Abstract

We study how to learn multiple dictionaries from a dataset, and approximate any data point by the sum of the codewords each chosen from the corresponding dictionary. Although theoretically low approximation errors can be achieved by the global solution, an effective solution has not been well studied in practice. To solve the problem, we propose a simple yet effective algorithm Group \( K \)-Means. Specifically, we take each dictionary, or any two selected dictionaries, as a group of \( K \)-means cluster centers, and then deal with the approximation issue by minimizing the approximation errors. Besides, we propose a hierarchical initialization for such a non-convex problem. Experimental results well validate the effectiveness of the approach.

1 Introduction

\( K \)-means is a well-known clustering algorithm and has been widely applied in numerous applications. The algorithm aims to partition \( N \) \( P \)-dimensional points into \( K \) clusters in which each point belongs to the cluster with the nearest mean. Let \( \mathcal{X} = \{ x_1, \ldots, x_N \} \subset \mathbb{R}^P \) be the dataset and \( \mathcal{D} = \{ d_1, \ldots, d_K \} \subset \mathbb{R}^P \) be the cluster centers. The clusters \( \mathcal{D} \) are learned by minimizing

\[
\sum_{x \in \mathcal{X}} \min_k \| x - d_k \|_2^2, \tag{1}
\]

where \( \| \cdot \|_p \) denotes the \( l_p \) norm. The objective function can be iteratively minimized [7]. Each iteration involves an assignment step and an update step. In the former step, the nearest center of each point is calculated, while the latter computes the mean of the points assigned into the same cluster. Each point can be represented by the index of the nearest cluster center, which requires \( \lceil \log_2 K \rceil \) bits.

The assignment of each point requires \( O(KP) \) time cost. When the number of clusters is huge, it is prohibitive to perform the exact \( K \)-means due to the high time cost. To solve the scalability issue, we can split the \( P \)-dimensional vector into \( M \) subvectors as in [4, 5, 8]. Then the standard \( K \)-means algorithm is applied on each subvector, resulting in \( K^M \) cluster centers but with \( O(KP) \) assignment time cost. The number of bits required to represent each point is \( \log_2 K^M = M \log_2 K \).

Recently, multiple dictionaries are proposed in [9, 3, 1]. Each dictionary contributes one codeword and the summation of these codewords is used to approximate one data point. Let \( \mathcal{D}^r = \)
Algorithm 1 Iterative optimization in gk-means

Input: Dataset $X = \{x_1, \cdots, x_N\}$, number of dictionaries $C$  
Output: Multiple dictionaries $\{D^c, c \in \{1, \cdots, C\}\}$

1: Initialize multiple dictionaries $\{D^c, c \in \{1, \cdots, C\}\}$ by Sec. 2.3.1
2: Initialize the assignments $\{k_1, \cdots, k_C\}$ for each point $x \in X$ by Sec. 2.3.2
3: while !converged do
4: Update multiple dictionaries by Sec. 2.2
5: Compute assignments by Sec. 2.1
6: end while

$\{d^c_1, \cdots, d^c_K\} \subset \mathbb{R}^P$ be the $c$-th dictionary with $c \in \{1, \cdots, C\}$. The objective is to minimize

$$\sum_{x \in X} \min_{k_1, \cdots, k_C} \left\| x - \sum_c d^c_{k_c} \right\|_2^2$$

(2)

to learn the dictionaries $\{D^c\}_{c=1}^C$. In [9], the problem is studied on the subvector, and can be seen as a special case where the subvector is equal to the full vector or the number of subvectors is 1. This problem is also explored in [10], but with an additional constraint to make the scheme more suitable for Euclidean approximate nearest neighbor search. To represent each point, we need $C \log_2 K$ bits to indicate which codewords are selected from all the dictionaries.

It is easily verified based on [9] that a global optimal solution can give a lower distortion error than [5, 8] under the same code lengths. However, it is very challenging to obtain the global solution due to the non-convexity of the problem. In [9], an intuitive recursive algorithm is proposed, but the complexity is exponential with the number of dictionaries, and it is less scalable with a larger $C$.

In this paper, we propose a simple yet effective algorithm, named Group $K$-Means (shorted as gk-means)\(^2\) to solve the problem. Specifically, we take each dictionary or any two consecutive dictionaries as a group of $K$-means clusters, and solve the assignment with a linear time complexity to the number of dictionaries. Due to the non-convexity of the problem, we propose a hierarchical scheme composed of multiple stages to initialize the dictionaries. Each stage solves a subproblem where a portion of the entries in the dictionaries are enforced to be 0. Experimental results have verified the effectiveness of our approach.

2 Group $K$-means

To minimize Eqn. (2), we iteratively perform the assignment step and the update step as shown in Alg. 1 and introduced in the first two subsections. The former computes the assignments $(k_1, \cdots, k_C)$ of each point $x$ based on the dictionaries and the assignments in the previous iteration. The latter updates the multiple dictionaries based on the current assignments. Besides, the initialization of the dictionaries and the assignments is introduced in the last subsection.

2.1 Assignment Step

2.1.1 Order-1 Group Assignment

In Eqn. (2), each point is approximated by the summation of multiple codewords, and each codeword is chosen from a different dictionary. We first take each dictionary as a group of clusters on the residual. For the $c_1$-th dictionary, the residual is defined as

$$y = x - \sum_{c \neq c_1} d^c_{k_c}.$$  

(3)

The assignments $\{k_c, c \neq c_1\}$ are from the previous iteration. We can also assert that the quantization error between $y$ and any codeword $d^c_{k_{c_1}} \in D^{c_1}$ equals the distortion error between $x$ and the

\(^2\)The algorithm is similar with [2], but we conduct the research independently and apply it in data/feature compression and image retrieval.
Furthermore, we propose the scheme for computing the assignments over all groups until the assignments do not change. If the number of iterations needed to scan all the groups for one point is greater than a constant, we refer to this scheme as one group of clusters, we call this scheme Group Assignment (GA), where any two dictionaries can be taken as a group of clusters.

Algorithm 2 Assignment Step in the current iteration

Input: \( \mathcal{X} = \{x_i\}_{i=1}^N \), \( \{d^c_k\}_{c=1,k=1}^{C,K} \), \( \{k_c\}_{c=1}^C \), assignments \( \{k_{c_1}\}_{c_1=1,k_{c_1}=1}^C \) for each \( x \in \mathcal{X} \) in the previous iteration.

Output: \( \{k_{c_1}\}_{c_1=1,k_{c_1}=1}^C \) for each \( x \in \mathcal{X} \) in the current iteration

1: Compute \( \{T_{k_{c_1},k_{c_2}}\} \) according to Eqn. (3)
2: for \( x \in \mathcal{X} \) do
3: Compute \( \{S_{k_{c_1}}\}_{c_1=1,k_{c_1}=1}^C \) according to Eqn. (7)
4: while ! converged do
5: Compute \( k_{c_1},c_1 \in \{1, \cdots, C\} \) by Sec. 2.1.1
6: end while
7: end for

The second item in Eqn. (6) is independent of the point \( x \), and thus we can pre-compute a lookup table \( \{T_{k_{c_1},k_{c_2}}\} \) before scanning all the points. For each point, we compute \( \{S_{k_{c_1}}\} \) before scanning all the group centers. Then, the computation of Eqn. (4) only requires \( O(C) \) addition by Eqn. (6), and the complexity of multiplication is reduced to \( O(KCP) \) from \( O(SKCP) \). Since each dictionary is referred to as one group of clusters, we call this scheme Order-1 Group Assignment (shorted as \( O_1GA \)).

2.1.2 Order-2 Group Assignment

Furthermore, we propose the scheme Order-2 Group Assignment (shorted as \( O_2GA \)), where any two dictionaries can be taken as a group of clusters.

For the \( c_1 \)-th and \( c_2 \)-th dictionaries, we obtain the residual similarly as Eqn. (3) by

\[
y = x - \sum_{c \neq c_1,c \neq c_2} d^c_{kc}.
\]
Each pair of \((k_{c1}, k_{c2})\) can construct a cluster center \(d_{k_{c1}}^{c1} + d_{k_{c2}}^{c2}\). Thus, we compute the assignment as
\[
(k_{c1}, k_{c2}) = \arg \min_{k_{c1}, k_{c2}} \frac{1}{2} \| y - d_{k_{c1}}^{c1} - d_{k_{c2}}^{c2} \|^2 
\]
\[
= \arg \min_{k_{c1}, k_{c2}} (S_{k_{c1}}^{c1} + \sum_{c \neq c2} T_{k_{c1}, k_{c}}^{c1,c}) + (S_{k_{c2}}^{c2} + \sum_{c \neq c1} T_{k_{c2}, k_{c}}^{c2,c}) + T_{k_{c1}, k_{c2}}^{c1,c2},
\]
where \(S_{k_{c1}}^{c1}\) and \(T_{k_{c1}, k_{c}}^{c1,c2}\) are defined in Eqn. (7) and Eqn. (8), respectively. To compute (11), we need only \(O(K^2)\) addition rather than multiplication. The formulation is general for any \(c1 \neq c2\).

Discussion. The assignment algorithm is illustrated in Alg. 2 for \(O_1GA\) and \(O_2GA\). Note that the iteration in Line 4 is important because the assignments \(\{k_c, c \neq c1\}\) or \(\{k_c, c \neq c1, c \neq c2\}\) may change after all the dictionaries are scanned once, and the assignment \(k_{c1}\) or \(k_{c1}, k_{c2}\) can be re-computed to further reduce the distortion error.

The scheme \(O_2GA\) can be straightforwardly extended to \(O_nGA\). If \(n\) equals \(C\), the global optimal assignment can be obtained. However, the time cost of all addition in Eqn. (11) is \(O(K^n)\) and is exponential with \(n\). Thus, we set \(n = 1, 2\) experimentally. Besides, the complexity is linear with the number of dictionaries \(C\), and is much lower than the exponential complexity of \(O_2GA\). Intuitively, the distortion induced by \(O_2GA\) should be lower than or equal to that by \(O_1GA\). However, this assertion cannot be guaranteed. One reason is that in the iterative optimization, the dictionaries are also optimized and become qualitatively different even after one update step. Given different dictionaries, we cannot assert the superiority of \(O_2GA\) over \(O_1GA\). However, in most cases, the superiority is demonstrated experimentally.

2.2 Update Step

The objective function in Eqn. (2) is quadratic w.r.t. the multiple dictionaries. Thus, the dictionaries can be updated by setting the derivative w.r.t. the dictionaries as 0. In the following, we derive the equivalent results from the mean of the centers, which is much similar with the traditional \(K\)-means.

Given the assignment \(\{k_c\}\) for the \(i\)-th point, we first introduce an indicator function
\[
r_{i,k} = \begin{cases} 1, & k_c = k \text{ for } x_i \\ 0, & \text{otherwise}. \end{cases}
\]
(12)
It represents whether the assignment of the \(i\)-th point on the \(c\)-th dictionary is \(k\). Then, the residual in Eqn. (3) can be written for the \(i\)-th point as
\[
y_i = x_i - \sum_{c \neq k} r_{i,k}^c d_k^c.
\]
(13)
Next, we update the center \(d_{k_{c1}}^{c1}\) by the mean of the residuals within the cluster, i.e.
\[
d_{k_{c1}}^{c1} = \frac{\sum_i r_{i,k_{c1}}^c y_i}{\sum_i r_{i,k_{c1}}^c}, \text{ if } \sum_i r_{i,k_{c1}}^c \neq 0.
\]
(14)
Substituting Eqn. (13) into Eqn. (14) and simplifying the equation, we have
\[
\sum_i r_{i,k_{c1}}^c x_i = \sum_{k,c} \left( \sum_i r_{i,k_{c1}}^c r_{i,k}^c \right) d_k^c.
\]
(15)
Since Eqn. (15) holds for any \(c1 \in \{1, \cdots, C\}\) and \(k_{c1} \in \{1, \cdots, K\}\), the matrix form is \(W = DZ\), where
\[
W = \begin{bmatrix} w_1^1 & \cdots & w_K^1 & \cdots & w_1^C & \cdots & w_K^C \end{bmatrix},
\]
(16)
\[
w_{k_{c1}}^c = \sum_i r_{i,k_{c1}}^c, k_{c1} \in \{1, \cdots, K\}, c \in \{1, \cdots, C\}
\]
(17)
\[
D = \begin{bmatrix} d_1^1 & \cdots & d_K^1 & \cdots & d_1^C & \cdots & d_K^C \end{bmatrix}.
\]
(18)
The element of \( Z \in \mathbb{R}^{KC \times KC} \) in the \( (c_1 - 1)K + k_1 \)-th row and the \( (c_2 - 1)K + k_2 \)-th column is
\[
Z_{c_1,c_2}^{k_1,k_2} = \sum_i c_i^{c_1,k_1} r_{c_2}^{c_2,k_2}, k_1, k_2 \in \{1, \cdots, K\}, c_1, c_2 \in \{1, \cdots, C\},
\]
which can be interpreted as the number of points whose assignments on the \( c_1 \)-th dictionary and on the \( c_2 \)-th dictionary are \( k_1 \) and \( k_2 \), respectively. Then, we can solve the dictionaries \( D \) by the matrix (pseudo)inversion.

### 2.3 Initialization

Since the problem of minimizing Eqn. 2 is non-convex, different initializations fall into different local minima, and thus the initialization is quite important.

#### 2.3.1 Initialization of Dictionaries

One direct method is to randomly sample the points from the dataset to construct the dictionaries as in \([9]\). Empirically, we find this scheme works well for cases with a small number of dictionaries (e.g. \( C = 2 \) as in \([9]\)), but the performance degrades for a larger \( C \). In this work, we propose two initialization schemes. The first is based on the traditional \( K \)-means and the second is a hierarchical scheme based on \([8][9]\).

**K-Means-based initialization** is to run the traditional \( K \)-means algorithm on the residual repeatedly. Specifically, we first set the residual by the original dataset, i.e. \( y = x, \forall x \in X \), and the index of the to-be-initialized dictionary as \( c = 1 \). Then, the \( K \)-means is performed on \( \{y\} \) to obtain the \( K \) cluster centers as the first dictionary \( \{d_1^c, \cdots, d_K^c\} \). After this, we update the residual of each point by \( y \leftarrow y - d_k^c \), where \( k \) is the assignment of \( y \), and \( c \leftarrow c + 1 \). The \( K \)-means algorithm is repeatedly run to obtain the second dictionary. By alternately updating the residual and performing the \( K \)-means on the residual, we can get all the dictionaries as an initialization.

**Hierarchical Initialization** can ensure that in theory the approach performs not worse than the vector partitioning approaches (e.g. \([8]\)) under the same code length. The basic idea is to solve \( \log_2 C \) subproblems where different constraints are applied on the multiple dictionaries. Let \( D^c = [d_1^c \cdots d_K^c] \) and \( b^c \in \{0, 1\}^K, \|b^c\|_1 = 1 \). The index of 1 in \( b^c \) represents which codeword is selected. We can rewrite the objective of Eqn. (2) as
\[
\sum_x b^c, \|b^c\|_1 = 1 \left\| x - \begin{bmatrix} D^1 & \cdots & D^C \end{bmatrix} \begin{bmatrix} b^1 \\ \vdots \\ b^C \end{bmatrix} \right\|_2^2.
\]

Before introducing the approach in a general case, we take \( C = 4 \) as an example. First, we minimize Eqn. (20) with the dictionaries \( D = [D^1 \quad D^2 \quad D^3 \quad D^4] \) constrained to be
\[
D = R_1 \begin{bmatrix} D_{1,1}^1 & 0 & 0 & 0 \\ 0 & D_{2,1}^1 & 0 & 0 \\ 0 & 0 & D_{3,1}^1 & 0 \\ 0 & 0 & 0 & D_{4,1}^1 \end{bmatrix}, R_1^T R_1 = I,
\]
where \( R_1 \) is a rotation matrix and \( D_{m,1}^1, m \in \{1, 2, 3, 4\} \) is a real matrix of size \( P/4 \times K \). The notation \( D_{u,v} \) denotes the block in the \( u \)-th row and \( ((u-1)2^{s-1} + v) \)-th column of \( D \) in the \( s \)-th subproblem. This subproblem is studied in \([8]\), and can be solved by alternating optimizations with regard to \( R_1, \{D_{m,1}^1\} \) and \( \{b^c\} \). We initialize \( R_1 \) by an identity matrix and \( \{D_{m,1}^1\} \) by randomly choosing the data points on the corresponding subvector. The optimal solution is used to initialize the second subproblem where the objective function remains the same but the constraint is relaxed to be
\[
D = R_2 \begin{bmatrix} D_{2,1}^2 & D_{2,2}^2 & 0 & 0 \\ 0 & D_{2,1}^2 & 0 & 0 \end{bmatrix}, R_2^T R_2 = I.
\]
\(^3\)We assume \( C \) is a power of 2. Meanwhile, the dimension \( P \) is assumed to be divisible by \( C \) in the following. This algorithm can easily adapt to general cases.
The initialization of the second subproblem is as follows
\[
R_2 = R_1^*, D_2^{1,1} = \begin{bmatrix} D_1^{1,1} & * \\ 0 & 0 \end{bmatrix}, D_2^{1,2} = \begin{bmatrix} 0 & * \\ D_1^{2,1} & 0 \end{bmatrix}, D_2^{2,1} = \begin{bmatrix} D_1^{3,1} & * \\ 0 & 0 \end{bmatrix}, D_2^{2,2} = \begin{bmatrix} 0 & * \\ D_1^{4,1} & 0 \end{bmatrix},
\] (23)
where the asterisk * denotes the optimal solution. This subproblem is studied in [9], and it is verified that the distortion can be lower than ck-means [8]. We solve the subproblem in a similar manner with [9], except that the assignment step is replaced by that in Sec. 2.1. Finally, D is initialized by
\[
D^1 = R_2^*\begin{bmatrix} D_2^{1,1} & * \\ 0 & 0 \end{bmatrix}, D^2 = R_2\begin{bmatrix} D_2^{1,2} & * \\ 0 & 0 \end{bmatrix}, D^3 = R_2^*\begin{bmatrix} 0 & * \\ D_2^{2,1} & 0 \end{bmatrix}, D^4 = R_2\begin{bmatrix} 0 & * \\ D_2^{2,2} & 0 \end{bmatrix}.
\] (24)

In summary, each subproblem enforces different levels of restrictions on the multiple dictionaries. In the first subproblem, the restriction is most severe, and most of the elements are constrained to be 0. Then it is relaxed gradually in the subsequent subproblems. Generally, the s-th (s ∈ {1, · · · , log2 C}) subproblem is constrained by \( R_s^T R_s = I \) and
\[
D = R_s \begin{bmatrix} D_s^{1,1} & \cdots & D_s^{1,2^{s-1}} \\ & \ddots & \\ & & D_s^{C/2^{s-1},1} & \cdots & D_s^{C/2^{s-1},2^{s-1}} \end{bmatrix}.
\] (25)

The initialization of the (s + 1)-th subproblem is \( R_{s+1} = R_s^* \) and
\[
D_{s+1}^{u,v} = \begin{cases} D_s^{2u-1,v*}, & \text{if } u \in \{1, \cdots, C/2^s\}, v \in \{1, \cdots, 2^{s-1}\}; \\
0, & \text{otherwise}. \end{cases}
\] (26)
\[
D_{s+1}^{u,v} = \begin{cases} 0, & \text{if } u \in \{1, \cdots, C/2^s\}, v \in \{2^{s-1} + 1, \cdots, 2^s\}. \end{cases}
\] (27)

The final initialization for Eqn. (2) is
\[
D^v = R_{log_2 C}^* \begin{bmatrix} D_{log_2 C}^{0,v*} & \vdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & 0 \end{bmatrix}, 1 \leq v \leq C/2; D^v = R_{log_2 C}^* \begin{bmatrix} 0 \\ \vdots \\ 0 \end{bmatrix}, C/2 + 1 \leq v \leq C.
\]

2.3.2 Initialization of assignments

In Sec. 2.1, the assignment is based on the residual defined in Eqn. (3) and Eqn. (9) for O1GA and O2GA, respectively. To initialize the assignment, we only use the initialized \( k_c \) to compute the residual. Taking O1GA as an example, we compute the residual by \( y = x - \sum_{c=1}^{c_1} d_{k_c} \) for the \( c_1 \)-th dictionary. After iterating \( c_1 \) from 1 to \( C \), we refine the assignment by Alg. 2. This is also applied to encode new data points after obtaining the dictionaries. That is, we initialize the assignments first and then refine them by Alg. 2. Similar ideas can be applied to initialize the assignments for O2GA.

3 Experiments

3.1 Settings

We conduct the experiments on three widely-used high-dimensional datasets: SIFT1M [5], GIST1M [3], and MNIST [6]. SIFT1M has 10^5 training features, 10^5 query features, and 10^6 database features. Each feature is a 128-dimensional SIFT descriptor. GIST1M has 5 × 10^5 training features, 10^5 query features and 10^6 database features with each being a 960-dimensional GIST feature. MNIST contains 60,000 database images (also used as the training set) and 10,000 query images. Each image has 28 × 28 pixels, and we vectorize it as a 784-dimensional feature vector.

The accuracy is measured by the relative distortion, which is defined as the objective function of Eqn. (2) with the optimized solutions divided by \( \sum_{x \in X} ||x||_2^2 \). This indicator is important in data compression, approximate nearest neighbor (ANN) search [9], etc. The accuracy is better with a lower distortion. Due to the space limitation, we report the experiments on the application of ANN search in the supplementary material.
We compare our approach with ck-means [8] and optimized Cartesian k-means (ock-means) [9] under the same code length. Let \( M_{ck} \) and \( M_{ock} \) be the numbers of subvectors in ck-means and ock-means respectively, and let \( C_{ock} \) and \( C_{pk} \) be the number of dictionaries on each subvector of ock-means and the number of dictionaries of gk-means respectively. Then the code lengths of ck-means, ock-means, and gk-means are \( M_{ck} \log_2(K) \), \( M_{ock} C_{ock} \log_2(K) \) and \( C_{pk} \log_2(K) \), respectively. We set \( M_{ck} = M_{ock} C_{ock} = C_{pk} \) to make the code length identical for all the approaches. Following [8, 9], we set \( K = 256 \) to fit the index by one byte, and \( C_{pk} = 4, 8, 16 \) to obtain the code lengths 32, 64, 128, respectively. As for the initialization of gk-means shown in Sec. 2.3.1, 30 iterations are consumed both in each \( k \)-means for the \( k \)-means-based initialization and in each subproblem for the hierarchical initialization. The number of iterations in all the approaches is at most 100 or the iteration stops if it reaches convergence. It is expected that the performance gains with a larger number of iterations. Here we just fix the maximum iteration number for the comparison purpose. To minimize Eqn. (2), a multiple candidate matching pursuit (MCP) algorithm is proposed on each subvector in [9]. Since MCP is exponential with the number of dictionaries, we set \( C_{ock} = 2 \) by default as suggested in [9]. We also run MCP on the full vector with other values of \( C_{ock} \) and compare it with gk-means.

The term gk-means\((a, b)\) is used to distinguish different assignment approaches in Sec. 2.4 and different initialization schemes in Sec. 2.3: \( a = 1, 2 \) to represent \( O_1GA \) and \( O_2GA \), respectively; \( b = r, k, h \) to represent the random initialization, the \( k \)-means-based initialization, and the hierarchical initialization, respectively.
Table 1: Relative distortion ($\times 10^{-2}$) on the databases with different code lengths.

|            | gk-means     | ock-means   | ck-means   |
|------------|--------------|-------------|------------|
|            | (2, h)       | (2, k)      | (2, r)     | (1, h) | (1, k) | (1, r) |          |
| SIFT1M     |              |             |            |        |        |        |          |
| 32         | 20.47        | 21.14       | 23.78      |        |        |        |          |
| 64         | 20.63        | 22.22       | 22.48      | 21.59  | 22.48  | 21.14  |          |
| 128        | 11.56        | 14.10       | 14.45      | 13.37  | 14.10  | 13.37  |          |
| GIST1M     |              |             |            |        |        |        |          |
| 32         | 41.24        | 42.32       | 42.32      | 44.32  | 41.64  | 43.19  |          |
| 64         | 33.92        | 33.92       | 33.38      | 34.75  | 33.92  | 34.75  |          |
| 128        | 25.93        | 25.93       | 26.18      | 26.29  | 25.93  | 26.18  |          |
| MNIST      |              |             |            |        |        |        |          |
| 32         | 15.29        | 18.18       | 18.18      |        |        |        |          |
| 64         | 10.36        | 14.88       | 14.88      | 18.38  | 14.88  | 18.38  |          |
| 128        | 6.55         | 12.37       | 12.37      | 16.11  | 12.37  | 16.11  |          |

3.2 Results

The relative distortions on the training sets are illustrated in Fig. 1 with different numbers of iterations. In each iteration, we report the relative distortion after Line 5 in Alg. 1. Since ock-means and ck-means adopt a similar alternating optimization algorithm, we also collect the relative distortions before the end of each iteration. Certain curves stop before 100 iterations because of convergence.

O1GA vs O2GA. In most cases, O2GA is better than O1GA except for certain cases, e.g., the comparison of gk-means(1, r) and gk-means(2, r) in Fig. 1 (b). This may be because in the iterative optimization, different assignment algorithms generate different assignments, and the dictionaries are optimized in different directions. With different dictionaries, we cannot guarantee the superiority of O2GA over O1GA. In the cases where the O2GA is better, the improvement varies among different settings. For example in Fig. 1 (a) and Fig. 1 (d), the improvement of gk-means(2, h) over gk-means(1, h) is much more significant, while in Fig. 1 (b) and Fig. 1 (c), the difference is minor.

Comparison of initializations. Generally, the hierarchical initialization is the best; the second is the k-means-based, and the worst is the random initialization. Although we cannot guarantee this in theory, this observation is true under all the settings in practice in Fig. 1.

Comparison with ock-means and ck-means. From Fig. 1 we can see that the random initialization is almost always inferior, while the hierarchical initialization can always lead to a lower distortion than ock-means and ck-means. This also implies that the initialization is quite important to such a non-convex problem.

Similar observations can be found w.r.t. the relative distortion on the databases illustrated in Table 1.

Finally, we compare the gk-means and the MCMP [9] on the full vector ($M_{ock} = 1$). We evaluate the time cost on a Linux server with a CPU of 2660MHz and 48G memory. The experiment is conducted on SIFT1M, and the program runs in 24 threads to encode the $10^6$ database points.

The results are depicted in Table 2 Due to the high time cost, we cannot run MCMP with 8 dictionaries. Thus, we estimate the time cost as follows. The dictionaries are trained by gk-means(2, h), and the time cost is collected on 240 database points with the MCMP algorithm since we deploy 24 threads. The result is 2589.66 seconds and we multiply it by $10^6/240$ to estimate the time cost to encode the whole $10^6$ database points. The results of gk-means are tested with the best hierarchical initialization. From the results, we can see that in terms of time cost both gk-means(1, h) and gk-means(2, h) scale well with the number of dictionaries while MCMP does not. This is because the time cost of gk-means is linear to the number of dictionaries while MCMP is exponential. Meanwhile, the time cost of gk-means(1, h) is less than that of gk-means(2, h), because the complexity of the former is $O(K)$ while that of the latter is $O(K^2)$. In terms of the relative distortion, MCMP is slightly better than gk-means(2, h) which is better than gk-means(1, h).
Table 2: Encoding time and the relative distortion (R.d) on the database of SIFT1M.

|       | 2              | 4              | 8              |
|-------|----------------|----------------|----------------|
|       | Time (s)       | R.d.           | Time (s)       | R.d.           | Time (s) | R.d. |
| gk-means | 1 8.6 0.30  | 20.3 0.21  | 120.4 0.12  |
|       | 2 45.2 0.29  | 110.3 0.20  | 392.9 0.11  |
| MCMP  | 12.2 0.29    | 723.3 0.19  | 10790 250.0  |

4 Conclusion

We proposed a simple yet effective algorithm, named as group $k$-means, to effectively encode the data point. With the desirable low distortion errors, this approach can represent high-dimensional data points with less storage cost and facilitate data management. Future work includes applying it to applications, e.g., multimedia retrieval with inner product measurement and image compression.

Appendices

This appendix reports the experimental results of approximate nearest neighbor search, in which our group $K$-means (gk-means) is compared with other approaches.

Following [9], we compute the approximate distance between the query $q \in \mathbb{R}^P$ and the database point $x \in \mathbb{R}^P$ encoded as $(k_1, \cdots, k_C)$ by

$$\frac{1}{2} \left\| q - \sum_c d_{kc}^c \right\|_2^2 = \frac{1}{2} \| q \|_2^2 - \sum_c q^T d_{kc}^c + \left\| \sum_c d_{kc}^c \right\|_2^2. \quad (28)$$

The first item is consistent and can be omitted during distance evaluation. The third item is independent of the query and can be pre-computed from the code $(k_1, \cdots, k_C)$ and the dictionaries. No original data is required for the computation of the third item. To compute the second item, we can evaluate all the inner products $q^T d_{kc}^c$ for $c \in \{1, \cdots, C\}$ and $k \in \{1, \cdots, K\}$. Then, each distance computation only involves $O(C) + 1$ addition, which is comparable to ck-means [8].

For each query, we compare it with every database point by Eqn. 28 and rank all the points by the approximate distance. We take recall as the performance criterion to measure the proportion of the queries whose corresponding true nearest neighbors (by Euclidean distance) fall in the top ranked points.

As studied in the paper, initialization is important for the minimization of the objective function and we only report the results with the best hierarchical initialization scheme.

The results are shown in Fig. 2 on the three datasets with code length 32, 64, 128. The suffixes in the legends denote the code length. We can see gk-means(2, h) almost always outperforms the others. The performance of gk-means(1, h) is better than okc-means on SIFT1M and MNIST, but is worse on GIST1M. The performance varies because the data distributions among the datasets are different and the numerical optimization does not achieve the theoretically optimal solution. The advantage of gk-means(2, h) over gk-means(1, h) is because the local minimum issue of gk-means(1, h) is more severe. Besides, the performance comparison for ANN search is quite consistent with the relative distortion on the database as shown in Table 1 in the paper.
Figure 2: Recall on the three datasets with different code lengths.

References

[1] Artem Babenko and Victor S. Lempitsky. Additive quantization for extreme vector compression. In 2014 IEEE Conference on Computer Vision and Pattern Recognition, CVPR 2014, Columbus, OH, USA, June 23-28, 2014, pages 931–938, 2014.

[2] Christopher F. Barnes. A new multiple path search technique for residual vector quantizers. In Proceedings of the IEEE Data Compression Conference, DCC 1994, Snowbird, Utah, March 29-31, 1994, pages 42–51, 1994.

[3] Chao Du and Jingdong Wang. Inner product similarity search using compositional codes. CoRR, abs/1406.4966, 2014.

[4] Tiezheng Ge, Kaiming He, Qifa Ke, and Jian Sun. Optimized product quantization for approximate nearest neighbor search. In CVPR, pages 2946–2953, 2013.

[5] Hervé Jégou, Matthijs Douze, and Cordelia Schmid. Product quantization for nearest neighbor search. IEEE Trans. Pattern Anal. Mach. Intell., 33(1):117–128, 2011.

[6] Yann LeCun, Léon Bottou, Yoshua Bengio, and Patrick Haffner. Gradient-based learning applied to document recognition. Proceedings of the IEEE, 86(11):2278–2324, 1998.

[7] Stuart P. Lloyd. Least squares quantization in pcm. IEEE Transactions on Information Theory, 28(2):129–136, 1982.

[8] Mohammad Norouzi and David J. Fleet. Cartesian k-means. In CVPR, pages 3017–3024, 2013.

[9] Jianfeng Wang, Jingdong Wang, Jingkuan Song, Xin-Shun Xu, Heng Tao Shen, and Shipeng Li. Optimized cartesian k-means. ArXiv e-prints, abs/1405.4054, May 2014.

[10] Ting Zhang, Chao Du, and Jingdong Wang. Composite quantization for approximate nearest neighbor search. In ICML, 2014.