNS) algorithm.

The bound for Minkowski metric and quadratic metric was derived and applied to codeword search [24]. The partial distance search (PDS) [19], absolute error inequality criterion (AEI) [25] and the improved absolute error inequality criterion (IAEI) [26] are all special cases in the bound for Minkowski metric. An inequality was also derived from IAEI criterion to improve the codeword search of the image coding [27]. This inequality can be interpreted as the generalized form of the basic inequality used in ENNS algorithm [22]. The improved ENNS algorithm in paper [27] can be referred to as IENNS algorithm. In that algorithm, a vector is separated into two sub-vectors, one is composed of the first half of the coordinates and the other is composed of the remaining coordinates. Two inequalities based on the sums of its two sub-vectors are used to reject those codewords which cannot be rejected by ENNS algorithm. A new inequality was also derived based on Hadamard transform for efficient codeword search [29] demonstrated it is superior to ENNS and IENNS algorithms. An inequality for fast codeword search based on the mean-variance pyramid was also derived [28] and an inequality designed based on the training approach was also proposed for efficient codeword search [30].

2.2 Derivation of new inequality

Triangular inequality elimination (TIE) criteria are efficient methods for applying to nearest neighbor search. Let X be the set of objects and O be the set of medoids and x, y, z belong to the set X. Assume the distance measure existing for defining the mapping $d : X \times X \rightarrow R$, is used to fulfill the following metric properties:

$$d(x, y) \geq 0; \tag{4}$$

$$d(x, y) = 0 \quad iff \quad x = y \tag{5}$$

$$d(x, y) = d(y, x) \tag{6}$$

$$d(x, y) + d(y, z) \geq d(x, z) \tag{7}$$

Let o_1, o_2, o_3 be three different medoids and t be an object, then three criteria are obtained as follows:

- Criterion 1. Given the triangular inequality:

$$d(t, o_2) + d(t, o_1) \geq d(o_1, o_2); \tag{8}$$

$$if \quad d(o_1, o_2) \geq 2d(t, o_1), \tag{9}$$

$$then \quad d(t, o_2) \geq d(t, o_1). \tag{10}$$

- Criterion 2. Given the triangular inequality:

$$d(o_3, o_2) \leq d(t, o_2) + d(t, o_3); \tag{11}$$

$$if \quad d(t, o_1) + d(t, o_2) \leq d(o_3, o_2), \tag{12}$$

$$then \quad d(t, o_1) \leq d(t, o_3). \tag{13}$$

- Criterion 3. Assume $\quad d(t, o_1) \leq d(t, o_2);$

$$Given \quad d(t, o_2) - d(t, o_3) \leq d(o_3, o_2), \tag{14}$$

$$if \quad d(o_3, o_2) \leq d(t, o_2) - d(t, o_1) \tag{15}$$

$$then \quad d(t, o_3) \geq d(t, o_1). \tag{16}$$

In Criterion 1, these distances between all pairs of medoids are computed in advance. If $Eq.12$ is satisfied, then we omit the computation of $d(x, o_2)$ if $d(x, o_1)$ has already been calculated. In this paper, Criterion is modified for a squared error distance measure. A table is made to store the one-fourth of squared distance between medoids,

$$if \quad d^2(o_1, o_2)/4 \geq d^2(x, o_1),$$

$$then \quad d(x, o_2) \geq d(x, o_1).$$

By merging criteria 2 and 3, we may get the following criterion, i.e.,

$$if \quad d(x, o_1) \leq |d(o_3, o_2) - d(x, o_2)| \tag{17}$$

$$then \quad d(x, o_3) \geq d(x, o_1) \tag{18}$$

Set

$$o_2 = \vec{0} \quad (zero\ vector).$$

Hence

$$if \quad d(x, o_1) \leq |d(o_3, \vec{o}) - d(x, \vec{0})|, \tag{19}$$

$$then \quad d(x, o_3) \geq d(x, o_1). \tag{20}$$

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For Euclidean distance measure and given

$$d_{min} = d(x, o_1),$$

$$if \quad d_{min} \leq |\sqrt{\sum_{i=1}^{d} o_{3i}^2} - \sqrt{\sum_{i=1}^{d} x_i^2}|, \tag{21}$$

$$then \quad d(x, o_3) \geq d_{min}. \tag{22}$$

Since $\sqrt{\sum_{i=1}^{d} o_{3i}^2}$ can be calculated off line and $\sqrt{\sum_{i=1}^{d} x_i^2}$ is only computed once for the nearest neighbor search, the derived inequality ($Eq.$ 22 $Eq.$ 25) is very efficient for the problem of nearest neighbor search.

2.3 Previous medoid index

Most of the k-medoids-based algorithms have to examined whether a nonmedoid object is a good replacement for a current medoid. Since only one medoid is changed, most of the objects will belong to the cluster represented by the same medoid. By using this property, we may calculate the distance between the object and its previous medoid index firstly. Owing to the probability is very eminent for the object belong to the same medoid index, the distance is very small. If we get a very small distance between the object and one medoid, then it is easier to use Criterion 1 of *TIE*, partial distance search or the derived inequality to reduce the distance computation.

2.4 Utilization of memory

Assume k medoids $o_j, j = 1, \ldots, k$, are chosen from T objects $x_i,\ i = 1, \ldots, T$ and the number of dimension for each object or medoid is n. The size of the memory for all objects in the database is Tn. If the distance table for each pair of objects, $d(x_i, x_j)$, $i \neq j$, $i, j = 1, \ldots, T$ are stored, then the size of memory for the distance table is $\frac{T(T-1)}{2}$. If this memory is available, then the distance calculation need be performed just the once, whether for the *PAM*, *CLARA* and *CLARANS* algorithms. All these algorithms will thus be very efficient, and the computational complexity will be similar. Unfortunately, if object numbers are large, memory is not always available. We thus propose a new approach which uses only $T - k$ memory to store the distance, but it may reduce the number of distance computations from $(T - k)k$ to $T - 1 + r(k - 1)$ (i.e. from $O(Tk)$ to $O(T)$) for the test of the swap between object o_{new} and o_{old}. ,where r is the number of objects whose nearest medoids are swapped. The probability to swap the nearest medoid with any object is $1/k$, so $r \approx T/k$. Assume $NM(x_i)$ is the nearest medoid to

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the object x_i before swap, the total distance difference before and after the swap of object o_{new} and medoid o_{old} can be expressed as

$$D_t' - D_t = \sum_{i \neq new, NM(x_i) \neq o_{old}} \min[d(x_i, NM(x_i)), d(x_i, o_{new})] +$$

$$\min[d(o_{old}, o_j), d(o_{old}, o_{new}),\ j = 1, \ldots, k, j \neq old] +$$

$$\sum_{i \neq new, NM(x_i) = o_{old}, x_i \in S_p} d(x_i, o_p) - \sum_i d(x_i, NM(x_i)) \quad (23)$$

If the distances $d(x_i, NM(x_i))$, $i = 1, \ldots, T-k$ are stored, then only $(T - k - 1 - r)$ distances need to be computed for $d(x_i, o_{new})$, $i = 1, \ldots, T-k, i \neq new, NM(x_i) \neq o_{old}$ and k distances computation for $d(o_{old}, o_j)$ and $d(o_{old}, o_{new})$, $j = 1, \ldots, k, j \neq old$ and rk distances computation for $d(x_i, o_p)$, $i = 1, \ldots, T-k$, $NM(x_i) = o_{old}$. Since the size $(T-k)$ memory space is generally reasonable for the clustering of the objects with memory size Tn, it is useful approach. Note that this approach can be applied to *PAM*, *CLARA*, *CLARANS* and our proposed *CLASA* algorithms.

3 Experimental results

3.1 Databases

Three artificial databases were used for the experiments as follows:

1. 3,000 objects with 8 dimensions are generated from the Gauss-Markov source that is of the form $y_n = \alpha y_{n-1} + w_n$ where w_n is a zero-mean, unit variance, Gaussian white noise process, with $\alpha = 0.5$.
2. 12,000 objects with 2 dimensions collected from twelve elliptic clusters.
3. 5000 objects with 2 dimensions are generated from curve database. The object (x, y) is collected from the form $-2 \leq x \leq 2$ and $y = 8x^3 - x$.

3.2 Experiments

In this paper, four search strategies are presented. These four search strategies are applied to *CLARANS* algorithm. The *CLARANS-TP* algorithm is the first extended version of *CLARANS* algorithm that applies the first criterion of triangular inequality elimination (TIE). *CLARANS* algorithm with previous medoid index, TIE and PDS is referred to as *CLARANS-ITP*. *CLARANS* with the proposed utilization of memory is referred to as *CLARANS-M*. Application of the proposed new inequality, previous medoid index, the proposed utilization of memory and partial distance search algorithm to *CLARANS* is referred to as *CLARANS-MITmP*. Experiments were carried out to test the number of distances calculation and the average distance per object for *CLARANS*, *CLARANS-TP*, *CLARANS-ITP*, *CLARANS-M* and *CLARANS-MITmP* algorithms. Since the computation time depends not only on the clustering algorithm but also on the use of computation facility. It is better

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Table 1: Results of experiment for Gauss-Markov source.

seed	***CLARANS*** Count of distance (10^5)	***CLARANS-TP*** Count of distance (10^5)	***CLARANS-ITP*** Count of distance (10^5)	***CLARANS-M*** Count of distance (10^5)	***CLARANS-MITmP*** Count of distance (10^5)	Ave. dist.
1	37604	17658	12572	2330	1784	4.43227
2	53234	24865	17678	3293	2524	4.35912
3	37512	17629	12346	2324	1779	4.38063
4	40559	19101	13342	2511	1923	4.39766
5	39694	18521	13058	2458	1880	4.36724
6	41370	19318	13672	2563	1963	4.38396
7	32312	14962	10566	2004	1526	4.37978
8	39600	18442	12956	2455	1877	4.39364
9	36707	17091	11972	2276	1737	4.37717
10	35835	16671	11879	2221	1699	4.40632
Ave.	39443	18426	13004	2444	1869	4.38778

to choose one measure criterion so that the measure results are the same for all types of computers and this measure criterion is proportional to the computation time. That is why we choose the number of distance calculation as the benchmark. Squared Euclidean distance measure is used for the experiments. The Gauss-Markov source was used for the first experiment. 32 medoids are selected from 3000 objects. For *CLARANS* algorithm, the parameters *numlocal* and *maxneighbor* are set to 5 and 1200, respectively. Experimental results are shown in Table 1, comparing with *CLARANS*, *CLARANS-MITmP*, *CLARANS-M*, *CLARANS-ITP* and *CLARANS-TP* may reduce the computational complexity by 95.3%, 93.8%, 67% and 53.3%, respectively.

The twelve elliptic clusters were used for the second experiment. 12 medoids are selected from 12000 objects. For *CLARANS* algorithm, the parameters *numlocal* and *maxneighbor* are set to 5 and 1800, respectively. As shown in Fig. 1, comparing with *CLARANS*, *CLARANS-MITmP*, *CLARANS-M*, *CLARANS-ITP* and *CLARANS-TP* may reduce the computational complexity by 88.8%, 84%, 84.3% and 61.2%, respectively.

The curve database was used for the third experiment. 20 medoids are selected from 5000 objects. For *CLARANS* algorithm, the parameters numlocal and maxneighbor are set to 5 and 1250, respectively. As shown in Table 2, comparing with *CLARANS*, *CLARANS-MITmP*, *CLARANS-M*, *CLARANS-ITP* and *CLARANS-TP* may reduce the computational complexity by 94.3%, 90.2%, 92% and 74.4%, respectively.

4 Conclusions

In this paper, we derive a new inequality for the problem of nearest neighbor search, propose the utilization of memory and technique of previous medoid index for clustering algorithm. Four extended versions of *CLARANS* algorithm are presented. Experimental results based on Gauss-Markov, elliptic and curve databases demonstrate that applying the proposed hybrid method using derived new inequal-

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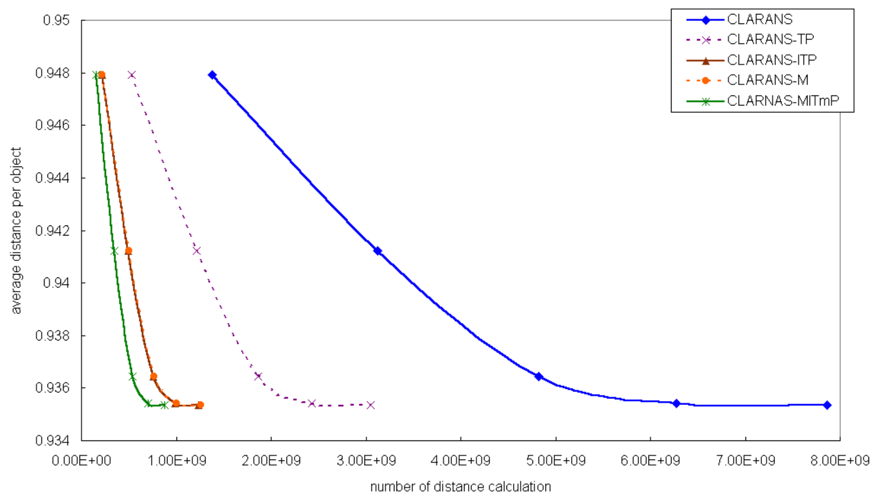

Figure 1: Performance comparison of *CLARANS*, *CLARANS-TP*, *CLARANS-ITP*, *CLARANS-M* and *CLARANS-MITmP* for twelve elliptic clusters.

Table 2: Results of experiment for curve clusters.

seed	*CLARANS* Count of distance (10^5)	*CLARANS-TP* Count of distance (10^5)	*CLARANS-ITP* Count of distance (10^5)	*CLARANS-M* Count of distance (10^5)	*CLARANS-MITmP* Count of distance (10^5)	Ave. dist.
1	65238	18049	5314	6380	3700	2.15118
2	62596	17214	5061	6074	3549	2.18127
3	70159	18097	5683	6894	3986	2.17871
4	71881	18528	5795	7029	4076	2.19157
5	57354	13927	4529	5604	3264	2.15642
6	62320	14631	4930	6095	3548	2.15689
7	65016	17204	5227	6360	3695	2.17072
8	63664	16960	5111	6198	3640	2.14399
9	55060	13399	4386	5384	3140	2.18530
10	48389	11093	3834	4739	2763	2.16522
Ave.	62166	15910	4987	6076	3536	2.16813

ity, previous medoid index, utilization of memory and partial distance search to *CLARANS* may reduce computational complexity from 88.8% to 95.3% comparing with *CLARANS*. Note that the proposed four search strategies may apply to the other clustering algorithms.

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