Inner Product Similarity Search using Compositional Codes

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Abstract

This paper addresses the nearest neighbor search problem under inner product similarity and introduces a compact code-based approach. The idea is to approximate a vector using the composition of several elements selected from a source dictionary and to represent this vector by a short code composed of the indices of the selected elements. The inner product between a query vector and a database vector is efficiently estimated from the query vector and the short code of the database vector. We show the superior performance of the proposed group \(M\)-selection algorithm that selects \(M\) elements from \(M\) source dictionaries for vector approximation in terms of search accuracy and efficiency for compact codes of the same length via theoretical and empirical analysis. Experimental results on large-scale datasets (\(1M\) and \(1B\) SIFT features, \(1M\) linear models and Netflix) demonstrate the superiority of the proposed approach.

1 Introduction

Similarity search \([1]\) is a fundamental research topic in the area of computational geometry and machine learning. It has attracted a lot of interests \([2]\) in computer vision and pattern recognition because of the popularity of large scale and high-dimensional multimedia data. Various technologies, such as index structures \([3, 4]\) and compact codes \([5, 6]\), have been developed to solve the similarity search problem under different similarity metrics \([7]\).

In this paper, we are interested in designing a compact code approach with a focus on inner product similarity. Inner product similarity search is an important task in many vision applications. In large scale retrieval of images from text queries and multi-class categorization, the PAMIR (Passive-Aggressive Model for Image Retrieval) approach \([5]\) trains a large number of linear models (each corresponds to a text query), and ranks the queries for a new image according to the scores evaluated over the linear models, which is an inner product similarity search problem. In the object detection task with a large number of object
classes [9], it consists of a step finding the top-responded filters by performing the convolution operation over sliding image windows and filters, which is also an inner product similarity search problem. The latent factor models widely used in recommendation systems [10] and document matching [11], such as matrix factorization [10], latent semantic index [12], and so on, also rely on inner product similarity search to find the best matches.

We propose a compact code approach to approximate inner product similarity search. Our approach is based on a vector approximation algorithm, using the composition of several vectors selected from a small set (source dictionary) as the approximation, which is not studied for compact codes and similarity search before. Then we use the indices of the selected vectors to form a compact code, which we call compositional codes, to describe the data vector. Finally, inner product between the query vector and the database vector can be efficiently estimated from the query vector and the code of the database vector.

The compositional way to vector approximation can be viewed as a quantization algorithm, finding the nearest element from a larger dictionary (called compositional dictionary) that is produced from a source dictionary. We study the way of using \( M \)-selection \( (M \)-combination with repetitions)\(^1\) to form the compositional dictionary, and show that it is equivalent to performing 1-selection from \( M \) identical source dictionaries respectively. This equivalence motivates us to generalize \( M \)-selection by using \( M \) different source dictionaries, yielding a so-called group \( M \)-selection algorithm that simultaneously learns source dictionaries and performs joint \( M \) 1-selections from source dictionaries. The advantage of group \( M \)-selection lies in more accurate vector approximation because of a larger compositional dictionary but with the compact code of the same length. Experimental results on finding similar SIFT features, searching for users with similar interests and discovering most relevant linear models show excellent search accuracy.

1.1 Related Work

Similarity search (or nearest neighbor search) has been studied in many research areas, including computational geometry, computer vision, machine learning, data mining and so on. A lot of algorithms have been developed for approximate nearest neighbor search, under the Euclidean distance [3, 1], the earth mover distance [7, 13], and so on. In this paper, we are interested in the nearest neighbor search problem, instead under the inner product similarity.

The challenges, compared with the well-studied similarity search under Euclidean distance, are analyzed in [14]. The main difficulty that inner product does not satisfy the triangle equality makes algorithms depending on it not suitable for inner product search. A cone tree based index structure [14] is designed for exact inner product similarity search. The fact that exact search under Euclidean distance in high-dimensional cases is even slower than the naive linear

\(^1\)In mathematics, an \( M \)-combination of a set \( S \) is a subset of \( M \) distinct elements of \( S \). An \( M \)-selection of a set \( S \) is a subset of \( M \) not necessarily distinct elements of \( S \).
scan algorithm is also observed under inner product similarity. Thus, we focus on approximate inner product similarity search and study the compact code approach.

There are many algorithms based on compact codes for similarity search with the Euclidean distance, including two main categories: hashing and compression-based source coding. The hashing category consists of random algorithms, such as locality sensitive hashing [5], and learning based algorithms such as spectral hashing [15], iterative quantization [16] and so on. These algorithms show promising performance for searching with Euclidean distance, but most of them cannot be directly applied for inner product similarity. The compression-based source coding category includes k-means, product quantization [6], and Cartesian k-means [17], which are shown to achieve superior performance over hashing codes with a little higher but still acceptable query time cost. The proposed approach belongs to the compression-based category, with a specific adaptation to inner product. The closely related approaches, product quantization and Cartesian k-means, we will show, are constrained versions of our proposed approach.

Recent research on hyperplane hashing [18, 19, 20] studies the problem of finding the points that are nearest to the hyperplane, which is related to inner product. Different from the maximum inner product problem our approach addresses, it is equivalent to finding the data vector that has the minimum inner product with the query vector. Concomitant hashing [20] is also able to solve the absolute maximum inner product problem. Approximate nearest subspace search [21], under the similarity based on the principal angles between subspaces, is related to the cosine similarity search. Those approaches address different problems and are not comparable to our approach.

2 Inner Product Similarity Search

Given a set of \( N d \)-dimensional database vectors \( X = \{ x_1, x_2, \cdots, x_N \} \) and a query \( q \), inner product similarity search aims to find a database vector \( x^* \) so that \( x^* = \arg \max_{x \in X} \langle q, x \rangle \).

In this paper, we study the approximate inner product similarity search problem with a focus on the compact coding approach, i.e., finding short codes to represent the database vectors. The objective includes three aspects: the code representing the database vector is compact; the similarity between a query \( q \) and a vector can be accurately approximated using the query and the compact code; and the evaluation over the query and the compact code can be quickly conducted.

The basic idea of our approach is to approximate a database vector \( x_n \) using a compositional vector, the summation \( \sum_{m=1}^{M} c_{nm} \) of \( M \) exemplar vectors \( \{ c_{n1}, c_{n2}, \cdots, c_{nM} \} \), where the exemplar vectors are selected from a collection of exemplars \( C \). The main work of this paper is to investigate its application to compact codes and effective and efficient inner product similarity approximation. Suppose that each example in \( C \) can be represented by a code of length
log $K$, where $K$ is the size of $C$. Then the compositional vector and thus the database vector can be represented by a short code of length $M \log K$.

The proposed approach also exploits the distributive property with respect to the inner product operation ($<\cdot, \cdot>$) over the addition operation: $<q, c_1 + c_2> = <q, c_1> + <q, c_2>$. With the distribution property, evaluating inner product between a query and the compositional vector takes $O(M)$ addition operation if the inner product values of $q$ with all vectors in $C$ are computed, whose time cost is neglectable when handling large scale data.

The vector approximation scheme using $M$ vectors is expected to have a better approximation, thus yielding a more accurate inner product approximation. This is guaranteed by the property that the inner product approximation error is upper-bounded if vector approximation is with an upper-bounded error (Euclidean distance with vector approximation has a similar property derived from the triangle inequality).

**Property 1.** Given a data vector $p$ and a query vector $q$, if the distance between $p$ and its approximation $\bar{p}$ is not larger than $r$, $\|p - \bar{p}\|_2 \leq r$, then the absolute difference between the true inner product and the approximate inner product is upper-bounded:

$$|<q, p> - <q, \bar{p}>| \leq r \|q\|_2. \quad (1)$$

The upper bound $r \|q\|_2$ is related to the $L_2$ norms of $q$, meaning that the bound depends on the query $q$ (in contrast, the upper bound for Euclidean distance does not depend on the query). However, the solution in inner product similarity search does not depend on the $L_2$ norm of the query as queries with different $L_2$ norm have the same solution, i.e., $x^* = \arg \max_{x \in X} <q, x> = \arg \max_{x \in X} s <q, x>$, where $s$ is an arbitrary positive number. In this sense, it also holds that more accurate vector approximation is potential to lead to better inner product similarity search.

### 3 Our Approach

In this section, we first introduce the basic vector approximation approach, $k$-means clustering, and connect it with the manner of using a 1-combination of a source dictionary to approximate the data vector. We then present the proposed compositional code approach, based on $M$-combination, $M$-selection and group $M$-selection. Finally, we give the analysis.

#### 3.1 $K$-means

$K$-means clustering is a method of vector quantization. It aims to partition the database points into $K$ clusters whose centers form a set $C$, in which each database point belongs to the cluster with the nearest center. In its application to data approximation, each database point is approximated by the nearest center, equivalently using the best 1-combination of $C$ to approximate a database
vector. The $K$-means clustering algorithm provides a way of jointly optimizing the center set $C$ and the 1-combination for each data vector.

### 3.2 Compositional Codes

We present the basic compositional code approach that uses $M$-combination over a set of samples denoted by $C$, i.e., using the compositional $\sum_{m=1}^{M} c_{nm} \in C$, to approximate the data vector $x_n$. This manner could be viewed as a two-step scheme: first producing a compositional dictionary formed by the $M$-combinations of $C$ that we call source dictionary and then finding the best element from the composite dictionary as the approximation of a data vector.

Instead of separately learning the source dictionary (e.g., using $k$-means clustering) and finding the optimal $M$-combinations, we use the way similar to sparse coding and $k$-means to jointly learn the source dictionary and $M$-combinations. We use a $K$-dimensional binary vector $b_n$ to represent an $M$-combination, where only $M$ entries in $b$ are valued as 1 and all others are 0, and a matrix $C$ of size $d \times K$ to represent the source dictionary with each column corresponding to an item of the source dictionary. The objective function is written as follows,

$$
\min_{C, b_1, \ldots, b_N} \sum_{n=1}^{N} \| x_n - C b_n \|_2^2.
$$

(2)

We relax the constraint in $M$-combination that the $M$ elements in $M$-combination are distinct and use $M$-selection in which the elements are not necessarily different. To mathematically formulate this case, we use a longer binary vector $b_n$ whose dimensionality is $K \times M$ to represent an $M$-selection for the data vector $x_n$. $b_n$ is a concatenation of $M$ subvectors, $b_n = [b_{n1}^T \ b_{n2}^T \cdots b_{nM}^T]^T$. In each subvector only one entry $b_{nm}$ is valued by 1 and all others are 0. The objective function can be formulated as follows,

$$
\min_{C, b_1, \ldots, b_N} \sum_{n=1}^{N} \| x_n - [C] b_n \|_2^2.
$$

(3)

Furthermore, we extend the $M$-selection scheme to a so-called group $M$-selection scheme. Group $M$-selection is a combination of the elements from $M$ sets $\{C_1, \ldots, C_M\}$ each of which is a matrix of size $d \times K$, taken 1 at a time from each of the $M$ sets. The whole formulation is then given as the following,

$$
\min_{C_1, \ldots, C_M, b_1, \ldots, b_N} \sum_{n=1}^{N} \| x_n - [C_1 C_2 \cdots C_M] b_n \|_2^2 \\
\text{s. t. } b_n = [b_{n1}^T \ b_{n2}^T \cdots b_{nM}^T]^T \\
\quad b_{nm} \in \{0, 1\}^K \\
\quad \| b_{nm} \|_1 = 1.
$$

(4)

The group $M$-selection case, similar to the $M$-selection case, also produces an approximation using the composition of $M$ elements, but differently $M$ source
dictionaries with each containing \( K \) elements are used to form the compositional dictionary. It, however, does not increase the code length and keeps the same length \( M \log K \), where each \( b_{nm} \) is represented by a code of length \( \log K \), denoted by \( y_{nm} \) which is the index of the non-zero entry in \( b_{nm} \) in our implementation. Note that in this case, the time consumption for computing the similarity table becomes to \( O(MKd) \). However, in the large scale similarity search case, the increase of such computation cost brought due to the increase of the number of elements in the source dictionaries (from \( K \) to \( KM \)) is neglectable because \( M \) in practice is chosen to be small so that the approximate inner product similarity evaluation cost \( O(M) \) is not large. Figure 1 illustrates the compositional dictionaries from \( K \)-means, \( M \)-combination, \( M \)-selection and group \( M \)-selection.

### 3.3 Optimization

We adopt alternating optimization, which is used in the Lloyd and sparse dictionary learning algorithms, to solve the optimization problem in Equation 4. To be clear, we denote \( D = [C_1 \cdots C_M] \). Our optimization algorithm alternatively optimizes the source dictionaries \( D \) and optimizes the group \( M \)-selection \( b_n \) for each data vector \( x_n \).

**Update the dictionary.** The objective function can be transformed as \( f(D, B) = \|X - DB\|_2^2 \), where \( X = [x_1 \cdots x_N] \) is the data matrix and \( B = [b_1 \cdots b_N] \) is the group \( M \)-selection matrix. This is a quadratic optimization problem w.r.t. the variable \( D \). Many algorithms have been designed to solve this problem. In this paper, we solve this problem using the closed-form solution. Let the derivative of \( f(D, B) \) with respect to \( D \) be zero: \( \frac{\partial f(D, B)}{\partial D} = 2(DBB^T - XB^T) = 0 \). Then we have the closed-form solution: \( D = XB^T(BB^T)^{-1} \). The online learning algorithm [22] can be also be borrowed for acceleration.

**Update the group \( M \)-selection \( b_n \).** Optimizing \( \{b_1, \cdots, b_N\} \) given the source dictionaries \( D \) can be decomposed into \( N \) independent subproblems \( \{\min_{b_n} (f_n(b_n) = \|x_n - Db_n\|_2^2)\}^N_{n=1} \) with the associated constraints, each of which optimizes the group \( M \)-selection \( b_n \) separately.

Intuitively, each subproblem selects one element from each source dictionary so that the composition of these elements is the closest to the data vector.

Figure 1: The illustrations of the compositional dictionaries learnt with (a) \( k \)-means, (b) \( M \)-combination, (c) \( M \)-selection, and (d) group \( M \)-selection, from a set of 1500 random 2D points. \( K = 5, M = 3 \). Each partition corresponds to a dictionary element.
The subproblem of minimizing $f_n(b_n)$ is a combinatorial problem and generally NP-hard. We propose to adopt a greedy algorithm, performing $M$ 1-selection optimizations over the $M$ source dictionaries in the best-first manner. The $m$-th iteration of the greedy algorithm consists of determining over which source dictionary 1-selection is performed from the remaining $(M - m - 1)$ source dictionaries that have not been selected and finding the best 1-selection over the selected source dictionary. The former issue is solved by selecting the best source dictionary over which the reconstruction error given the previous selected $(m - 1)$ 1-selections is the minimal. The latter issue is solved by selecting the element in the source dictionary that is the nearest to the residual (the difference of the data vector from the current approximate vector using the previous $(m - 1)$ 1-selections).

3.4 Search with Compositional Codes

Given that the database $\{x_n\}_{n=1}^{N}$ is represented by the compact codes $\{y_n\}_{n=1}^{N}$ with $y$ being $M$ codes $y_{n1}, y_{n2}, \cdots, y_{nM}$, we perform the linear scan search to find nearest neighbors, by computing the approximate similarity of a query $q$ with each database vector. The inner product similarity between $q$ and $x_n$ is approximated using the compact code, $\langle q, x_n \rangle \approx \langle q, \sum_{m=1}^{M} c_{y_{nm}} \rangle$. The distributive property shows that $\langle q, \sum_{m=1}^{M} c_{y_{nm}} \rangle = \sum_{m=1}^{M} \langle q, c_{y_{nm}} \rangle$, which takes $O(M)$ time if the inner products between the query and the dictionary elements have been already computed. As aforementioned, before linear scan, the search process first constructs the similarity table, storing inner products between the query $q$ and all the dictionary elements in $C$, whose time complexity is $O(MKd)$. In summary, the overall search time complexity is $O(MKd + NM)$.

When handling large scale data, the cost of computing the similarity table is relatively small and neglectable compared with the linear scan cost. In the case of searching over SIFT1M with $M = 8$ and $K = 256$, the time of computing the similarity table is about only 2% of the total search time and in the case of searching over SIFT1B with $M = 8$ and $K = 256$, the ratio for the cost of similarity table computation is even much smaller.

3.5 Analysis

Let’s see how to transform the group $M$-selection case formulated in Equation 4 to other cases. We introduce three constraints: $c1$: $C_1 = C_2 = \cdots = C_M$; $c2$: $b_{ni} \neq b_{nj}, \forall i \neq j, \forall n$; $c3$: $M = 1$. It is easy to show that the formulation in Equation 4 with an extra constraint $c1$ is equivalent to the $M$-selection case, that it with two extra constraints $c1$ and $c2$ is reduced to the $M$-combination case, and that it together with all the three extra constraints, $c1$, $c2$ and $c3$, is reduced to the $k$-means case. The reduction relations are summarized as the following property.

Property 2. The compositional code approach with group $M$-selection can be transformed to the ones with $M$-selection and $M$-combination and $k$-means by
successively adding extra constraints: Group $M$-selection $\rightarrow c_1 M$-selection $\rightarrow c_2 M$-combination $\rightarrow c_3 k$-means.

With regard to the optimal objective function values of $k$-means, $M$-combination, $M$-selection, and group $M$-selection that are denoted by $f^*_{km}$, $f^*_{mc}$, $f^*_{ms}$, and $f^*_{gms}$, respectively, we have the following property.

**Property 3.** Given the same database $X$ and the same variables of $K$ and $M$, we have (1) $f^*_{gms} \leq f^*_{ms}$; (2) $f^*_{ms} \leq f^*_{mc}$; (3) $f^*_{ms} \leq f^*_{km}$. There is no guarantee for $f^*_{mc} \leq f^*_{km}$.

The proofs of the first three inequalities in the above property is obvious and it is easily validated that the optimal solution of the $M$-selection ($M$-combination, $k$-means) case is (or forms) a feasible solution of the group $M$-selection ($M$-selection, $M$-selection) case. In contrast, we can find an example that the optimal solution of the $k$-means case cannot form a feasible solution of the $M$-combination case (e.g., in the case $K = M$).

We compute the cardinalities of the compositional dictionaries (the source dictionary in $k$-means is equivalently regarded as the compositional dictionary) in the four cases to show the difference of the four algorithms in another way. Generally, the objective value would be smaller if the cardinality of the compositional dictionary is larger. The cardinalities are summarized as follows.

**Property 4.** The cardinalities of the group $M$-selection case, the $M$-selection case, the $M$-combination case, and the $k$-means case are $K^M$, $\binom{K}{M}$, $\binom{K+M-1}{M}$, $\frac{(K+M-1)!}{M!(K-1)!}$, and $K$, respectively. We have $K^M \geq \binom{K}{M} \geq \binom{K+M-1}{M} = \frac{(K+M-1)!}{M!(K-1)!}$, and $K$, respectively. Property 3 shows that the group $M$-selection scheme produces the smallest objective values. In other words, the group $M$-selection scheme leads to the most accurate approximation on average. Based on the bound analysis in Property 5, it can be concluded that group $M$-selection can achieve the most accurate inner product approximation as given in the following corollary.

**Corollary 1.** On average, the group $M$-selection scheme results in more accurate inner product approximation (smaller error upper-bound) than $k$-means, $M$-combination, and $M$-selection given the same variables $M$ and $K$.

**Time Complexity.** Section 3.4 has described the search process and its time complexity. The following presents the time complexity for the training process. The training process is an iterative procedure and each iteration consists of two steps: dictionary learning and code updating. The dictionary learning step updates the dictionaries as a closed-form solution: $D = XB^T(BB^T)^{-1}$, which includes (sparse) matrix multiplication and matrix inversion, and its time complexity is $O(NMd + d(MK)^2 + NM^2 + (MK)^3)$. The code updating step involves computing the code for each vector, taking $O(M^2Kd)$, and thus takes $O(NM^2Kd)$ for all database vectors. In a word, the time complexity of the whole iteration process is $O(T(NM^2Kd + d(MK)^2 + (MK)^3))$ with $T$ being the
number of iterations and one can see that it is linear with respect to the number of vectors N and the dimension d. when training the codes for the SIFT1M dataset, the algorithm reaches convergence in 15 iterations and takes about 250 × 15 seconds (with a single Intel i7-2600 CPU (3.40GHz)) Our algorithm also benefits from parallel computing, and thus the practical time consumption is acceptable, for example, computing the codes from the 100M learning vectors for SIFT1B is completed within 5 hours.

Connections and Discussions. We summarize the relations with several closely-related algorithms. Detailed analysis is given in the supplementary material. Product quantization [6] and Cartesian k-means [17] can be viewed as a constrained version of the group M-selection algorithm: each subquantizer corresponds to a source dictionary in our approach and each source dictionary lies in a different subspace with the same dimension (in the case that each subspace is full-ranked). In comparison with order permutation [23] in which the similarity between permutation orders is used as a predictor of the closeness, our approach uses the composition of selected dictionary elements to approximate the vector and thus uses it for inner product similarity approximation.

The proposed M-selection and group M-selection schemes can be regarded as a sparse coding approach with group sparsity [24] in which the coefficients are divided into several groups and the sparsity constraints are imposed in each group separately. In particular, the coefficients in our approach that can be only valued by 0 or 1 are divided into M groups and for each group the non-sparsity degree is 1.

4 Experiments

We conduct the inner product similarity search experiments over four data sets: SIFT1M [6], SIFT1B [25], linear models (LM1M), and Netflix. The SIFT1M dataset consists of 1M 128-dimensional SIFT descriptors as the database vectors and 10K SIFT descriptors as the query vectors, which are extracted from the INRIA holidays images [26]. The SIFT1B dataset contains 1 billion SIFT features as the database vectors, 100M SIFT features as the learn vectors and 10K SIFT features as the query vectors, which are extracted from approximately 1 million images. The LM1M dataset consists of around 1M (890,912) linear models with the weight vector as the database vectors, which are learnt from 890,912 textual queries with the images frequently clicked in a commercial search engine for each textual query as the training samples using the PAMIR approach [8] and 100K 2048-dimensional image features as the queries. Net-
Figure 2: Performance comparison of $M$-combination, $M$-selection, and group $M$-selection. $(x, y) = (#(\text{NNs}), #(\text{bits}))$

flix [27] contains a rating matrix that 480,189 users gave to 17,770 movies and aims to predict user ratings for films. It is shown that inner product between the rating vectors that two users gave to 17,770 movies can be used to evaluate the similarity of users’ interest which can help recommend films to users. In our experiments, the dimension of the rating vector is reduced to 512 with PCA. The descriptions of the datasets are summarized in Table 1.

The search quality is measured with recall@$P$, which is defined as the fraction of relevant instances that are retrieved among the first $P$ positions. Relevant instances in our case are $R$-nearest neighbors under the inner product similarity. This measure is equivalent to the precision measure if $R = P$, or when evaluating the returned top $R$ results after performing a subsequent reranking scheme using the exact inner product similarity over the retrieved $P$ items, following an approximate search step. The true nearest neighbors under the inner product similarity are computed by comparing each query with all the database vectors using the raw features.

4.1 Empirical Analysis

We report the performance of compositional code using the proposed three schemes: $M$-combination, $M$-selection, and group $M$-selection. The results of searching different numbers of nearest neighbors with different numbers of bits at the same position 100 are shown in Figure 2. This result and all the following results are obtained by fixing $K = 256$ (i.e., each source dictionary is encoded with a byte) and tuning $M$ to vary the number of bits. We can see that group $M$-selection performs the best, which is consistent to the analysis that group $M$-selection is the best on average in vector approximation and inner product approximation. In addition, from the results in Figure 2 it can be observed that more bits result in better performance when searching the same number of nearest neighbors and the performance when searching more nearest neighbors with the same number of bits decreases.

4.2 Comparison

We compare our approach, compositional code with group $M$-selection (abbreviated as CC), with several compact coding algorithms, including product quan-
The experimental results over SIFT1M are shown in Figure 3. One can see that our approach (CC) is superior over other algorithms. Recall@500 with 64 bits for 1-NN, 10-NN and 100-NN is 20% larger than those from other algorithms. One can also observe that the improvement with 128 bits becomes smaller than with 64 bits. This is because all the algorithms with more bits result in smaller approximation error and thus the inner product approximation quality becomes closer. Figure 4 shows the results over a very large dataset, SIFT1B. We can see that there are consistent improvements and our approach achieves above 20% improvement for Recall@500 with 64 bits for 1-NN. In comparison with the hashing algorithm, our algorithm is much better in the case of using the same code length. Our experiment indicates that the query time cost of our algorithm is about 1.8 times of that of the hashing algorithm. However, our algorithm using the code of a half length still outperforms the hashing algorithm. For example, one can observed from Figure 4(b) that our method using 64 bits achieves about 1.5 search accuracy at $p = 1000$ compared with hashing using 128 bits and in this case the time cost is even smaller than hashing.

The experimental results over LM1M are shown in Figure 5. In this case, the inner product similarity search aims to find the linear models which the query image fits the best, equivalently meaning that the query image is most relevant to the textual queries associated with the linear models. The retrieved linear models can be viewed as soft attributes that can be applied to image search ranker. From the respect of large scale classification, our approach can
provide fast prediction for a large number of categories, which is a flat approach rather than hierarchical label trees recently studied (e.g. [29]). We present the performance to show how the approximate search algorithms are close to the exact search algorithm. From the results shown in Figure 5, we can see that the recall improvement @300 with 64 bits for 1-NN is above 3% over the second best, 14% over the others, and our approach performs the best.

We also show the performance over the Netflix dataset in Figure 6. The task in this experiment is that we retrieves the similar users by viewing the rating vector as the feature of one user, which can be applied to mine the films that the query user might be interested from the films rated by the similar users. One can see that our approach performs much better with 32 bits, showing the advantage of approach under very small codes, and the improvement with 64 bits is a little small, which might come from that the code of 64 bits is already able to well characterize the differences. One point observed from all the four comparisons is that our approach consistently performs the best while no other algorithm always performs the second best.

Last, we show the advantage in the potential application of learning large scale image classifiers, beyond similarity search. Image classification with a large scale is shown to achieve state-of-the-art performance with the use of high-dimensional signatures [30, 31]. [30, 31] show that data compression is necessary to support efficient in-RAM training with stochastic gradient decent (SGD) as the raw training features are too large to be loaded into the memory in normal PCs.

The training process [30, 31] needs to decompress the compact code and pass the decompressed version to the SGD iteration. It is expected that the decompressed version is as close as the raw feature as possible. Thus, we first use the closeness, i.e., the average feature approximation error \(E_i[\|x_i - \bar{x}_i\|_2^2]\) with \(\bar{x}\) being the decompressed vector, as a criterion. The performance is reported...
over the 4096-dimensional fisher vectors extracted from the INRIA holidays dataset that contains 500 query and 991 corresponding relevant images, and the UKbench Recognition Benchmark images that contains 10200 images. The conclusions from such two datasets hold for larger scale datasets. From the results shown in Tables 2 and 3, one can see that our approach can achieve the best vector approximation.

One popular category of classification algorithms in large-scale image classification is linear SVM or its variants, e.g., used in [30, 31], in which the training equivalently depends on the inner product approximation as the dual formulation is based on the kernel matrix formed by the inner products of the training features. So we also compare the inner product approximation accuracy \(E_{ij}[(x_i^T x_j - \bar{x}_i^T \bar{x}_j)^2]\) as shown in Tables 2 and 3. Here the inner product is evaluated in a symmetric way as the training algorithm can only use the decompressed features. Note that the computation cost of symmetric inner product, \(O(M^2)\), does not matter because the SGD algorithm does not really compute the inner product. In addition, we also show that such approximate (symmetric) inner product similarities is also superior in preserving the semantic similar-
Table 2: Performance comparison in the application of data compression using short codes over the holidays dataset. VAE = vector approximate error. IPAE = inner product approximation error

|        | 32 bits |       | 64 bits |       |       |       |
|--------|---------|-------|---------|-------|-------|-------|
|        | VAE     | IPAE  | MAP     | VAE   | IPAE  | MAP   |
| PQ     | 0.4526  | 0.0057| 0.4179  | 0.3775| 0.0044| 0.4780|
| OPQ    | 0.4014  | 0.0049| 0.4339  | 0.3221| 0.0030| 0.4787|
| CKM    | 0.3081  | 0.0054| 0.4843  | 0.2279| 0.0039| 0.5251|
| CC     | 0.1462  | 0.0020| 0.5245  | 0.0139| 0.0002| 0.6360|

Table 3: Performance comparison in the application of data compression using short codes over the UKBench dataset

|        | 32 bits |       | 64 bits |       |       |       |
|--------|---------|-------|---------|-------|-------|-------|
|        | VAE     | IPAE  | score   | VAE   | IPAE  | score |
| PQ     | 0.4629  | 0.0075| 1.871   | 0.4120| 0.0054| 2.180 |
| OPQ    | 0.3982  | 0.0050| 1.790   | 0.3232| 0.0025| 2.193 |
| CKM    | 0.3767  | 0.0059| 2.064   | 0.3079| 0.0037| 2.382 |
| CC     | 0.3076  | 0.0038| 2.152   | 0.2261| 0.0021| 2.551 |

5 Conclusion

This paper studies the approximate inner product similarity search problem and introduces a compact code approach, compositional code using group M-selection. Vector approximation of our approach is more accurate, without increasing the code length. The similarity search is efficient as evaluating the approximate inner product between a query and a compact code is computationally cheap. In the future, we will generalize our approach for search with Euclidean distance and other similarity measures.

6 Appendix: Proof

We rewrite Property 5 presented in the main paper in the following and then give the proof.

Property 5. Given a data vector p and a query vector q, if the distance between p and its approximation \( \bar{p} \) is not larger than r, \( \|p - \bar{p}\|_2 \leq r \), then the absolute difference between the true inner product and the approximate inner product is

\[ \left| \langle p, q \rangle - \langle \bar{p}, \bar{q} \rangle \right| \leq 2r \]

There is a similar theorem (Theorem 3.1) in [14] showing the maximum value of the approximate inner product in the same condition. Differently, we provide the upper-bound of the approximation error (including both maximum and minimum values of the approximate inner product) and present a more succinct proof.
upper-bounded:
\[ |\langle q, p \rangle - \langle q, \bar{p} \rangle| \leq r \|q\|_2. \quad (5) \]

Proof. The proof is simple and given as follows. Let \( \bar{p} = p + \delta \). By definition, we have \( \|\delta\|_2 \leq r \). Look at the absolute value of the inner product approximation error,

\[
\begin{align*}
\|\langle q, \bar{p} \rangle - \langle q, p \rangle\| \\
= \|\langle q, p + \delta \rangle - \langle q, p \rangle\| \\
= \|\langle q, p \rangle + \langle q, \delta \rangle - \langle q, p \rangle\| \quad (by \ the \ distributive \ property) \\
= \|\langle q, \delta \rangle\| \\
\leq \|\delta\|_2\|q\|_2 \\
\leq r\|q\|_2. 
\end{align*}
\]

Thus, the approximation error is upper-bounded by \( r\|q\|_2 \). \( \square \)

7 Appendix: Analysis

7.1 Connection to Product Quantization and Cartesian K-means

The idea of product quantization [6] is to decompose the space into a Cartesian product of \( M \) low dimensional subspaces and to quantize each subspace separately. A vector \( x \) is then decomposed into \( M \) subvectors, \( x^1, \ldots, x^M \). Let the quantization dictionaries over the \( M \) subspaces be \( C_1, C_2, \ldots, C_M \) with \( C_m \) being a set of centers \( \{c_{m1}, \ldots, c_{mK}\} \). A vector \( x \) is represented by the concatenation of \( M \) centers, \( [c_1^T c_2^T \cdots c_{mK}^T \cdots c_M^T]^T \) each of which \( c_{mk} \) is the one nearest to \( x^m \) in the \( m \)-th quantization dictionary, respectively.

Rewrite each center \( c_{mk} \) as a \( d \)-dimensional vector \( \tilde{c}_{mk} \) so that \( \tilde{c}_{mk} = [0^T, \ldots, (c_{mk})^T, \ldots, 0^T]^T \), i.e., all entries are zero except that the part corresponding to the \( m \)-th subspace is equal to \( c_{mk} \). The approximation of a vector \( x \) using the concatenation \( \tilde{x} = [c_1^T c_2^T \cdots c_{mK}^T \cdots c_M^T]^T \) is equivalent to the composition \( x = \sum_{m=1}^{M} \tilde{c}_{mk} \).

Cartesian \( k \)-means [17] extends the subspace decomposition by performing a rotation \( R(R^Tx) \) and then the product quantization in the rotated space, where the rotation and the subquantizers are jointly optimized. Similar to product quantization, the vector approximation in Cartesian \( k \)-means is equivalent to \( \tilde{x} = \sum_{m=1}^{M} \tilde{R} \tilde{c}_{mk} = \sum_{m=1}^{M} \tilde{c}_{mk} \).

From the above analysis, the vector approximation approach using product quantization and Cartesian \( k \)-means can be viewed as a constrained version of our approach, each subquantizer corresponds to a source dictionary in our approach and each source dictionary lies in a different subspace with the same dimension in the case that each subspace is full-ranked. If some subspaces are not full-ranked, the equivalence still holds.
7.2 Relation to Order Permutation

Order permutation [23] is an index algorithm for approximate nearest neighbor search. It aims to predict closeness between data vectors according to how they order their distances towards a distinguished set of anchor vectors (such as the \( k \)-means centers \( C \)). Each data vector sorts the anchor objects from closest to farthest to it, i.e., a permutation of anchor objects, \( \{c_{i_1}, c_{i_2}, \ldots, c_{i_t} \} \) (\( t \leq K \)), and the similarity between orders is used as a predictor of the closeness between the corresponding elements.

In contrast, our approach finds a partial permutation of the source dictionary and uses their composition (rather than the order) to approximate the data vector, yielding a compact code representation. In the query stage, the distance of the query to the approximated data vector, in a fast way by the efficient table-lookup and addition operations, is computed to approximate the closeness.

7.3 Connection to Sparse Coding

The aim of sparse coding is to find a set of \( K \) (over-complete) basis vectors \( \{\phi_k\} \) such that a data vector \( x \) as a linear combination of these basis vectors:

\[
x = \sum_{k=1}^{K} \alpha_k \phi_k,
\]

where there are few non-zero coefficients in the coefficient vector \( \alpha = [\alpha_1 \alpha_2 \cdots \alpha_K]^T \), i.e., \( \|\alpha\|_0 \) is small. The proposed \( M \)-combination scheme can be viewed as a special sparse coding approach in which the coefficients can be only valued as 0 or 1 and the sparsity is fixed, \( \|\alpha\|_0 = M \).

Coding with group sparsity [24] is an extension of sparse coding, in which the coefficients \( \{\phi_k\} \) are divided into several groups and the sparsity constraints are imposed in each group separately. The proposed \( M \)-selection and group \( M \)-selection schemes can be regarded as a special coding approach with group sparsity, where the coefficients that can be only valued by 0 or 1 are divided into \( M \) groups and for each group the non-sparsity degree is 1.

7.4 Time Complexity

In the main paper, we have shown that the time complexity of dictionary updating is \( O(NMd + d(MK)^2 + NM^2 + (MK)^3) \) and the time complexity of code computation (group \( M \)-selection updating) is \( O(NM^2Kd) \). The following gives detailed analysis on the time complexity.

The dictionary is updated in our algorithm by computing the closed-form solution:

\[
D = XB^T(BB^T)^{-1}.
\]

The computation consists of (1) the matrix multiplication operation: \( XB^T = E \), (2) the matrix multiplication operation: \( BB^T = Q \), (3) the inverse operation: \( Q^{-1} = R \), and (4) the multiplication operation: \( ER \). Note that \( X \) is a matrix of \( d \times N \), \( B = [b_1 \cdots b_N] \) and each \( b_n \) is a \( MK \)-dimensional vector with only \( M \) entries being 1 and all the others being 0. It can be easily shown that \( E \) is of size \( d \times N \), \( Q \) is of size \( MK \times MK \), and \( R \) is of size \( MK \times MK \). Step (1) takes \( O(NMd) \) due to the sparse matrix \( B \). Step (2) can be transformed to \( BB^T = \sum_{n=1}^{N} b_n b_n^T \). Because \( b_n \) is a sparse vector, \( b_n b_n^T \) takes \( O(M^2) \) instead of \( O(M^2K^2) \). Step (3) takes \( O((MK)^3) \).
Table 4: The average vector approximation error for the database vectors, and the average inner product approximation error between the query vector and the nearest 100 database vectors using 64 bits. VAE = vector approximate error. IPAE = inner product approximation error.

|        | SIFT1M | SIFT1B | Netflix | LinerModels |
|--------|--------|--------|---------|-------------|
| PQ     | 2.319  | 8.915  | 2.540   | 1.707       |
| OPQ    | 2.842  | 8.238  | 3.282   | 2.153       |
| CKM    | 2.134  | 6.835  | 2.346   | 1.318       |
| CC     | 1.626  | 2.148  | 1.773   | 0.460       |

Table 5: The average vector approximation error for the database vectors, and the average inner product approximation error between the query vector and the nearest 100 database vectors using 128 bits.

|        | SIFT1M | SIFT1B | Netflix | LinerModels |
|--------|--------|--------|---------|-------------|
| PQ     | 1.058  | 3.191  | 1.070   | 5.075       |
| OPQ    | 1.406  | 2.398  | 1.620   | 5.610       |
| CKM    | 0.992  | 2.768  | 1.047   | 4.269       |
| CC     | 0.797  | 0.868  | 0.850   | 1.252       |

, and step (4) takes $O(d(MK)^2)$. In summary, the whole time complexity is $O(NM^2 + d(MK)^2 + NM^2 + (MK)^3)$.

The code (group $M$-selection) is updated by optimizing $b_n$ separately. Each $b_n$ is computed as $\min b_n = ||x_n - Db_n||_2^2$. We solve it by a greedy algorithm, performing $M$ 1-selection optimizations over the $M$ source dictionaries in the best-first manner. The $m$-th optimization involves selecting the best 1-selection over $(M - m - 1)$ source dictionaries, each of which contains $K d$-dimensional exemplar vectors. It costs $O((M - m - 1)(Kd))$ to select the best exemplar vector. There are $M$ optimizations to be performed, thus the cost of updating $b_n$ is $\sum_{m=1}^{M} O((M - m - 1)(Kd)) = O(M^2Kd)$. In summary, the time complexity of updating all $b_n$ is $O(NM^2Kd)$.

8 Appendix: More Experimental Results

In the main paper, we show the inner product similarity search performance over four datasets. Here we report the average approximation error using the composition of the selected vectors as the vector approximation over the database vectors, and the average inner product approximation error using the approximated vector between the query vector and the nearest 100 database vectors as shown in Tables 4 and 5. One can observe that the average vector approximation error of our approach is the smallest and the inner product approximation error is also the smallest. This gives another evidence that our approach can achieve the best similarity search performance.
9 Appendix: Future Work

Adaptation to cosine similarity search. Inner product is equivalent to cosine similarity in the case that the database vectors are of the same $L_2$ norm. Our approach finds the optimal composition, however, without making the composition vector keep the same norm. In the future, we will study the way of approximating the vector with maintaining the $L_2$ norm, e.g. extending spherical $k$-means clustering.

Extension to similarity search under Euclidean distance. The experiments show that using the compact codes learnt from our approach for Euclidean distance based similarity search achieves better search accuracy than product quantization and Cartesian $k$-means. Because the distributive property with respect to the Euclidean distance operation over the addition operation does not hold ($d^2(q, \sum_{m=1}^M c_{mk_m}) \neq \sum_{m=1}^M d^2(q, c_{mk_m})$), the general time cost of evaluating the approximate Euclidean distance using the codes produced from our approach is $\Theta(M^2)$, which is a little large. If the $M$ source dictionaries (i.e., the $M$ subspaces spanned by the $M$ source dictionaries) are mutually orthogonal ($\langle c_{si}, c_{rj} \rangle = 0, \forall s \neq r, \forall i, j$), the time cost is reduced to $\Theta(M)$ with the constant coefficient 2 because $\|q - \sum_{m=1}^M c_{mk_m}\|_2^2 = \|q\|_2^2 + \sum_{m=1}^M c_{mk_m}^2 - 2 \times q^T \sum_{m=1}^M c_{mk_m}$.

However, we have the following equation:

$$\|q - \sum_{m=1}^M c_{mk_m}\|_2^2 = (q - \sum_{m=1}^M c_{mk_m})^T(q - \sum_{m=1}^M c_{mk_m}) \quad (12)$$

(from orthogonality constraints between the items of different dictionaries) \quad (14)

$$= q^Tq - 2q^T\left(\sum_{m=1}^M c_{mk_m}\right) + \sum_{m=1}^M c_{mk_m}^T c_{mk_m} \quad (15)$$

$$= q^Tq - 2q^T\left(\sum_{m=1}^M c_{mk_m}\right) + \sum_{m=1}^M c_{mk_m}^T c_{mk_m} + (M - 1)q^Tq - (M - 1)q^Tq \quad (16)$$

$$= \sum_{m=1}^M(q^Tq - 2q^Tc_{mk_m} + c_{mk_m}^T c_{mk_m}) - (M - 1)q^Tq \quad (17)$$

$$= \sum_{m=1}^M \|q - c_{mk_m}\|_2^2 - (M - 1)\|q\|_2^2. \quad (18)$$

The above equations show that, given a query, it is enough to compute the first part, $\sum_{m=1}^M \|q - c_{mk_m}\|_2^2$, to find the nearest neighbors as the second part, $(M - 1)\|q\|_2^2$, is the same for all the database vectors. Thus, it can be concluded that
$(M - 1)$ addition operations are enough, if we have precomputed the distance table from the query to dictionary items as PQ and Cartesian $k$-means do.

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