Parallel D2-Clustering: Large-Scale Clustering of Discrete Distributions

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Abstract—The discrete distribution clustering algorithm, namely D2-clustering, has demonstrated its usefulness in image classification and annotation where each object is represented by a bag of weighed vectors. The high computational complexity of the algorithm, however, limits its applications to large-scale problems. We present a parallel D2-clustering algorithm with substantially improved scalability. A hierarchical structure for parallel computing is devised to achieve a balance between the individual-node computation and the integration process of the algorithm. Additionally, it is shown that even with a single CPU, the hierarchical structure results in significant speed-up. Experiments on real-world large-scale image data, Youtube video data, and protein sequence data demonstrate the efficiency and wide applicability of the parallel D2-clustering algorithm. The loss in clustering accuracy is minor in comparison with the original sequential algorithm.

Index Terms—Discrete Distribution, Transportation Distance, Clustering, D2-Clustering, Parallel Computing, Large-Scale Learning, Image Annotation, Sequence Clustering.

1 INTRODUCTION

The transportation problem is about finding an optimal matching between elements in two sets with different Radon measures under a certain cost function. The problem was initially formulated by French mathematician G. Monge in the late 18th century [29], and later by Russian mathematician L. Kantorovich in 1942 [16]. The solution of a transportation problem defines a metric between two distributions, which is normally known as the Kantorovich-Wasserstein metric. With the wide applications of the transportation problem in different fields, there are several variants, as well as names, of the corresponding transportation metric. Readers can refer to [31] for these applications.

The Kantorovich-Wasserstein metric is better known as the Mallows distance [26] in the statistics community because C. L. Mallows used this metric (with \(L_2\)-norm as the cost function) to prove some asymptotic property. In the computer science community, the metric is often called the Earth Mover’s Distance (EMD) [32]. Hereafter we refer to the Kantorovich-Wasserstein metric as the Mallows distance. It is not until the recent decade that the Mallows distance has received much attention in data mining and machine learning.

The advantages of the Mallows distance over a usual histogram-based distance include its effectiveness with sparse representations and its consideration of cross-term relationships. We have found abundant applications of the Mallows distance in video classification and retrieval [34], [38], sequence categorization [21], and document retrieval [36], where objects are represented by discrete distributions. The Mallows distance is also adopted in a state-of-the-art real-time image annotation system named ALIPR [22], in which a clustering algorithm on discrete distributions was developed.

Clustering is a major unsupervised learning methodology for data mining and machine learning. The K-means algorithm is one of the most widely used algorithms for clustering. To a large extent, its appeal comes from its simple yet generally accepted objective function for optimization. The original K-means proposed by MacQueen [24] only applies to the Euclidean space, which is a fundamental limitation. Though there are quite a few attempts to extend K-means to various distances other than the Euclidean distance [18], [27], [28], these K-means’ variants generally work on vector data. In many emerging applications, however, the data to be processed are not vectors. In particular, bags of weighted vectors, which can be formulated as discrete distributions with finite but arbitrary support, are frequently used as descriptors for objects in information and image retrieval [3]. The discrete distribution clustering algorithm, also known as the D2-clustering [22], tackles this type of data by optimizing an objective function defined in the same spirit as that used by K-means, specifically, to minimize the sum of distances between each object and its nearest centroid.

Because linear programming is needed in D2-clustering and the number of unknown variables grows with the number of objects in a cluster, the computational cost would normally increase polynomially with the sample size (assuming the number of clusters is...
roughly fixed). For instance, ALIPR takes several minutes to learn each semantic category by performing D2-clustering on 80 images in it. However, it will be difficult for ALIPR to include over 1,000 training images in one semantic category, because on a CPU with a clock speed of 2 GHz, the category may demand more than a day to cluster. There are some alternative ways [14], [40] to perform the clustering faster, but they generally perform some indirect or sub-optimal clustering instead of the optimization based D2-clustering.

The clustering problems researchers tackle today are often of very large scale. For instance, we are seeking to perform learning and retrieval on images from the Web containing millions of pictures annotated by one common word. This leads to demanding clustering tasks even if we perform learning only on a fraction of the Web data. Adopting bags of weighted vectors as descriptors, we will encounter the same issue in other applications such as video, biological sequence, and text clustering, where the amount of data can be enormous. In such cases, D2-clustering is computationally impractical.

Given the application potential of D2-clustering and its theoretical advantage, it is of great interest to develop a variant of the algorithm with a substantially lower computational complexity, especially under a parallel computing environment. With the increasing popularity of large-scale cloud computing in information systems, we are well motivated to exploit parallel computing.

### 1.1 Preliminaries

D2-clustering attempts to minimize the total squared Mallows distance between the data and the centroids. Although this optimization criterion is also used by K-means, the computation in D2-clustering is much more sophisticated due to the nature of the distance. The D2-clustering algorithm is similar to K-means in that it updates the iterate of the partition and the update of the centroids. There are two stages within each iteration. First, the cluster label of each sample is assigned to be the label of its closest centroid; and secondly, centroids are updated by minimizing the within-cluster sum of squared distances. To update the partition, we need to compute the Mallows distance between a sample and each current centroid. To update the centroids, an embedded iterative procedure is needed which involves a large-scale linear programming problem in every iteration. The number of unknowns in the optimization grows with the number of samples in the cluster. Suppose \( v_1, v_2, \ldots, v_n \) are discrete distributions within a certain cluster currently and \( v_i = \{ (t_1^{(i)}, p_z^{(i)}) , \ldots, (t_i^{(i)}, p_z^{(i)}) \} \), \( i = 1, 2, \ldots, n \), the following optimization is pursued in order to update the centroid \( z = \{ (z^{(1)}, p_z^{(1)}), \ldots, (z^{(s')}, p_z^{(s')})) \).

\[
\varepsilon = \min_{z^{(r)}, p_z^{(r)}} \sum_{i=1}^{n'} \sum_{1 \leq r \leq s'} D^2(z, v_i) 
\]

where

\[
D^2(z, v_i) = \min_{w_r, \alpha} \sum_{r=1}^{s'} \sum_{\alpha=1}^{t_i} \sum_{i=1}^{n'} w_r,\alpha \parallel z(r) - v_i^{(\alpha)} \parallel^2, 
\]

subject to:

\[
p_z^{(r)} \geq 0, r = 1, \ldots, s', \sum_{r=1}^{s'} p_z^{(r)} = 1, \\
\sum_{\alpha=1}^{t_i} w_r,\alpha = p_z^{(r)}, i = 1, \ldots, n', r = 1, \ldots, s', \\
\sum_{r=1}^{s'} p_z^{(\alpha)} = p_v^{(\alpha)}, i = 1, \ldots, n', \alpha = 1, \ldots, t_i, \\
w_r,\alpha \geq 0, i = 1, \ldots, n', \alpha = 1, \ldots, t_i, r = 1, \ldots, s'.
\]

If \( z \) is fixed, \( D(z, v_i) \) is in fact the Mallows distance between \( z \) and \( v_i \). However in (1), we cannot separately optimize \( D(z, v_i) \), \( i = 1, \ldots, n' \), because \( z \) is involved and the variables \( w_r,\alpha \) for different \( i \)'s affect each other through \( z \). To solve the complex optimization problem, the D2-clustering algorithm adopts the following iterative strategy.

**Algorithm 1. Centroid Update Process of D2-Clustering.**

**Step 1** Fix \( z^{(r)} \)'s and update \( p_z^{(r)} \), \( r = 1, \ldots, s' \), and \( w_r,\alpha \), \( i = 1, \ldots, n' \), \( r = 1, \ldots, n', \alpha = 1, \ldots, t_i \). In this case the optimization (1) of \( p_z^{(r)} \)'s and \( w_r,\alpha \)'s reduces to a linear programming.

**Step 2** Then fix \( p_z^{(r)} \)'s and \( w_r,\alpha \)'s and update \( z^{(r)} \), \( r = 1, \ldots, s' \). In this case the solution of \( z^{(r)} \)'s to optimize (1) are simply weighted averages:

\[
z^{(r)} = \frac{\sum_{i=1}^{n'} \sum_{\alpha=1}^{t_i} w_r,\alpha p_v^{(\alpha)}}{\sum_{i=1}^{n'} \sum_{\alpha=1}^{t_i} w_r,\alpha}, r = 1, \ldots, s'.
\]

**Step 3** Calculate the objective function \( \varepsilon \) in (1) using the updated \( z^{(r)} \)'s, \( p_z^{(r)} \)'s, and \( w_r,\alpha \)'s. Terminate the iteration until \( \varepsilon \) converges. Otherwise go back to Step 1.

The linear programming in Step 1 is the primary cost in the centroid update process. It solves \( p_z^{(r)}, w_r,\alpha \), \( r = 1, \ldots, s', i = 1, \ldots, n', \alpha = 1, \ldots, t_i \), a total of \( s' + s\sum_{i=1}^{n} t_i \) \( \approx n s^2 \) parameters when \( s' \) is set to be the average of the \( t_i \)'s. The number of constraints is \( 1 + n s' + \sum_{i=1}^{n} t_i \approx 2 n s'^2 \). Hence, the number of parameters in the linear programming grows linearly with the size of the cluster. Because it costs polynomial time to solve the linear programming problem [17], D2-clustering is much more complex than K-means algorithm in computation.

The analysis of the time complexity of K-means remains an unsolved problem because the number of iterations for convergence is difficult to determine. Theoretically, the worst case time complexity for K-means is \( \Omega(2^n) \) [2]. Arthur et al. [11] show recently that K-means has polynomial smoothed complexity, which reflects the fact that K-means will converge in a relatively short time in real cases (although no tight upper or lower bound of time complexity has been proved). In practice, K-means usually converges fast, and seldom costs an exponential number of iterations. In many cases K-means converges...
in linear or even sub-linear time. Although there is still a gap between the theoretical explanation and practice, we can consider K-means algorithm with at most polynomial time.

Although the D2-clustering algorithm interlaces the update of clustering labels and centroids in the same manner as K-means, the update of centroids is much more complicated. As described above, to update each centroid involves an iterative procedure where a large-scale linear programming problem detailed in has to be solved in every round. This makes D2-clustering usually polynomially more complex than K-means.

The computational intensiveness of D2-clustering limits its usages to only small-scale problems. With emerging demands to extend the algorithm to large-scale datasets, e.g., online image datasets, video resources, and biological databases, we exploit parallel processing in a cluster computing environment in order to overcome the inadequate scalability of D2-clustering.

1.2 Overview of Parallel D2-Clustering
To reduce the computational complexity of D2-clustering, we seek a new parallel algorithm. Parallelization is a widely adopted strategy for accelerating algorithms. There are several recent algorithms that parallelize large-scale data processing. By distributing parallel processes to different computation units, the overall processing time can be greatly reduced.

The labeling step of D2-clustering can be easily parallelized because the cluster label of each point can be optimized separately. The centroid update stage described by (1), which is the performance bottleneck of D2-clustering, makes the parallelization difficult. Unlike K-means’ centroid update, which is essentially a step of computing an average, the computation of a centroid in D2-clustering is far more complicated than any linear combination of the data points. Instead, all the data points in the corresponding cluster will play a role in the linear programming problem in (1).

The averaging step of K-means can be naturally parallelized. We divide the data into segments, and compute a local average of each segment in parallel. All the local averages can then be combined to a global average of the whole group of data. This is usually how K-means is being parallelized. To the best of our knowledge, there is no mathematical equivalence of a parallel algorithm for the linear programming problem in D2-clustering. However, we can adopt a similar strategy to parallelize the centroid update in D2-clustering: dividing the data into segments based on their adjacency, computing some local centroids for each segment in parallel, and combining the local centroids to a global centroid. Heuristically we can get a good estimation of the optimal centroid in this way, considering that the notion of centroid is exactly for a compact representation of a group of data. Hence, a centroid computed from the local centroids should represent well the entire cluster, although some loss of accuracy is expected.

The most complex part in the parallelization of D2-clustering is the combination of local centroids. Same as the computation of local centroids, the combination operation also involves a linear programming with polynomial time in terms of data size. To achieve a low overall runtime, we want to keep both linear programming problems at a small scale, which cannot be achieved simultaneously when the size of the overall data is large. As a result, we propose a new hierarchical structure to conduct parallel computing recursively through multiple levels. This way, we can control the scale of linear programming in every segment and at every level.

We demonstrate the structure of the algorithm in Fig. 1, which will be explained in detail in Section 2.1. In short, we adopt a hierarchically structured parallel algorithm. The large dataset is first clustered into segments, within each of which D2-clustering is performed in parallel. The centroids generated for each segment are passed to the next level of the hierarchy and are treated as data themselves. The data size in the new level can still be large, although it should be much smaller than the original data size. At the new level, the same process is repeated to cluster data into segments and perform D2-clustering in parallel for each segment. When the amount of data at a certain level is sufficiently small, no further division of data is needed and D2-clustering on all the data will produce the final result. We can think of the granularity of the data becoming coarser and coarser when the algorithm traverses through the levels of the hierarchy. Details about each step will be introduced in the following sections.

Particularly for implementation, parallel computing techniques, such as Message Passing Interface (MPI) and MapReduce can be applied. In the current work, MPI is used to implement the parallel algorithm.

1.3 Outline of the Paper
The remainder of paper is organized as follows. The parallel D2-clustering algorithm and its performance analysis are presented in Section 2. Experimental results and comparison with other methods are described in Section 3. Finally, we conclude in Section 4.

2 Parallel D2-clustering Algorithm
In this section, we present the parallel D2-clustering algorithm. Hereafter, we refer to the original D2-clustering as the sequential algorithm. We will describe the hierarchical structure for speeding up D2-clustering and a weighted version of D2-clustering which is needed in the parallel algorithm but not the sequential. We will also describe in detail the coordination among the individual computation nodes (commonly called the slave processors) and the node that is responsible for integrating the results (called the master processor). Finally, we analyze the computational complexity of the parallel algorithm and explain various choices made in the algorithm in order to achieve fast speed.
Fig. 1. An illustration of the structure of the parallel D2-clustering algorithm. Crossings are data to be clustered at each level. Different shadings denote different segments to perform local D2-clustering, which can be done in parallel within a level. Dots are cluster centroids. Centroids at a certain level become data points at the next level. The clustering stops going to a higher level until we get the desired number of clusters.

2.1 Hierarchical Structure

Fig. 1 illustrates the hierarchical structure used for parallel processing. All input data are denoted by crossings at the bottom level (Level 1) in Fig. 1. Because of the large data size, these data points (each being a discrete distribution) are divided into several segments (reflected by different shadings in the figure) which are small enough to be clustered by the sequential D2-clustering. D2-clustering is performed within each segment. Data points in each segment are assigned with different cluster labels, and several cluster centroids (denoted by blue dots in the figure) are obtained.

These cluster centroids are regarded as good summarization for the original data. Each centroid approximates the effect of the data assigned to the corresponding cluster, and is taken to the next level in the hierarchy. Obviously, the number of data points to be clustered at the second level is much reduced from the original data size although it can still be large for sequential D2-clustering. Consequently, the data may be further divided into small segments which sequential D2-clustering can handle. In our implementation, we keep the size of a segment at different levels roughly the same. When the algorithm proceeds to higher levels, the number of segments decreases. The hierarchy terminates when the data at a level can be put in one segment.

In short, at each level, except the bottom level, we perform D2-clustering on the centroids acquired from the previous level. Fig. 1 shows that the data size at the third level is small enough for not proceeding to another level. Borrowing the terminology of a tree graph, we can call a centroid a parent point and the data points assigned to its corresponding cluster child points. The cluster labels of the centroids at a higher level are inherited by their child points, and propagate further to all the descendent points. To help visualize the tree, in Fig. 1 data points in one cluster at a certain level are connected to the corresponding centroid using dashed lines. And the red arrows between levels indicate the correspondence between a centroid and a data point at the next level. To determine the final clustering result for the original data, we only need to trace each data point through the tree and find the cluster label of its ancestor at the top level.

In such a hierarchical structure, the number of centroids becomes smaller and smaller as the level increases. Therefore it is guaranteed that the hierarchy can terminate. Also since D2-clustering is conducted within small segments, the overall clustering can be completed fast. More detailed discussion about the complexity of the algorithm will be provided in a later section.

2.2 Initial Data Segmentation

We now describe the initial data segmentation method. In this step, we want to partition the dataset into groups all smaller than a certain size. The partitioning process is in a similar spirit as the initialization step of the LBG algorithm proposed by Linde et al. [24], an early instance of K-means in signal processing. The whole dataset is iteratively split into partitions until a stopping criterion is satisfied. And within each iteration, the splitting is an approximation of, and computationally less expensive than, an optimal clustering.

Fig. 2 illustrates the iterative process containing a series of binary splitting. Different from the initialization of the LBG algorithm, which splits every segment into two parts, doubling the total number of segments in every iteration, our approach only splits one segment in each round. The original data are split into two groups using a binary clustering approach (to be introduced later). Then we further split the segments by the same process repetitively. Each time we split the segment containing the most data points into two clusters, until all segments are small enough.

As shown by Fig. 2, in each round of dividing a group of data into two segments, we aim at good clustering so
that data points in each segment are close. On the other hand, this clustering step needs to be fast since it is a preparation before conducting D2-clustering in parallel. The method we use is a computationally reduced version of D2-clustering. It is suitable for clustering bags of weighted vectors. Additionally, it is fast because of some constraints imposed on the centroids. We refer to this version as the constrained D2-clustering.

The constrained D2-clustering is a reduced version of D2-clustering. We denote each data point to be clustered as \( v_i = \{(\epsilon_i^{(1)}, \pi_i^{(1)}), \ldots, (\epsilon_i^{(t_i)}, \pi_i^{(t_i)})\} \), \( i = 1, \ldots, n \), and \( k \) initial centroids as \( z_j = \{(\epsilon_j^{(1)}, \pi_j^{(1)}), \ldots, (\epsilon_j^{(s_j)}, \pi_j^{(s_j)})\} \), \( j = 1, \ldots, k \). Parameters \( t_i \) and \( s_j \) are the numbers of support vectors in the corresponding discrete distributions \( v_i \) and \( z_j \). And \( C(i) \in \{1, \ldots, k\} \) denotes the cluster label assigned to \( v_i \). The D2-clustering and constrained D2-clustering algorithms are described below.

Algorithm 2. D2-Clustering and Constrained D2-Clustering.

\begin{enumerate}
\item Select some random centroids as the initialization.
\item Allocate a cluster label to each data point \( v_i \) by selecting the nearest centroid.
\end{enumerate}

\( C(i) = \arg \min_j D(v_i, z_j), \) where \( D(v_i, z_j) \) is the Mallows distance between \( v_i \) and \( z_j \).

\begin{enumerate}
\item [Step 3] (For D2-clustering only) Solve \( 1 \) to update \( z_j \), the centroid of each cluster, using the data points \( \{v_i : C(i) = j\} \) assigned to the cluster. Algorithm 1, which is also an iterative process, is invoked here to solve \( z_j \).
\item [Step 3* (For constrained D2-clustering only)] Keep \( \mu^{(r)}_j = 1/s_j, r = 1, \ldots, s_j \) fixed when invoking Algorithm 1 to solve \( z_j \). The linear programming \( 1 \) can thus be separated into several smaller ones and runs much faster. The result of \( z_j \) will be a uniform weighted bag of vectors containing support vectors at optimized locations.
\item [Step 4] Suppose the objective function in \( 1 \) converges to \( \varepsilon \). Calculate the overall objective function for the clustering:
\[ \varepsilon(C) = \sum_{j=1}^{s_j} \varepsilon_j. \]
If \( \varepsilon(C) \) converges, the clustering finishes; otherwise go back to Step 2.
\end{enumerate}

The difference between D2-clustering and constrained D2-clustering is the way to update centroids in Step 3 of the above algorithm. As discussed previously in Section 1.1, we need to solve a large-scale linear programming problem in Algorithm 1 to update each \( z_j \) in D2-clustering. The linear programming involves the optimization of \( p^{(r)}_j \) and \( w^{(r)}_{r, \alpha} \), \( r = 1, \ldots, s_j, \alpha = 1, \ldots, t_i \), \( i : C(i) = j \) (\( w^{(r)}_{r, \alpha} \) is the matching weight between the \( r \)-th vector of \( z_j \) and the \( \alpha \)-th vector of \( v_i \)). This makes D2-clustering computationally complex.

In the constrained D2-clustering algorithm, we replace Step 3 by Step 3* in the D2-clustering algorithm. We simplify the optimization of D2-clustering by assuming uniform \( p^{(j)}_{z_j} = 1/s_j, r = 1, \ldots, s_j \), for any \( j = 1, \ldots, k \). With this simplification, in the linear programming problem in Step 1 of Algorithm 1, we only need to solve \( w^{(j)}_{r, \alpha} \)’s. Moreover, \( w^{(j)}_{r, \alpha} \)’s can be optimized separately for different \( i \)’s, which significantly reduces the number of parameters in a single linear programming problem. More specifically, instead of solving one linear programming problem with a large number of parameters, we solve many linear programming problems with a small number of parameters. Due to the usual polynomial complexity of the linear programming problems, this can be done much faster than the original D2-clustering.

2.3 Weighted D2-clustering

Data segments generated by the initialization step are distributed to different processors in the parallel algorithm. Within each processor, a D2-clustering is performed to cluster the segment of data. Such a process is done at different levels as illustrated in Fig. 1.

Clustering at a certain level usually produces unbalanced clusters containing possibly quite different numbers of data points. If we intend to keep equal contribution from each original data point, the cluster centroids passed to a higher level in the hierarchy should be weighted and the clustering method should take those weights into account. We thus extended D2-clustering to a weighted version. As will be shown next, the extension is straightforward and results in little extra computation.

It is obvious that with weighted data, the step of nearest neighbor assignment of centroids to data points will not be affected, while the update of the centroids under a given partition of data will. Let us inspect the optimization in \( 1 \) for updating the centroid \( z \) of one cluster. When data \( v_i \) have weights \( \omega_i \), a natural extension of the objective function is
\[ \min_{z^{(r)} \in \mathbb{D}} \sum_{i=1}^{n'} \omega_i D^2(z, v_i) \]
where \( D(z, v_i) \) is defined in \( 1 \).

In Step 1 of Algorithm 1, we fix \( z_j^{(r)}, r = 1, \ldots, s_j \), and solve a linear programming problem with objective function \( 5 \) under the same constraints specified in \( 1 \) to get the vector weights \( p^{(r)}_{z_j^{(r)}} \)’s and a matching \( w^{(r)}_{r, \alpha} \) between \( z_j \) and each \( v_i, i : C(i) = j \). Then in Step 2, the update for \( z_j^{(r)} \) is revised to a weighted version:
\[ z_j^{(r)} = \frac{\sum_{i : C(i) = j} \omega_i \sum_{\alpha=1}^{t_i} w^{(j)}_{r, \alpha} v_i^{(\alpha)}}{\sum_{i : C(i) = j} \omega_i \sum_{\alpha=1}^{t_i} w^{(j)}_{r, \alpha}}. \]

Because the optimal solution of centroid is not affected when the weights are scaled by a common factor, we simply use the number of original data points assigned to each centroid as its weight. The weights can be computed recursively when the algorithm goes through levels in the hierarchy. At the bottom level, each original data point is assigned with weight 1. The weight of a data point in a parent level is the sum of weights of its child data points.

2.4 Algorithmic Description

With details in several major aspects already explained in the previous sections, we now present the overall
flow of the parallel D2-clustering algorithm. The parallel
program runs on a computation cluster with multiple
processors. In general, there is a “master” processor
that controls the flow of the program and some other
“slave” processors in charge of computation for the
sub-problems. In the implementation of parallel D2-
clustering, the master processor will perform the ini-
tial data segmentation at each level in the hierarchi-
cal structure specified in Fig. 1 and then distribute
the data segments to different slave processors. Each
slave processor will cluster the data it received by the
weighted D2-clustering algorithm independently, and
send the clustering result back to the master processor.
As soon as the master processor receives all the within-
segment clustering results from the slave processors,
it will combine these results and set up the data for
clustering at the next level if necessary.

The current work adopts MPI for implementing the
parallel program. In order to keep a correct work flow
for both master and slave processors, we use synchro-
nized communication ways in MPI to perform message
passing and data transmission. A processor can broad-
cast its local data to all others, and send data to (or receive data
from) a specific processor. Being synchronized, all these
operations will not return until the data transmission
is completed. Further, we can block the processors until
all have reached a certain blocking point. In this way,
different processors are enforced to be synchronized.

Because the communication is synchronized, we can
divide the overall work flow into several steps for both
the master and slave processors. To better explain the
algorithm, in particular how the master and slave pro-
cessors interact, we describe the working processes of
both the master and slaves together based on these steps,
although they are essentially different sets of instructions
performed at different CPU cores respectively.

The work flow is illustrated in Fig. 3. There are one
master processor (on the left of the figure) and M slave
processors (on the right of the figure). The master pro-
cessor will read the original set of discrete distributions
X = \{x_1, x_2, \ldots, x_N\} and maintain the clustering label
C(i) ∈ \{1, \ldots, k'\} for each data entry x_i, as well as
the corresponding cluster centroids Z = \{z_1, z_2, \ldots, z_k'\}.
Initially the weight of each data entry is set to be \omega_i = 1,
i = 1, \ldots, N. At each level, there are three steps. In each
step, either the master processor or the slave processors
are idle, passively waiting and receiving incoming data,
and the other one is performing computation (which
are marked by dashed and solid icons in the figure
respectively). Suppose the targeted number of clusters is
k and the sequential (weighted) D2-clustering is applied
to segments of data containing no more than \tau entries.
The algorithm has a hierarchical structure and iteratively
performs clustering level by level. And each iteration
contains the following three steps.

**Algorithm 3. Parallel D2-Clustering.**

**Step 1 Data segmentation in the master’s side.**
- The master processor segments the data objects \(\hat{G}\) (con-
taining \(n\) objects) at current level into \(m\) groups, \(G_1, \ldots, G_m\), each of which contains no more than \(\tau\) entries, using
the constrained D2-clustering introduced in Section 2.3.
The indices of data entries assigned to segment \(G_j\) are stored in
array \(L_j\). For each segment \(G_j\), the master processor sends
the segment index \(\mu_j\) data in the segment and their weights
to the slave processor with index \((\mu_j \ mod\ M)\).
- Each slave processor will listen to and receive any incoming
data segment from the master processor in this step. It will store data in the segment \(V_{\mu_j} = \{v_{\mu_j, 1}, v_{\mu_j, 2}, \ldots, v_{\mu_j, n_{\mu_j}}\}\) and

**Fig. 3.** Work flow and communication among master and
slave processors in parallel D2-clustering for one iteration.
Within each iteration (level), there are three synchronized
steps for the master and slave processors. In each step,
one of the master or slave side is performing computation
(marked in solid line) and the other is idle and waiting for
incoming data and message (marked in dashed line).
the corresponding weights \( W_\mu = \{\omega_\mu,1, \omega_\mu,2, \ldots, \omega_\mu,n_\mu\} \) locally for clustering. In addition, the index of the corresponding segment, \( \mu \), is also transmitted and kept in the slave processor. Since the number of data segments \( n \) might be larger than the number of slave processors \( M \), the master processor uses a modular operation to distribute different segments to different slave processors and each slave processor may handle multiple segments sequentially. The segment indices help the master processor manage the data distribution and identify the result of a certain segment when it is returned by a slave processor in the next step.

**Step 2 Parallel D2-clustering in the slaves’ side.**

- **The master processor** listens to the clustering results, including both the labels \( C_\mu \) (containing \( n_\mu \) labels) and centroids \( Z_\mu \) (containing \( k_\mu \) centroids), as well as the index \( \mu \), for each segment, and is blocked until it receives all segments’ results.

- **Each slave processor** will perform weighted D2-clustering on \( V_\mu \) with weights \( W_\mu \) by Algorithm 1 (using 3 and 4) when updating centroids. Then a set of centroids \( Z_\mu = \{z_{\mu,1}, \ldots, z_{\mu,k_\mu}\} \) and cluster labels \( C_\mu = \{C_\mu(1), \ldots, C_\mu(n_\mu)\} \) are acquired, where \( C_\mu(i) \) is assigned to centroid \( z_{\mu,j} \). After this it sends back the segment index \( \mu \), the set of centroids \( Z_\mu \), and cluster labels \( C_\mu \) to the master processor.

**Step 3 Work flow control in the master’s side.**

- **The master processor** will merge the clustering results of all the segments and then determine whether to proceed to the next level. The current overall centroid list is set to \( Z = \emptyset \) at the beginning. The centroids \( Z_\mu \) for group \( G_\mu \) are appended to \( Z \) one by one. And the labeling list of \( G_\mu \), \( C(i), i = 1, \ldots, n_\mu \), is updated once a new group of centroids is being added. Let the most recent list \( Z \) before adding \( Z_\mu \) be \( Z^{(\mu-1)} \), then \( Z(0) = Z \), \( \bar{C}(i) \) is computed by (5).

\[
\bar{C}(L_\mu(i)) = C_\mu(i) + |Z^{(\mu-1)}|, \quad i = 1, \ldots, n_\mu.
\]  

(5)

After all \( Z_\mu \) has been merged to \( Z \) and all \( \bar{C}(i) \) is computed, we update the cluster label of a data entry in the original dataset (bottom level), \( C(i) \), by inheriting label from its ancestor in \( G \).

\[
C(i) = \overline{C}(C(i)), \quad i = 1, \ldots, N.
\]  

(6)

Assume \( k_\mu \) is the number of clusters in segment \( G_\mu \) and \( k' = \sum_{\mu=1}^M k_\mu \). At the end of the current level of clustering, we get a list of centroids, \( Z = \{z_1, z_2, \ldots, z_{k'}\} \), and the cluster labels \( C(1), C(2), \ldots, C(N) \) for the original data. If \( k' \leq k \), clustering is accomplished. The master processor will output \( Z \) and \( C \), and sends a termination signal to all the processors. Otherwise, clustering at a higher level is needed. Let \( \omega'_\mu = \omega_\mu, i = 1, \ldots, n_\mu \). Update \( G = Z \) and assign new weights to each entry in \( G \) by \( \omega_i = \sum_{C(j) = i} \omega'_j, \quad i = 1, \ldots, k' \). Then the master processor will go back to Step 1 and send signals to slave processors to tell them also to return to Step 1.

- **The slave processors** are blocked in this step, doing nothing until the master processor tells them the next action, either to return to Step 1 and receive new data, or to terminate.

### 2.5 Run-Time Complexity

In this section, we analyze the time complexity of the parallel D2-clustering algorithm.

As described in Section 2.1 for D2-clustering, the computational complexity of updating the centroid for one cluster in one iteration is polynomial in the size of the cluster. The total amount of computation depends on computation within one iteration as well as the number of iterations. Again, as discussed in Section 2.1 even for K-means clustering, the relationship between the number of iterations needed for convergence and the data size is complex. In practice, we often terminate the iteration after a pre-specified number of rounds (e.g., 500) if the algorithm has not converged before that. As a result, in the analysis of computational complexity, we focus on the time needed to complete one iteration and assume the time for the whole algorithm is a multiple of that, where the multiplication factor is a large constant.

Suppose there are \( N \) data entries in total and we want to cluster them into \( k \) clusters. Assuming the clusters are of similar sizes, each cluster contains roughly \( \frac{N}{k} \) data entries. The sequential D2-clustering algorithm will run in approximately \( O(\frac{N}{k} \tau) \) time, where \( \gamma \) is the degree of the polynomial time required by linear programming for computing the centroid of one cluster. In many applications, when \( N \) increases, the number of clusters \( k \) may stay the same or increase little. As a result, the time for D2-clustering increases polynomially with \( N \).

Now consider the time required by the parallel D2-clustering. The sequential D2-clustering is then performed on segments of data with sizes no larger than \( \tau \). Each segment is clustered into \( c \) groups with roughly equal size \( e \). Thus, \( \gamma = \frac{N}{\tau} \). After clustering every data segment, the number of data to be processed at the next level of the hierarchy shrinks from \( N \) to \( \frac{N}{\tau} \), since we use each cluster centroid to summarize data entries assigned to the corresponding cluster.

Based on the run-time analysis on the sequential clustering, the time for clustering one segment of data is \( O(e^\gamma) = O(\tau e^{\tau-1}) \). The combined CPU time used for clustering all segments is then \( O(N e^{\gamma-1}) \). The actual time for performing clustering also depends on the number of available parallel CPU cores. Assuming there are \( M+1 \) CPUs, where \( M \) is the number of CPUs performing slave clustering operations and there is one CPU serving as the master. When \( M \geq \frac{N}{\tau} \), it can be guaranteed that each segment is distributed to a unique CPU. Therefore the actual time used is \( O(\tau e^{\tau-1}) \). When \( M < \frac{N}{\tau} \), there will be some CPUs handling more than one clustering jobs sequentially, so the actual time is \( O\left(\frac{N}{\tau} e^{\tau-1}\right) \).

In addition to clustering the segments, it also takes time to divide data into segments by the approach described in Section 2.2. The data segments are generated by a binary tree-structured clustering process. For the simplicity of analysis, we assume the tree is balanced. The time to split a node is linear to the number of data entries in the node; and the time for creating \( \frac{N}{\tau} \) segments is \( O\left(\frac{N}{\tau} \log \frac{N}{\tau}\right) \). Similarly, there is also some computation for initialization when clustering each segment, which takes \( O(\tau \log \frac{N}{\tau}) \) time. When \( \tau \) is large, the initialization cannot be neglected for run-time analysis. In summary, the overall actual time for performing clustering at the first level in Fig. 1 is
\[ T(1) = O \left( N \log \frac{N}{\tau} + \frac{e^{\gamma-1} + \log \frac{N}{\min(M, \frac{N}{e})}}{e} N \right). \] (7)

The hierarchical clustering may not reach the desired number of clusters at the first level, where \( \frac{N}{e} > k \), the algorithm proceeds to the next level, where each cluster centroid will be treated as a data entry. If we keep the same values for parameters \( \tau, e, \) and \( M \), the time for the second level clustering can be calculated simply using (7) with \( N \) replaced by \( \frac{N}{e} \). More generally, we can obtain the time complexity for any \( l \)-th level, \( l \geq 2 \), by

\[ T(l) = O \left( \frac{N}{e^{l-1}} \log \frac{N}{\tau e^{l-1}} + \frac{e^{\gamma-1} + \log \frac{N}{\min(M, \frac{N}{e^{l-1}} e^{l-1})}}{e} N \right). \] (8)

Obviously \( T(l) > eT(l+1) \). The algorithm will terminate at level \( L \) when \( \frac{N}{e^L} \leq k \). Hence, the highest level \( L = \lceil \log \frac{N}{k} \rceil \). And the total run-time is \( T(1) + \ldots + T(L) < \frac{1}{e-1} T(1) \leq 2T(1) \). The last inequality comes from the fact \( e \geq 2 \) (if \( e = 1 \), there is essentially no clustering). We thus see that the computational order of the total run-time is the same as that of \( T(1) \).

With fixed \( N \) and \( \tau \), the complexity \( T(1) \) in (7) indicates that a small value of \( e \) is favored. Another benefit of having a small \( e \) is that a centroid can better represent a small number of data entries. We set \( e = 5 \) in our implementation. We do not go as low as \( e = 2 \) because more levels will be needed which makes the coordination among processors harder to track.

To achieve small \( T(1) \), (7) shows that there is a trade-off for \( \tau \). Given the number of slave CPUs, \( M \), which is inherently determined by the hardware, we try to choose a sufficiently large \( \tau \) so that the number of segments \( \frac{N}{e} \) is no greater than \( M \). This ensures that no CPU needs to process multiple segments sequentially. Moreover, large \( \tau \) will reduce the time for generating the segments, which corresponds to the first term in (7). On the other hand, when \( \tau \) is large, assuming \( \frac{N}{e} \leq M \), the second term in (7) is in the linearithmic order of \( \tau \). Hence, \( \tau \) should not be unnecessarily large. If \( M \) slave processors are guaranteed, \( \tau = \frac{N}{e} \) is a good choice. In our implementation, we observe that the sequential D2-clustering can handle 50 data entries and 10 clusters (5 entries per cluster) at satisfactory speed. We thus set \( \tau = 50 \) and \( e = 5 \) in the parallel algorithm by default.

Comparing the two terms in (7), the first term dominates when \( N \) is large. Otherwise, the second term dominates because \( e^{\gamma-1} \) can be substantial. Assuming parameters \( M, \tau, \) and \( e \) are fixed, when \( \frac{N}{e^L} \leq M, T(1) \) will be dominated by a constant given in the second term. As \( N \) grows, \( T(1) \) will eventually be dominated by the first term, which is a linearithmic order \( (O(N \log N)) \).

Based on the analysis above, we can see the speedup of the parallel D2-clustering over the original sequential algorithm, which runs in time \( O\left(\frac{N^2}{k}\right) \). Usually \( N \gg k \), so the sequential algorithm has to solve a large linear program when \( N \) is large. In the parallel algorithm, during the update of a centroid, on average \( e \) data entries are handled, rather than \( \frac{N}{e} \). There is thus no large-scale linear programming. Even when there is only one CPU, i.e., \( M = 1 \), (that is, essentially no parallel processing), the “parallel” algorithm based on the hierarchy will have run-time \( O\left(\frac{N}{e^{\gamma-1} + \log \frac{N}{k}}\right) \), which is linearithmic order in \( N \) rather than polynomial order. If we have enough CPUs to guarantee \( M \) is always no smaller than \( \frac{N}{e} \), the second term of (7) is always a constant with respect to \( N \). When \( N \) is large, the first term \( O\left(\frac{N}{e^{\gamma-1}}\right) \) dominates, which is much lower in order than \( O\left(\frac{N^2}{k}\right) \).

### 3 Experiments

To validate the advantage and usefulness of this algorithm, we conduct experiments on four different types of dataset, including image, video, protein sequence, and synthetic datasets. Though our work was originally motivated by image concept learning, we apply the parallel D2-clustering algorithm to different scenarios. Readers in these related areas may therefore find applications that are suitable to embed the algorithm into.

First, we test the algorithm on images crawled from Flickr in several experiments. When crawling images from Flickr, we use the Flickr API to perform keyword query for certain concepts, and download top \( N \) images with highest values of interestingness. The number of images \( N \) is different in different experiments. Typically it is at a scale of thousands, much larger than the scale the sequential D2-clustering has been applied. If such clustering is performed for multiple concepts, the training dataset for image tagging can easily reach several millions, which is quite large for image annotation.

For such image datasets, each image is first segmented into two sets of regions based on the color (LUV components) and texture features (Daubechies-4 wavelet coefficients) respectively. We then use two bags of weighted vectors \( U \) and \( V \), one for color and the other for texture, to describe an image as \( I = (U, V) \). The distance between two images, \( I_i = (U_i, V_i) \) and \( I_j = (U_j, V_j) \), is defined as

\[ D(I_i, I_j) = (D^2(U_i, U_j) + D^2(V_i, V_j))^{1/2}, \] (9)

where \( D(\cdot, \cdot) \) is the Mallows distance. It is straightforward to extend the D2-clustering algorithm to the case of multiple discrete distributions using the combined distance defined in (9). See [22] for details. The order of time complexity increases simply by a multiplicative factor equal to the number of distribution types, the so-called super-dimension.

Second, we adopt videos queried and downloaded from Youtube. We represent each video by a bag of weighted vectors, and conduct parallel D2-clustering on these videos. Then we check the accordance between the clustering result and the videos’ genre.

For the video clustering, we adopt the features used in [59]. Edge Direction Histogram (EDH), Gabor (GBR), and Grid Color Moment (GCM) features are extracted from each frame. A video is segmented into several sub-clips based on the continuity of these three features.
among nearby frames [24]. Using the time percentage of each sub-clip as the weight of its average feature vector, we represent the video by a bag of weighted vectors by combining all sub-clips.

Third, we download the SwissProt protein data [3] and apply clustering on a subset of this dataset. Prosite protein family data [13] provides the class labels of these protein sequences. Using the Prosite data, we can select protein sequences from several certain classes as the experiment dataset, which contains data gathering around some patterns. Each protein sequence is composed of 20 types of amino acids. We count the frequency of each amino acid in a sequence, and use the frequency as the signature of the sequence.

At last, we synthesize some bags of weighted vectors following certain distribution and cluster them.

The parallel program is deployed on a computation cluster at The Pennsylvania State University named “CyberStar” consisting of 512 quad-core CPUs and therefore 2048 computation units. Since \( M = 2048 \), theoretically it can be guaranteed that at each level every data segment can be processed in parallel by a unique CPU core when the data size is several thousands. In practice the system will put a limit to the maximal number of processors each user can occupy at a time because it is a publicly shared server.

In this section, we first evaluate objectively the D2-clustering algorithm on image datasets with different topics and scales. Then we show the D2-clustering results for the image, video, protein, and synthetic datasets respectively.

### 3.1 Comparison with Sequential Clustering

In order to compare the clustering results of the parallel and sequential D2-clustering, we have to run the experiment on relatively small datasets so that the sequential D2-clustering can finish in a reasonable time. In this experiment, 80 concepts of images, each including 100 images downloaded from Flickr, are clustered individually using both approaches. We compare the clustering results obtained for every concept.

It is in general challenging to compare a pair of clustering results, as shown by some sincere efforts devoted to this problem [41]. The difficulty comes from the need to match clusters in one result with those in another. There is usually no obvious way of matching. The matter is further complicated when the numbers of clusters are different. The parallel and sequential clustering algorithms have different initializations and work flows. Clearly we cannot match clusters based on a common starting point given by initialization. Moreover, the image signatures do not fall into highly distinct groups, causing large variation in clustering results.

We compare the clustering results by three measures.

First, we assess the quality of clustering by the generally accepted criterion of achieving small within-cluster dispersion, specifically, the mean squared distance between a data entry and its corresponding centroid.

Second, we define a distance between two sets of centroids. Let the first set of centroids be \( Z = \{ z_1, \ldots, z_k \} \) and the second set be \( Z' = \{ z'_1, \ldots, z'_{k'} \} \). A centroid \( z_i \) (or \( z'_j \)) is associated with a percentage \( p_i \) (or \( p'_j \)) computed as the proportion of data entries assigned to the cluster of \( z_i \) (or \( z'_j \)). We define a Mallows-type distance \( D(Z, Z') \) based on the element-wise distances \( D(z_i, z'_j) \), where \( D(z_i, z'_j) \) is the Mallows distance between two centroids, which are both discrete distributions. We call \( D(Z, Z') \) Mallows-type because it is also the square root of a weighted sum of squared distances between the elements in \( Z \) and \( Z' \). The weights satisfy the same set of constraints as those in the optimization problem for computing the Mallows distance.

\[
\tilde{D}^2(Z, Z') = \sum_{i=1}^{k} \sum_{j=1}^{k'} w_{i,j} D^2(z_i, z'_j),
\]

subject to:

\[
\sum_{j=1}^{k'} w_{i,j} = p_i, \quad \sum_{i=1}^{k} w_{i,j} = p'_j,
\]

\[
w_{i,j} \geq 0, i = 1, \ldots, k, j = 1, \ldots, k'.
\]

We refer to \( D(Z, Z') \) as the MM distance (Mallows-type weighted sum of the squared Mallows distances).

Third, we use a measure for two ways of partitioning a dataset, which is proposed in [41]. This measure only depends on the grouping of data entries and is irrelevant with centroids. We refer to it as the categorical clustering distance. Let the first set of clusters be \( \mathcal{P} = \{ P_1, P_2, \ldots, P_k \} \) and the second be \( \mathcal{P}' = \{ P'_1, P'_2, \ldots, P'_{k'} \} \). Then the element-wise distance \( D_{p}(P_i, P'_j) \) is the number of data entries that belong to either \( P_i \) or \( P'_j \) but not the other. The distance between the partitions \( \tilde{D}_{p}(\mathcal{P}, \mathcal{P}') = \sum_{i=1}^{k} \sum_{j=1}^{k'} w_{i,j} D_{p}(P_i, P'_j) \) is again a Mallows-type weighted sum of \( D_{p}(P_i, P'_j), i = 1, \ldots, k, j = 1, \ldots, k' \). See [41] for details.

For each concept category, the number of clusters is set to 10. The mean squared distance from an image signature to its closest centroid is computed based on the clustering result obtained by the parallel or sequential D2-clustering algorithm. These mean squared distances are plotted in Fig. 4(a). We also compute the mean squared distance using randomly generated clusters for each concept. The random clustering is conducted 10 times and the average of the mean squared distances is recorded as a baseline. The random clusters, unsurprisingly, have the largest mean squared distances. In comparison, the parallel and sequential algorithms obtain close values for the mean squared distances for most concepts. Typically the mean squared distance by the parallel clustering is slightly larger than that by the sequential clustering. This shows that the parallel clustering algorithm compromises the tightness of clusters slightly for speed.

Fig. 4(b) compares the clustering results using the MM distance between sets of centroids acquired by different methods. For each concept \( i \), the parallel algorithm generates a set of centroids \( Z_i = \{ z_{i1}, \ldots, z_{ik_i} \} \).
and the sequential algorithm generates a set of centroids \( Z'_i = \{ z'_1, \ldots, z'_c \} \). The solid curve in Fig. 4(b) plots \( D^2(Z_i, Z'_i) \) for each concept \( i \). To demonstrate that \( D(Z_i, Z'_i) \) is relatively small, we also compute \( D(Z_i, Z'_j) \) for all pairs of concepts \( i \neq j \). Let the average \( d^2_i = \frac{1}{c-1} \sum_{j \neq i} D^2(Z_i, Z'_j) \), where \( c = 80 \) is the number of concepts. We use \( d^2_i \) as a baseline for comparison and plot it by the dashed line in the figure. For all the concepts, \( d^2_i \) is substantially larger than \( D(Z_i, Z'_i) \), which indicates that the set of centroids \( Z_i \) derived from the parallel clustering is relatively close to \( Z'_i \) from the sequential clustering. Another baseline for comparison is formed using random partitions. For each concept \( i \), we create 10 sets of random clusters, and compute the average over the squared MM distances between \( Z_i \) and every randomly generated clustering. Denote the average by \( d^2_i \), shown by the dashed dot line in the figure. Again comparing with \( d^2_i \), the MM distances between \( Z_i \) and \( Z'_i \) are relatively small for all concepts \( i \).

Fig. 4(c) plots the categorical clustering distance defined in (1) between the parallel and sequential clustering results for every image concept. Again, we compute the categorical clustering distance between the result from the parallel clustering and each of 10 random partitions. The average distance is shown by the dash line in the figure. For most concepts, the clustering results from the two algorithms are closer than those from the parallel algorithm and random partition. However, for many concepts, the categorical clustering distance indicates substantial difference between the results of the parallel and sequential algorithm. This may be caused to a large extent by the lack of distinct groups of images within a concept.

In summary, based on all the three measures, the clustering results by the parallel and sequential algorithms are relatively close.

3.2 Scalability Property

In Section 2.5 we derive that the parallel D2-clustering runs in approximately linearithmic time, while the sequential algorithm scales up poorly due to its polynomial time complexity. In order to demonstrate this, we perform clustering on sets of images with different sizes using both the parallel and sequential D2-clustering with different conditions, and examine the time consumed.

Fig. 5 shows the running time on sets of images in the concept “mountain”. In the plot, both axes are in log-log scales. All versions of clusterings are performed on datasets with sizes 50, 100, 200, 400, 800, 1600, 3200, and 6400. We test the parallel D2-clustering algorithm in three cases with identical parameters \( \tau = 50 \) and \( e = 5 \). In the first case, there is only one slave CPU handling all the clustering requests sent by the master CPU (i.e. there are two CPUs employed in total). All clustering requests are therefore processed sequentially by the only slave processor. In the second case, there are 16 slave CPUs (i.e. 17 CPUs in total). In the third case, the conditions are the same to the second case, but the data segmentation is implemented by a Vector Quantization (VQ) approach instead of the approach in Section 2.2. For comparison, the original sequential D2-clustering algorithm is also tested on the same datasets.

Fig. 5 shows the parallel algorithm scales up approximately at linearithmic rate. On a log-log plot, this means the slope of the curve is close to 1. The number of slave CPUs for the parallel processing, as discussed in Section 2.5 contributes a linear difference (the second term in (7)) to the run-time between the first and second parallel cases. When \( N \) is small, the linear difference may be relatively significant and make the single CPU case much slower than the multiple CPU case. But the difference becomes less so when the dataset is large because there is a dominant linearithmic term in the run-time expression. Nevertheless, in either case, the parallel algorithm is much faster than the sequential algorithm. The slope of the curve on the log-log plot for...
the sequential algorithm is much larger than 1, indicating at least polynomial complexity with a high degree. As a matter of fact, the parallel algorithm with 16 slave CPUs takes 88 minutes to complete clustering on the dataset containing 6400 images, in contrast to almost 8 hours consumed by the sequential algorithm running only on the dataset of size 200. Because the time for the sequential D2-clustering grows dramatically with the data size, we can hardly test it on dataset larger than 200.

For the last parallel case, we include VQ in the segmentation in order to further accelerate the algorithm. Based on the analysis in Section 2.5, we know that data segmentation takes a lot of time at each level of the algorithm. In the VQ approach, we quantify the bag of weighted vectors to histograms and treat them as vectors. These histograms are then segmented by K-means algorithm in the segmentation step. The clustering within each segment is still D2-clustering on the original data. However the time spent for segmentation is much shorter than the original approach in Section 2.2.

In Fig. 5 the acceleration is reflected by the difference between the run-time curves of parallel D2-clustering with and without VQ segmentation when \( N \) is large. When \( N \) is small and the data segmentation is not dominant in the run-time, VQ will usually not make the clustering faster. In fact due to bad segmentation of such a coarse algorithm, the time consumed for D2-clustering within each segment might be longer. That is the reason why the parallel D2-clustering with VQ segmentation is slower than its counterpart without VQ segmentation (both have same parameters and 16 slave CPUs employed) in Fig. 5 when \( N \) is smaller than 800.

Theoretically VQ can reduce the order of the clustering from linearithmic to linear (referred by (7)). However because the quantization step loses some information, the clustering result might be less accurate. This can be reflected by the MM distance (defined in (10)) between the parallel D2-clustering with VQ segmentation and the sequential D2-clustering results on a dataset containing 200 images, which is 19.57 on average for five runs. Compared to 18.41 as the average MM distance between the original parallel D2-clustering and sequential D2-clustering results, the VQ approach makes the parallel clustering result less similar to the sequential clustering result which is regarded as the standard.

No matter whether VQ is adopted, the experiment shows the acceleration of parallel D2-clustering over the sequential algorithm, which verifies the run-time analysis in Section 2.5. Applying the algorithm, we can greatly increase the scale of the discrete distribution clustering problems.

3.3 Visualization of Image Clustering

Simulating the real image annotation application, the parallel D2-clustering algorithm is applied to a set of 1488 images downloaded from Flickr \((\tau = 50, e = 5)\). These images are retrieved by query keyword “mountain”. For such a set, we do not have ground truth for the clustering result, and the sequential D2-clustering cannot be compared because of its unrealistic running time. We thus visualize directly the clustering result and attempt for subjective assessment.

The 1488 images are clustered into 13 groups by the parallel D2-clustering algorithm using 873 seconds (with 30 slave CPUs). At the end, there are 7 clusters with sizes larger than 100, for each of which 20 images closest to the corresponding cluster centroid are displayed in Fig. 6. In the figure we try to manually arrange similar clusters close, and dissimilar ones far away based on the Mallows distances between the cluster centroids. Fig. 6 shows that images with similar color and texture
are put in the same clusters. More clustering results for images with different concepts are shown in Fig. 4. For all the datasets, visually similar images are grouped into the same clusters. The parallel algorithm has produced meaningful results.

3.4 Video Clustering

To demonstrate the application of parallel D2-clustering on video clustering, we download 450 videos from Youtube. They are all 5 to 20 minutes in length, and come from 6 different queries, which are “news”, “soccer”, “lecture”, “movie trailer”, “weather forecast”, and “tablet computer review”. Each category contains 75 videos. We compare the clustering result with the category label to check the correctness of the algorithm.

It should be emphasized that video classification is a complicated problem. Since our algorithm is an unsupervised clustering algorithm rather than a classification method, we cannot expect it to classify the videos with a high accuracy. In addition, though not the major concern in this paper, the visual features for segmenting and describing videos are crucial for the accuracy of the algorithm. Here we only adopt some easy-to-implement simple features for demonstration. Therefore the purpose of this experiment is not to pursue the best video classification, but to demonstrate the reasonable results of the parallel D2-clustering algorithm on videos. The videos’ class labels, which serve as the ground truth, are used as a reference to show whether similar videos can be clustered into a same group.

In this experiment, we set \( \tau = 30 \), \( e = 5 \), and request 15 slave CPUs (\( M = 15 \)) to cluster the data. As mentioned above, we adopt three visual features, EDH, GBR, and GCD, to segment and describe each video. We extract the features and form the video descriptors before the clustering. Typically a video will be segmented into 10 to 30 sub-clips, depending on its content and length. In addition, the feature vector itself is high in dimension (73 for EDH, 48 for GBR, and 225 for GCD). As a result, each video is represented by a large bag of weighted vectors.

### TABLE 1

| Cluster (Size) | C1 (36) | C2 (40) | C3 (111) | C4 (40) | C5 (72) | C6 (75) |
|---------------|---------|---------|----------|---------|---------|---------|
| Soccer        | 43      | 5       | 1        | 1       | 8       | 10      |
| Tablet        | 19      | 23      | 14       | 1       | 9       | 4       |
| News          | 9       | 13      | 27       | 8       | 17      | 5       |
| Weather       | 4       | 0       | 31       | 32      | 0       | 2       |
| Lecture       | 4       | 2       | 32       | 0       | 17      | 13      |
| Trailer       | 2       | 3       | 6        | 0       | 20      | 43      |

By applying the parallel D2-clustering algorithm, we can get a clustering result for this high dimensional problem in 847 seconds. 6 major clusters (C1-C6) are generated and Table 1 is the confusion table. We then try to use the clustering result for classification by assigning each cluster with the label corresponding to its majority class. For these six clusters, the unsupervised clustering achieves a classification accuracy of 47.5%.

3.5 Protein Sequence Clustering

In bioinformatics, composition-based methods for sequence clustering and classification (either DNA \([19, 20]\) or protein \([11]\)) use the frequencies of different compositions in each sequence as the signature. Nucleotides and amino acids are basic components of DNA and protein sequence respectively and these methods use a nucleotide or amino acid histogram to describe a sequence. Because different nucleotide or amino acid pairs have different similarities determined by their molecular structures and evolutionary relationships, cross-term relations should be considered when we compute the distance between two such histograms. As a result, the Mallows distance would be a proper metric in composition-based approaches. However, due to the lack of effective clustering algorithms under the Mallows distance, most existing clustering approaches either ignore the relationships between the components in the histograms and treat them as variables in a vector, or perform clustering on some feature vectors derived from the histograms. In this case, D2-clustering will be especially appealing. Considering the high dimensionality and large scale of biological data, parallel algorithm is necessary.

In this experiment, we perform parallel D2-clustering on 1,500 protein sequences from Swiss-Prot database, which contains 519,348 proteins in total. The 1,500 proteins are selected based on Prosite data, which provides class labeling for part of Swiss-Prot database. We randomly choose three classes from Prosite data, and extract 500 protein sequences from Swiss-Prot database for each class to build our experiment dataset.

Each protein sequence is transformed to a histogram of amino acid frequencies. There is a slight modification in the computation of the Mallows distance between two such histograms over the 20 amino acids. In Equation (11), the squared Euclidean distance between two support vectors is replaced by a pair-wise amino acid distance provided in the PAM250 mutation matrix \([30]\). Given any two amino acids \( A \) and \( B \), we can get the probabilities of \( A \) mutated to \( B \) and \( B \) mutated to \( A \) from the matrix. The distance between \( A \) and \( B \) is defined as

\[
D_{\text{PAM250}}(A, B) = \log \left( P(A|B) \right) + \log \left( P(B|A) \right) .
\] (11)

Because the support vectors for each descriptor are the 20 types of amino acids and hence symbolic, we will skip the step to update support vectors in the centroid update of D2-clustering (refer to Step 2 in Algorithm 1) in the implementation of the parallel D2-clustering algorithm in this case. We set \( \tau = 30 \), \( e = 5 \), and request 7 slave processors to perform the parallel clustering (\( M = 7 \)). We let the program generate 5 clusters and the clustering finishes in about 7 hours. Considering the high dimensionality of the histograms and the scale of the dataset, this is a reasonable time. Three out of the five clusters are
Fig. 7. Visualized clustering results on four image concepts. Each concept contains 1,000 images from Flickr. They are clustered by the parallel D2-clustering algorithm and top ranked images in large clusters are displayed. Visually similar images are grouped into same clusters, though images in a same cluster do not always stand for similar semantics.

major ones, which contain more than 99% of the dataset. Fig. 8(a) describes the clustering centroids.

If we do not consider cross-term differences in the distance between two histograms and use Euclidean distance as the metric, the clustering is reduced to K-means. Therefore in this application, we are able to apply K-means on the dataset. Running on the multi-CPU server, the K-means algorithm is also implemented by parallel programs. We parallelize K-means in two different ways. In the first one, we apply the approach in [15], which is to perform centroid update and label update in parallel for different segments of data and then combine partial result linearly. In this way the parallelization is equivalent to the original K-means on the whole dataset. In the second way, we adopt the same hierarchical clustering structure, as in Fig. 1 used in the parallel D2-clustering algorithm and only replace the Mallows distance by the Euclidean distance. Thus within each data segment at any level of the hierarchy, the locally performed clustering is K-means. However there will be some loss of accuracy since several data are grouped and treated as one object at higher levels’ clustering, and will never be separated thereafter. For short, we refer to the first implementation as parallel K-means and the second one as hierarchical K-means.

Fig. 8(b) and Fig. 8(c) show the clustering centroids generated by parallel K-means and hierarchical K-means, running on the same dataset with identical parameters. Apparently, none of parallel K-means’ or hierarchical K-means’ centroids reveals distinct patterns compared with the centroids acquired by parallel D2-clustering. In order to prove the fact objectively, we compute the Davies-Bouldin index (DBI) [7] for all the three clustering results as the measurement of their tightness. DBI is defined as

$$DB = \frac{1}{k} \sum_{j=1}^{k} \max_{l \neq j} \left( \frac{\sigma_j + \sigma_l}{d(z_j, z_l)} \right),$$

(12)

where $k$ is the number of clusters, $z_j$ is the centroid of cluster $j$, $d(z_j, z_l)$ is the distance from $z_j$ to $z_l$, and $\sigma_j$ is the average distance from $z_j$ to all the elements in cluster $j$. DBI is the average ratio of intra-cluster dispersion to inter-cluster dispersion. Lower DBI means a better clustering result with tighter clusters.

**TABLE 2**

| Distance used in (12) | Parallel D2 | Parallel K-means | Hierarchical K-means |
|-----------------------|-------------|------------------|----------------------|
| Squared Mallows       | 1.55        | 2.99             | 2.01                 |
| Squared $L_2$         | 1.69        | 5.54             | 2.04                 |

We compute DBI using both the squared Mallows
distance and the squared Euclidean distance as $d(\cdot)$ in (12) for each clustering result. Table 2 shows the result. Parallel D2-clustering gains the lowest DBI in both cases. This indicates good tightness of the clusters generated by parallel D2-clustering. In contrast, the two implementations of K-means generate looser clusters than parallel D2-clustering. Though both can complete very fast, their clustering results are less representative.

3.6 Evaluation with Synthetic Data

Except for all the above experiments on real data, we also apply the algorithm on a synthetic dataset. The synthetic data are bags of weighted vectors. We carefully sample the vectors and their weights so that the data gather around several centroids, and their distances to the corresponding centroids follow the Gamma distribution, which means they follow a Gaussian distribution in a hypothetical space. By using this dataset, we have some ideally distributed data with class labels.

We create a synthetic dataset containing 15 clusters, each composed of 100 samples around the centroid. The clusters are well separated. The upper bound for the number of clusters in the algorithm is set 20. It takes about 8 minutes to cluster the data (with 30 slave CPUs). Then 17 clusters are generated. We try to match these 17 clusters to the ground truth clusters: 9 of the 17 clusters are identical to their corresponding true clusters; 5 clusters with sizes close to 100 differ from the true clusters only by a small number of samples; 2 clusters combine precisely into one true cluster; and at last a small cluster of size 8 may have formed from some outliers. It is evident that for this synthetic dataset, the parallel D2-clustering has produced a result close to the ground truth.

4 Conclusion

As a summary, a novel parallel D2-clustering algorithm with dynamic hierarchical structure is proposed. Such algorithm can efficiently perform clustering operations on data that are represented as bags of weighted vectors. Due to the introduction of parallel computing, the speed of the clustering is greatly enhanced, compared to the original sequential D2-clustering algorithm. By deploying the parallel algorithm on multiple CPUs, the time complexity of D2-clustering can be improved from high-ordered polynomial to linearithmic time, with minimal approximation introduced. The parallel D2-clustering algorithm can be embedded into various applications, including image concept learning, video clustering, and sequence clustering problems. In the future, we plan to further develop image concept learning and annotation applications based on this algorithm.

Acknowledgments

This material is based upon work supported by the National Science Foundation under Grant No. 1027854, 0347148, and 0936948. The computational infrastructure was provided by the Foundation through Grant No. 0821527. Part of the work of James Z. Wang and Jia Li is done while working at the Foundation.

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