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A Parallel K-means Clustering Algorithm with MPI

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***Abstract*—Clustering is one of the most popular methods for data analysis, which is prevalent in many disciplines such as image segmentation, bioinformatics, pattern recognition and statistics etc. The most popular and simplest clustering algorithm is K-means because of its easy implementation, simplicity, efficiency and empirical success. However, the real-world applications produce huge volumes of data, thus, how to efficiently handle of these data in an important mining task has been a challenging and significant issue. In addition, MPI (Message Passing Interface) as a programming model of message passing presents high performances, scalability and portability. Motivated by this, a parallel K-means clustering algorithm with MPI, called MKmeans, is proposed in this paper. The algorithm enables applying the clustering algorithm effectively in the parallel environment. Experimental study demonstrates that MKmeans is relatively stable and portable, and it performs with low overhead of time on large volumes of data sets.**

Keywords-clustering, K-means algorithm, MPI, parallel computing

I. INTRODUCTION

Clustering is a method of unsupervised learning and a common technique for data analysis used in many disciplines, including image segmentation, bioinformatics, pattern recognition and statistics etc [1].

K-means is a well-known clustering algorithm for its simplicity and easy implementation. K-means was ranked second of top 10 algorithms in data mining by the ICDM Conference in October 2006, while C4.5 was ranked first [2]. Compared with other clustering algorithms, K-means algorithm has three major advantages covering simple implementation, efficient when handling a large data sets and a solid theoretical foundation based on the greedy optimization of Voronoi partition [3].

With the development of information technology, data volumes are becoming increasingly mass. Cloud computing is a form of technology that uses the Internet to maintain data and application. It is based on the development of distributed computing, parallel computing and grid computing [4]. Meanwhile, "Top 10 obstacles and opportunities for Cloud Computing" are presented in [5], which predict that cloud computing will grow and believe that computing, storage and networking must all focus on the horizontal scalability of virtualized resources rather than the performance of single node.

MPI (Message Passing Interface) is a library specification for message passing, which is proposed as a standard program model. MPI is an application programmer interface of message passing, together with protocol and semantic specifications for how its features must behave in any implementation [6]. MPI aims to maintain the high performance, scalability and portability.

Many scholars focus on the studies in the fields of parallel and distributed clustering. More specifically, (1) Rasmussen et al. suggested that the parallel processing using an array processor like the DAP (Distributed Array Processor) can provide significant speedups over serial processing for the hierarchic agglomerative cluster analysis of large data sets [7]. (2) Olson et al. considered parallel algorithms for hierarchical clustering using several inter-cluster distance metrics and parallel computer architectures [8]. (3) Zhao et al. proposed a fast parallel K-means clustering algorithm based on MapReduce. The proposed algorithm can scale well and efficiently to process large data sets on commodity hardware [9].

However, our contributions in this paper are as follows:

a) MKmeans, a parallel K-means clustering algorithm with MPI, is proposed.

b) The configuration of MPI parallel development platform based on open resource project Eclipse and MPICH in Windows is implemented. Our method can be ported to Linux or other platforms.

c) Experimental results illustrate that our MKmeans algorithm is relatively stable and portable, it improves the time performance of clustering on large data sets. Meanwhile, MPI is quite appropriate for the parallel and distributed computing environment.

The rest of this paper is organized as follows. Section 2 gives the related work. Section 3 mainly presents our MKmeans algorithm in detail. Section 4 shows our experimental results and performance evaluation. Finally, Section 5 concludes the paper and outlines our future work.

II. RELATED WORK

Related work including K-means clustering algorithm, MPI and Weka are involved in this section. More precisely, an outline on K-means is summarized in Section *A*, the brief introduction of MPI is given in Section *B* and a classical experimental tool Weka is described in Section *C*.

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A. K-means

The most popular and the simplest partitional algorithm is K-means [10]. K-means has a rich and diverse history as it was independently discovered in different scientific fields by Steinhaus (1956), Lloyd (proposed in 1957, published in 1982), Ball and Hall (1965), and MacQueen (1967) [1]. K-means is a method of data analysis. The objective is to partition N data objects into K clusters ($K<N$) such that the objects in the same cluster are as similar as possible and as dissimilar as possible in different clusters.

Main steps of the K-means algorithm are described by Jain and Dubes [11] as follows:

a) Select an initial partition with K clusters; repeat steps b and c until cluster memberships stabilize.

b) Generate a new partition by assigning each pattern to its closest cluster center.

c) Compute new cluster centers.

B. MPI

Message Passing Interface (MPI) is a standard developed by the Message Passing Interface Forum (MPIF). MPI is a standard library specification designed to support parallel computing in a distributed memory environment. The first version (version1.0) was published in 1994 and the second version (MPI-2) was published in 1997 [12]. Both point-to-point and collective communication are supported.

MPI is an API library consisting of hundreds of function interfaces called by computers such as computer clusters communicate with one another in the parallel development environment.

MPI is a language-independent communications protocol. FORTRAN, C and C++ can directly call the API library. The goals of MPI are high performance, scalability and portability.

The standards of MPI are as follows [13]:

a) Point-to-point communication
b) Collective operations
c) Process groups
d) Communication contexts
e) Process topologies
f) Bindings for Fortran 77 and C
g) Environmental management and inquiry
h) Profiling interface

C. Weka

Weka is a comprehensive suite of Java class libraries that implement many state-of-the-art machine learning and data mining algorithms [14]. Weka contains implementations of algorithms for classification, clustering, association rule mining, along with graphical user interfaces and visualization utilities for the data exploration and algorithm evaluation.

K-means algorithm is the most widely used clustering algorithm. SimpleKMeans from Weka is a simplified version of K-means [15]. Clustering data using the K-means algorithm can use either the Euclidean distance (default) or the Manhattan distance. If the Manhattan distance is used, centroids are calculated as the component-wise median rather than the mean.

III. MKMEANS – A PARALLEL K –MEANS ALGORITHM WITH MPI

In this section, we will propose an implementation of a parallel K-means algorithm based on MPI, called MKmeans. Before introducing our MKmeans algorithm, we first give a short description of the SKmeans (Sequential K-means) algorithm in Section *A*, because MKmeans is composed of SKmeans and MPI. Second, we give the detailed description of MKmeans in Section *B*.

A. SKmeans Algorithm

The clustering algorithm K-means is one of the most popular partitioning clustering algorithms. The main processing in the algorithm is to define K centroids (one for each cluster). These centroids should be placed in a cunning way because different locations cause different results [3]. In the SKmeans algorithm, the objective function J is defined as Formula (1). SKmeans aims to minimize the objective function, i.e., a squared error function. In (1), J refers to the distance index of N data objects from the corresponding cluster centroids. In Formula (1), x_n ($1 \leqslant n \leqslant N$) indicates a data point, and c_k ($1 \leqslant k \leqslant K$) specifies the cluster centroid. $\|x_n - c_k\|^2$ is the distance measure between x_n and c_k.

In our SKmeans algorithm, the number of clusters K is a user-specified parameter. First, read N objects from the input file. The initial K-centroids are randomly selected, defined as μ_k ($1 \leqslant k \leqslant K$). Second, the SKmeans algorithm iteratively assigns each object into the corresponding cluster by the minimum distance. When all objects are assigned, update the K centroids. This process will be repeated until the user-specified threshold is met. The SKmeans algorithm is shown in Figure 1.

$$J = \sum_{n=1}^{N} \sum_{k=1}^{K} \|x_n - c_k\|^2 \quad (1)$$

$$\mu_k = \frac{1}{N_k} \sum_{n \in c_k} x_n \quad (2)$$

SKmeans algorithm

Input: number of clusters K, number of data objects N

Output: K centroids

1: Read N objects from the file;
2: Randomly select K points as the initial cluster centroids, denoted as μ_k ($1 \leqslant k \leqslant K$);
3: Calculate J in Formula (1), denoted by J';
4: Assign each object n ($1 \leqslant n \leqslant N$) to the closest cluster;
5: Calculate new centroid of each cluster μ_k in Formula (2) ;
6: Recalculate J in Formula (1);
7: Repeat steps 3-6 until $J' - J <$ threshold;
8: Output the clustering results: K centroids;

Figure 1. SKmeans clustering algorithm

MKmeans algorithm

Input: number of clusters K, number of data objects N
Output: K centroids

1: MPI_INIT// start the procedure;
2: Read N objects from the file;
3: Partition N data objects evenly among all processes, and assume that each process has N' data objects;
4: For each process, install steps 5-11;
5: Randomly select K points as the initial cluster centroids, denoted as μ_k ($1 \leqslant k \leqslant K$);
6: Calculate J in Formula (1), denoted as J';
7: Assign each object n ($1 \leqslant n \leqslant N$) to the closest cluster;
8: Calculate the new centroid of each cluster μ_k in Formula (2) ;
9: Recalculate J in Formula (1);
10: Repeat steps 6-9 until $J' - J <$ threshold;
11: Generate the cluster id for each data object;
12: Generate new cluster centroids according to the clustering results of all processes at the end of each iteration;
13: Generate a final centroid set *Centroid* by Function Merge and output the clustering results: K centroids;
14: MPI_FINALIZE// finish the procedure;

Figure 2. MKmeans clustering algorithm

Function Merge

Input: n centroid sets from $Centroid_1$ to $Centroid_n$ ($n*K$ centroids)
Output: a centroid set *Centroid* (K centroids)

1: Initialize a centroid set *Centroid* as empty;
2: If any centroid set $Centroid_i$ ($i=1,...,n$) is empty, exit and the final centroid set is *Centroid*, otherwise, go to step 3;
3: Find a vector of centroids ($c_1, ..., c_K$) with the minimum inner distance, which is defined as Formula (3), and then delete c_i from $Centroid_i$, in addition, add $\bar{c}$ into *Centroid.* Go to step 2;
4: Output K centroids;

Figure 3. Merge function

B. MKmeans Algorithm

Figure 2 shows the processing flow of our MKmeans algorithm, which is the key algorithm in our work. This algorithm utilizes K-means and the MPI parallel framework, it is hence simple and portable.

All initialization is implemented by the MPI_INIT function, which is the first call of MPI program. It is the first executable statement of all of the MPI program. To start the MPI environment, it means the beginning of the parallel codes. The MPI_FINALIZE function is the last call of MPI program, and it ends the running of MPI program. It is the last executable statement of MPI program, otherwise, results of the procedure is unpredictable. MPI_FINALIZE symbolizes the end of the parallel codes.

In our MKmeans algorithm, the parallelism is implemented by the data parallelism. The parallel processing in MKmeans is consistent with that of SKmeans. Data objects are evenly partitioned in all processes and cluster centroids are replicated. The global operation for all cluster centroids is performed at the end of each iteration in order to generate new cluster centroids. Finally, output the clustering results: K centroids, I/O time and clustering time.

We assume that processes are n, which MKmeans generates n new data sets from the original data set. Since each data set uses K-means algorithm to generate K centroids, we can get n centroid sets from $Centroid_1$ to $Centroid_n$. Therefore, our goal is to merge the n centroid sets into a final centroid set. In our MKmeans algorithm, a simple merging algorithm is applied to ensemble with a greedy style, shown in Figure 3.

The Function *Merge* aims to find a vector of centroids ($c_1, ..., c_K$) with the minimum inner distance. In addition, the Euclidean distance is used to calculate the inner distance, denoted as Distance. In Formula (3), c_i comes from centroid set $Centroid_i$ ($i=1,...,K$) and $\bar{c}$ is the centroid.

$$D(c_1,...,c_K) = \sum_{i=1}^{K} Distance\ (c_i, \bar{c}) \qquad (3)$$

It is obvious that the calculation of each inner distance is independent. Therefore, all calculations can be performed in parallel. The Function *Merge* merges $n*K$ centroids into new K centroids, which are the final centroids.

IV. EXPERIMENTS

In this section, we first give the experimental environment in Section *A*. Second, we give the description of experimental data sets in Section *B*. Last, we give the experimental results and analysis in Section *C*.

A. Experimental environment

The hardware platform in this paper uses a PC with the configuration: Intel Xeon 5110 dual-core processor, 2GB RAM, 250GB hard driver; the software environment uses the following configuration: the operation system is Windows XP Professional Service Pack 3, the parallel and distributed environment is the Windows version of MPICH2, Java development platform is the JDK 1.6; Network environment is 100M- LAN.

In terms of aforementioned platform, eclipse SDK 3.2.1 is used to develop procedures. Considering the fairness of comparison, the configuration of MPI parallel development platform is based on open resource project Eclipse in Windows, and the experimental platform has a C/C++ complier based on MinGW (Minimalist GNU for Windows).

B. Data sets

All experimental data sets are selected from the UCI Machine Learning Dataset Repository [16]. The information of all data sets is illustrated as shown in Table 1.

In this table, seven testing data sets are listed corresponding to the number of instances. As the number of instances increases, the space consumption of data sets also increases, denoted as size.

C. Experimental results and analysis

In our experiments, the time cost is the key performance. The I/O time and clustering time are calculated respectively in MKmeans and SKmeans. To reflect the fairness and authenticity of the proposed algorithms, the number of processes is 1 in MKmeans.

Table 2 reports the results of the aforementioned two algorithms, including the I/O time, the clustering time and the total running time. Figure 4 compares the clustering running time of seven data sets in our algorithm with other different algorithms directly. From this figure, we can see that with the increasing of the size of data sets, the clustering time of MKmeans is slightly lower than that of SKmeans. However, the total time cost of MKmeans is higher than that of SKmeans on each testing data set, a preliminary analysis is that the I/O time occupies a large proportion. If our algorithm MKmeans is run in a large cluster, or as the number of processes increases, the experimental results will be more significant. In sum, we conclude that our MKmeans algorithm enables improving the time performance of clustering on large-scale data sets and MPI is quite appropriate for the parallel and distributed computing environment.

Table 3 illustrates the total time overheads of SKmeans and WKmeans. To make a convenient comparison in the experiments, WKmeans is based on the SimpleKMeans algorithm from Weka. In Figure 5, we can see that the time cost of WKmeans is significantly higher than that of SKmeans, and SKmeans performs much more stable on the overhead of time in the large data sets compared to WKmeans. MKmeans and SKmeans share the similar idea, it is hence to conclude that MKmeans is also a stable clustering algorithm.

Table 1. Description of data sets

Code Number of Data Sets	*Name of Data Sets(.arff)*	*Size(KB)*	*Number of Instances*
1	zoo	14.0	101
2	breast-cancer	28.7	286
3	credit-a	33.5	690
4	vowel	90	990
5	segment	298	2310
6	hypothyroid	303	3772
7	letter	703	20000

Table 2. Comparison results between MKmeans and SKmeans

Code Number of Data Sets	*MKmeans(ms)*			*SKmeans(ms)*		
	I/O	*Clustering*	*Total*	*I/O*	*Clustering*	*Total*
1	12.5	0.2	12.7	0.0	0.0	0.0
2	22.2	0.2	22.4	0.0	0.0	0.0
3	48.6	7.6	56.2	15.6	0.0	15.6
4	72.0	8.8	80.8	15.6	15.6	31.2
5	179.3	45.4	224.7	46.9	46.9	93.8
6	251.3	57.9	309.2	31.3	62.5	93.8
7	1268.2	268.8	1537.0	171.9	281.3	453.2

Table 3. Overheads of time in SKmeans and WKmeans

Code Number of Data Sets	*SKmeans(ms)*	*WKmeans(ms)*
1	0.0	78
2	0.0	78
3	15.6	156
4	31.2	219
5	93.8	562
6	93.8	625
7	453.2	6297

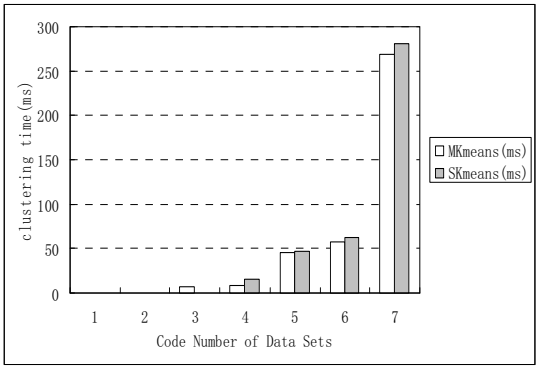

Figure 4. Clustering time of MKmeans and Skmeans

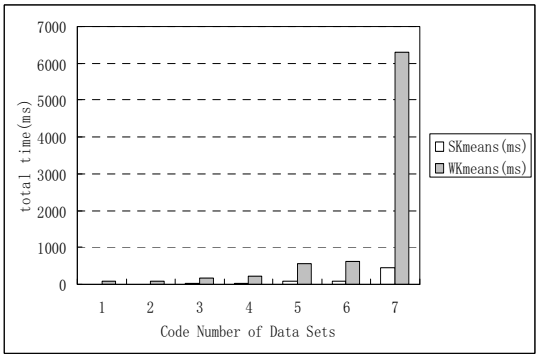

Figure 5. The total time overheads of SKmeans and WKmeans

V. CONCLUSIONS

We proposed a parallel K-means algorithm based on MPI (called MKmeans) in this paper. Meanwhile, the configuration of MPI parallel development platform based on open resource project Eclipse and MPICH in Windows is implemented, whose ideas and methods can be ported to Linux or other platforms. Experimental results show that MKmeans is relatively stable and portable, and it is efficient in the clustering on large data sets.

However, how to study the cluster validity of MKmeans with theoretical analysis, how to study the effect of clustering performance varying with the number of processes, how to compare the clustering performance in MPI and Map-Reduce are our future work [17].

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