New Loss Functions for Fast Maximum Inner Product Search

Ruiqi Guo  Quan Geng  David Simcha  Felix Chern  Sanjiv Kumar  Xiang Wu
Google Research  New York, NY 10011  
{guorq, qgeng, dsimcha, fchern, sanjivk, wuxiang} @google.com

Abstract

Quantization based methods are popular for solving large scale maximum inner product search problems. However, in most traditional quantization works, the objective is to minimize the reconstruction error for datapoints to be searched. In this work, we focus directly on minimizing error in inner product approximation and derive a new class of quantization loss functions. One key aspect of the new loss functions is that we weight the error term based on the value of the inner product, giving more importance to pairs of queries and datapoints whose inner products are high. We provide theoretical grounding to the new quantization loss function, which is simple, intuitive and able to work with a variety of quantization techniques, including binary quantization and product quantization. We conduct experiments on standard benchmarking datasets to demonstrate that our method using the new objective outperforms other state-of-the-art methods.

1 Introduction

Maximum inner product search (MIPS) has become a popular paradigm for solving large scale classification and retrieval tasks. For example, in recommendation systems, user queries and documents are embedded into dense vector space of the same dimensionality and MIPS is used to find the most relevant documents given a user query [1]. Similarly, in extreme classification tasks [2], MIPS is used to predict the class label when a large number of classes, often on the order of millions or even billions are involved. Lately, MIPS has also been applied to training tasks such as scalable gradient computation in large output spaces [3], efficient sampling for speeding up softmax computation [4] and sparse updates in end-to-end trainable memory systems [5].

To formally define Maximum Inner Product Search (MIPS) problem, consider a database $X = \{x_i\}_{i=1,2,...,N}$ with $N$ datapoints, where each datapoint $x_i \in \mathbb{R}^d$ in a $d$-dimensional vector space. In the MIPS setup, given a query $q \in \mathbb{R}^d$, we would like to find the datapoint $x \in X$ that has the highest inner product with $q$, i.e., we would like to identify

$$x^* := \arg \max_{x_i \in X} \langle q, x_i \rangle.$$  

Exhaustively computing the exact inner product between $q$ and $N$ datapoints is often very expensive and sometimes infeasible. Several techniques have been proposed in the literature based on hashing and quantization to solve the approximate maximum inner product search problem efficiently, and the quantization based techniques have shown strong performance [6][8]. Quantizing each datapoint $x_i$ to $x_i^*$ not only reduces storage costs and memory bandwidth bottlenecks, but also permits efficient computation of distances. It avoids memory bandwidth intensive floating point operations through Hamming distance computation and look up table operations [9][11]. In most traditional quantization works, the objective in the quantization procedures is to minimize the reconstruction error for the datapoints to be searched.

In this paper, we propose a new class of loss functions in quantization to improve the performance of MIPS. Our contribution is threefold:
• We derive a novel class of loss functions for quantization, which departs from regular reconstruction loss by weighting each pair of \( q \) and \( x \) based on its inner product value. We prove that such weighting leads to an effective loss function, which can be used by a wide class of quantization algorithms.

• We devise algorithms for learning the codebook, as well as quantizing new datapoints, using the new loss functions. In particular, we give details for two families of quantization algorithms, binary quantization and product quantization.

• We show that on large scale standard benchmark datasets, such as Glove100, the change of objective yields a significant gain on the approximation of true inner product, as well as the retrieval performance.

This paper is organized as follows. We first briefly review previous literature on quantization for Maximum Inner Product Search, as well as its links to \( \ell_2 \) nearest neighbor search in Section 2. Next, we give our main result, which is the derivation of our objective in Section 3. Applications of the new loss functions to binary quantization and product quantization are given in Section 4. Finally, we present the experimental results in Section 5.

2 Related Works

There is a large body of similarity search literature on inner product and nearest neighbor search. We refer readers to [12, 13] for a comprehensive survey. Some methods also transform MIPS problem into its equivalent form of \( \ell_2 \) nearest neighbor using transformation such as [14, 15], but in general are less successful than the ones that directly work in the original space. In general, these bodies of works can be divided into two families: (1) representing the data as quantized codes so that similarity computation becomes more efficient (2) pruning the dataset during the search so that only a subset of data points is considered.

Typical works in the first family include binary quantization (or binary hashing) techniques [16] and product quantization techniques [17], although other families such as additive quantization [18] and ternary quantization [19] also apply. There are many subsequent papers that extend these base approaches to more sophisticated codebook learning strategies, such as [20] for binary quantization and [21] for product quantization. There are also lines of work that focus on learning transformations before quantization [22]. Different from these methods which essentially minimize reconstruction error of the database points, we argue in Section 3 that reconstruction loss is suboptimal in the MIPS context, and any quantization method can potentially benefit from our proposed objective.

The second family includes non-exhaustive search techniques such as tree search [23], graph search [24], or hash bucketing [25] in nearest neighbor search literature. There also exist variants of these for MIPS problem [26]. Some of these approaches lead to larger memory requirement, or random access patterns due to the cost of constructing index structures in addition to storing original vectors. Thus they are usually used in combination with linear search quantization methods, in ways similar to inverted index [10].

3 Problem Formulation

Common quantization techniques focus on minimizing the reconstruction error (sum of squared error) when \( x \) is quantized to \( \tilde{x} \). It can be shown that minimizing the reconstruction errors is equivalent to minimizing the expected total inner product quantization errors over the query distribution:

\[
\mathbb{E}_q \sum_{i=1}^{N} \left\| \langle q, x_i \rangle - \langle q, \tilde{x}_i \rangle \right\|^2 = \mathbb{E}_q \sum_{i=1}^{N} \left\| \langle q, x_i - \tilde{x}_i \rangle \right\|^2.
\]

Under the assumption that \( q \) is isotropic, i.e., \( \mathbb{E}[qq^T] = cI \), where \( I \) is the identity matrix and \( c \in \mathbb{R}^+ \), the objective function becomes

\[
\sum_{i=1}^{N} \mathbb{E}_q \left\| \langle q, x_i - \tilde{x}_i \rangle \right\|^2 = \sum_{i=1}^{N} \mathbb{E}_q (x_i - \tilde{x}_i)^T qq^T (x_i - \tilde{x}_i) = c \sum_{i=1}^{N} \left\| x_i - \tilde{x}_i \right\|^2
\]
Therefore, the objective becomes minimizing the reconstruction errors of the database points \( \sum_{i=1}^{N} \| x_i - \hat{x}_i \|^2 \), and this has been considered extensively in the literature.

One key observation about the above objective function (1) is that it takes expectation over all possible combinations of datapoints \( x \) and queries \( q \). However, it is easy to see that not all pairs of \((x, q)\) are equally important. The approximation error on the pairs which have a high inner product is far more important since they are likely to be among the top ranked pairs and can greatly affect the search result, while for the the pairs whose inner product is low the approximation error matters much less. In other words, for a given datapoint \( x \), we should quantize it with a bigger focus on its error with those queries which have high inner product with \( x \).

Following this key observation, we propose a new loss function by weighting the approximation error of the inner product based on the value of true inner product. More precisely, let \( w(t) \geq 0 \) be a monotonically non-decreasing function, and consider the following inner-product weighted quantization error

\[
\sum_{i=1}^{N} E_q[w(\langle q, x_i \rangle) \langle q, x_i - \hat{x}_i \rangle^2] = \sum_{i=1}^{N} \int w(t)E_q[\langle q, x_i - \hat{x}_i \rangle^2 | \langle q, x_i \rangle = t]dP(\langle q, x_i \rangle \leq t). \tag{2}
\]

One common choice can be \( w(t) = I(t \geq T) \), in which case we care about all pairs whose inner product is greater or equal to certain threshold \( T \), and disregard the rest of the pairs.

One key result of this work is to decompose the inner-product weighted quantization errors based on the direction of the datapoints. We show that the new loss function (2) can be expressed as a weighted sum of the parallel and orthogonal components of the residual errors with respect to the raw datapoints. Formally, let \( r(x, \hat{x}) := x - \hat{x} \) denote the quantization residual function. Given the datapoint \( x \) and its quantizer \( \hat{x} \), we can decompose the residual error into two parts, the one parallel to \( x \) and the one orthogonal to \( x \):

\[
orl(x, \hat{x}) := \langle x - \hat{x}, x \rangle \cdot \frac{x}{\|x\|}, \tag{3} \]
\[
orl(x, \hat{x}) := (x - \hat{x}) - \norl(x, \hat{x}), \tag{4} \]

so that \( r(x, \hat{x}) = r_{\|}(x, \hat{x}) + r_{\perp}(x, \hat{x}) \). Because the norm of \( q \) does not matter to the ranking result, without loss of generality we can assume \( \|q\| = 1 \) to simplify the derivation below.

**Theorem 3.1.** Assuming the query \( q \) is uniformly distributed in \( d \)-dimensional unit sphere. Given the datapoint \( x \) and its quantizer \( \hat{x} \), conditioned on the inner product \( \langle q, x \rangle = t \) for some \( t > 0 \), we have

\[
E_q[\langle q, x - \hat{x} \rangle^2 | \langle q, x \rangle = t] = \frac{t^2}{\|x\|^2} \|r_{\|}(x, \hat{x})\|^2 + \frac{1 - \frac{t^2}{\|x\|^2}}{d-1} \|r_{\perp}(x, \hat{x})\|^2. \tag{5}
\]

**Proof.** First, we can decompose \( q := q_{\|} + q_{\perp} \) with \( q_{\|} := \langle q, x \rangle \cdot \frac{x}{\|x\|} \) and \( q_{\perp} := q - q_{\|} \) where \( q_{\|} \) is parallel to \( x \) and \( q_{\perp} \) is orthogonal to \( x \). Then, we have

\[
E_q[\langle q, x - \hat{x} \rangle^2 | \langle q, x \rangle = t] = E_q[\langle q_{\|}, r_{\|}(x, \hat{x}) \rangle + \langle q_{\perp}, r_{\perp}(x, \hat{x}) \rangle^2 | \langle q, x \rangle = t]
\]
\[
= E_q[\langle q_{\|}, r_{\|}(x, \hat{x}) \rangle^2 | \langle q, x \rangle = t] + E_q[\langle q_{\perp}, r_{\perp}(x, \hat{x}) \rangle^2 | \langle q, x \rangle = t]. \tag{6}
\]

The last step uses the fact that \( E_q[\langle q_{\|}, r_{\|}(x, \hat{x}) \rangle] E_q[r_{\|}(x, \hat{x})] | \langle q, x \rangle = t \) = 0 due to symmetry. The first term of (6). \( E_q[\langle q_{\|}, r_{\|}(x, \hat{x}) \rangle^2 | \langle q, x \rangle = t] = \|r_{\|}(x, \hat{x})\|^2 E_q[\|q_{\|}\|^2 | \langle q, x \rangle = t] = \|r_{\|}(x, \hat{x})\|^2. \) For the second term, since \( q_{\perp} \) is uniformly distributed in the \((d-1)\) dimensional subspace orthogonal to \( x \) with the norm \( \sqrt{1 - \frac{t^2}{\|x\|^2}} \), we have \( E_q[r_{\perp}(x, \hat{x})^2 | \langle q, x \rangle = t] = \frac{t^2}{\|x\|^2} \|r_{\perp}(x, \hat{x})\|^2. \)

Therefore,

\[
E_q[\langle q, r(x, \hat{x}) \rangle^2 | \langle q, x \rangle = t] = \frac{t^2}{\|x\|^2} \|r_{\|}(x, \hat{x})\|^2 + \frac{1 - \frac{t^2}{\|x\|^2}}{d-1} \|r_{\perp}(x, \hat{x})\|^2. \tag{5} \]

\( \square \)
With the base case of $I_0$ we plot

$$E_q[(q, r(x, \hat{x}))^2 | (q, x) = t] = t^2 ||r_\parallel(x, \hat{x})||^2 + \frac{1-t^2}{d-1} ||r_\perp(x, \hat{x})||^2.$$  

Now we are ready to compute the inner-product weighted quantization error (2) for the case when $w(t) = 1 (t \geq T)$ (one can do similar derivations for any reasonable $w(t)$). Without loss of generality, for simplicity we show results below for when $q$ and $x$ are unit-normed.

**Proposition 1.** Assuming the query $q$ is uniformly distributed in the $(d-1)$-dimensional unit sphere with $\|q\| = 1$, and all datapoints $x_i$ are unit-normed, given $T > 0$,

$$\sum_{i=1}^{N} E_q[I((q, x_i) \geq T) (q, x_i - \hat{x}_i)^2] \propto (d-1) \lambda(T) \sum_{i=1}^{N} ||r_\parallel(x_i, \hat{x}_i)||^2 + \sum_{i=1}^{N} ||r_\perp(x_i, \hat{x}_i)||^2,$$

where $\lambda(T)$ is defined as

$$\lambda(T) := \frac{\int_{t=0}^{T} t^2 dP((q, x) \leq t)}{\int_{t=0}^{T} (1-t^2) dP((q, x) \leq t)}.$$  

We can show that $\lambda(T)$ can be analytically computed, and $\lambda(T) \to \frac{T^2}{1-T^2} \propto \frac{d^2}{d}$ as the dimension $d \to \infty$.

**Theorem 3.2.** $\lambda(T) = \frac{\int_{0}^{\arccos T} \sin^{d-2} \theta d\theta}{\int_{\arccos T}^{\pi} \sin^{d} \theta d\theta} - 1.$

*Proof.* Let $\theta := \arccos t$, and $\alpha := \arccos T$. Note that $\frac{dP((q,x) \leq t)}{dt}$ is proportional to the surface area of $(d-1)$-dimensional hypersphere with a radius of $\sin \theta$. Thus we have $\frac{dP((q,x) = t)}{dt} \propto S_{d-1} \sin^{d-2} \theta$, where $S_{d-1}$ is the surface area of $(d-1)$-sphere with unit radius.

Thus, $\lambda(T)$ can be re-written as:

$$\lambda(T) = \frac{\int_{0}^{\arccos T} \cos \alpha \cos^2 \theta S_{d-1} \sin^{d-2} \theta d\theta}{\int_{\arccos T}^{\pi} \sin^2 \theta S_{d-1} \sin^{d-2} \theta d\theta} = \frac{\int_{0}^{\arccos T} \sin^{d-2} \theta d\theta}{\int_{0}^{\arccos T} \sin^2 \theta d\theta} - 1.$$  

Denote $I_d = \int_{0}^{\alpha} \sin^d \theta d\theta$,

$$I_d = -\cos \alpha \sin^{d-1} \alpha + \int_{0}^{\alpha} \cos^2 \theta (d-1) \sin^{d-2} \theta d\theta$$  

$$= -\cos \alpha \sin^{d-1} \alpha + (d-1) \int_{0}^{\alpha} \sin^{d-2} \theta d\theta - (d-1) \int_{0}^{\alpha} \sin^d \theta d\theta$$  

$$= -\cos \alpha \sin^{d-1} \alpha + (d-1) I_{d-2} - (d-1) I_d.$$  

This gives us a recursive formula to compute $I_d$ when $d$ is a positive integer:

$$I_d = -\cos \alpha \sin^{d-1} \alpha \frac{d}{d} + \frac{d-1}{d} I_{d-2}$$

(8)

With the base case of $I_0 = \alpha$, and $I_1 = 1 - \cos \alpha$, the exact value of $\lambda = \frac{I_{d-2}}{I_d} - 1$ can be computed explicitly in $O(d)$ time.

We furthermore prove that the limit of $\lambda(T)$ exists and that it equals $\frac{(d-1)T^2}{1-T^2}$ as $d \to \infty$. In Figure 1a, we plot $\lambda$ with $T = 0.2$ and we can see it approaches its limit quickly as $d$ grows.

**Theorem 3.3.** When $T \geq 0$, we have $\lim_{d \to \infty} \lambda(T) = \frac{T^2}{1-T^2}$.

*Proof.* See the Section A.1 of Appendix.
Therefore, motivated by minimizing the inner product approximation errors for pairs of queries and datapoints whose inner product is significant, given a quantization scheme (e.g., vector quantization, product quantization, additive quantization), we propose to minimize the weighted quantization error

\[
\mu \sum_{i=1}^{N} ||r\parallel (x_i, \tilde{x}_i)||^2 + \sum_{i=1}^{N} ||r_\perp (x_i, \tilde{x}_i)||^2,
\]

(9)

where \(\mu := (d-1)\lambda(T)\) is a hyperparameter depending on the datapoint dimension \(d\) and the threshold \(T\) imposed on the inner product between queries and datapoints. Note that when the hyperparameter \(\mu\) is set to be 1, (9) is reduced to the traditional reconstruction errors of the datapoints.

4 Application to Quantization Techniques

In this section, we derive algorithms for applying new loss functions in (9) to common quantization techniques, including vector quantization, product quantization and binary quantization.

4.1 Vector Quantization

Recall that in vector quantization, given a set of \(N\) datapoints, we want to find a codebook of size \(k\) and quantize each datapoint as one of the \(k\) codes. The goal is to minimize the total squared quantization error. Formally, the traditional vector quantization solves

\[
\min_{c_1, c_2, \ldots, c_k \in \mathbb{R}^d} \sum_{i=1}^{N} \|x_i - \tilde{x}_i\|^2,
\]

One of the most popular quantization algorithms is the \(k\)-Means algorithm, where we iteratively partition the datapoints into \(k\) quantizers where the centroid of each partition is set to be the mean of the datapoints assigned in the partition.

Motivated by minimizing the inner product quantization error for cases when the inner product between queries and datapoints is high, our proposed objective solves:

\[
\min_{\tilde{x}_i \in \{c_1, c_2, \ldots, c_k\}, 1 \leq i \leq N} \sum_{i=1}^{N} \left( \mu \|r\parallel (x_i, \tilde{x}_i)\|^2 + \|r_\perp (x_i, \tilde{x}_i)\|^2 \right),
\]

(10)

where \(\mu\) is a hyperparameter as a function of \(d\) and \(T\) following (9).

We solve (10) through a \(k\)-Means style Lloyd’s algorithm, which iteratively minimizes the new loss functions by assigning datapoints to partitions and updating the partition quantizer in each iteration. The assignment step is computed by enumerating each quantizer and finding the quantizer that minimizes (10). The update step finds the new quantizer \(\tilde{x}^* \in \mathbb{R}^d\) for a partition of datapoints \(x_1, x_2, \ldots, x_m \in \mathbb{R}^d\), i.e.,

\[
\tilde{x}^* = \min_{\tilde{x} \in \mathbb{R}^d} \sum_{i=1}^{m} \left( \mu \|r\parallel (x_i, \tilde{x})\|^2 + \|r_\perp (x_i, \tilde{x})\|^2 \right),
\]

(11)

Because of the changed objective, the best quantizer is no longer the center of the partition. Since (11) is a convex function of \(\tilde{x}\), there exists an optimal solution. The update rule given a fixed partitioning can be found by setting the partial derivative of (11) with respect to each codebook entry to zero. This algorithm provably converges in a finite number of steps. See Algorithm 1 in Appendix for a complete outline of the algorithm. Note that, in the special case that \(\mu = 1\), it reduces to regular \(k\)-Means algorithm.

**Theorem 4.1.** The optimal solution of (11) is

\[
\tilde{x}^* := \mu \left( 1 + \frac{\mu - 1}{m} \sum_{i=1}^{m} \frac{x_i x_i^T}{\|x_i\|^2} \right)^{-1} \frac{1}{m} \sum_{i=1}^{m} x_i.
\]

**Proof.** See Section 7.2 of the Appendix.
Theorem 4.2. Algorithm [7] converges in finite number of steps.

Proof. This immediately follows from the fact that the loss defined in (10) is always non-increasing during both assignment and averaging steps under the changed objective.  

4.2 Product Quantization

A natural extension of vector quantization is product quantization, which works better in high dimensional spaces. In product quantization, the original vector space \( \mathbb{R}^d \) is decomposed as the Cartesian product of \( m \) distinct subspaces of dimension \( \frac{d}{m} \), and vector quantizations are applied in each subspace separately. For example, let \( x \in \mathbb{R}^d \) be written as

\[
x = (x^{(1)}, x^{(2)}, \ldots, x^{(m)}) \in \mathbb{R}^d,
\]

where \( x^{(j)} \in \mathbb{R}^{\frac{d}{m}} \) is denoted as the sub-vector for the \( j \)-th subspace. We can quantize each of the \( x^{(j)} \) to \( \tilde{x}^{(j)} \) with its vector quantizer in subspace \( j \), for \( 1 \leq j \leq m \). With product quantization, \( x \) is quantized as \( (\tilde{x}^{(1)}, \ldots, \tilde{x}^{(m)}) \in \mathbb{R}^d \) and can be represented compactly using the assigned codes.

Using our proposed loss objective (9), we minimize the following loss function instead of the usual objective of reconstruction error:

\[
\min_{A \in \{1,2,\ldots,k\}^{N \times m}} \sum_{i=1}^{N} \left( \mu ||r_\parallel((x_i, \tilde{x}_i))||^2 + ||r_\perp((x_i, \tilde{x}_i))||^2 \right),
\]

where \( \tilde{x}_i \) denotes the product quantization of \( x_i \), i.e.,

\[
\tilde{x}_i := (C_{1,A_{i,1}}, C_{2,A_{i,2}}, \ldots, C_{m,A_{i,m}}).
\]

To optimize (13), we apply the vector quantization of Section 4.1 over all subspaces, except that the subspace assignment is chosen to minimize the global objective over all subspaces (13), instead of using the objective in each subspace independently. Similar to the update rule is found by setting the derivative of loss in (13) with respect to each codebook entry to zero. The complete algorithm box of Algorithm (1) is found in Section 7.4 of the Appendix.

4.3 Binary Quantization

Another popular family of quantization function is binary quantization. In such a setting, a function \( h(x) \) is learned to quantize datapoints into binary codes, which saves storage space and can speed up distance computation. There are many possible ways to design such a binary quantization function. We follow the setting of Dai et al. [22], which explicitly minimizes reconstruction loss and has been shown to outperform earlier baselines. In their paper, a binary auto-encoder is learned to quantize and dequantize binary codes:

\[
\tilde{x} = g(h(x)); \text{ where } h(x) \in \{0,1\}^h
\]

where \( h(\cdot) \) is the “encoder” part which binarizes original datapoint into binary space and \( g(\cdot) \) is the “decoder” part which reconstructs the datapoints given the binary codes. The authors of the paper uses \( h(x) = sign(W_h^T x + b_h) \) as the encoder function and \( g(h) = W_g^T h \) as the decoder functions, respectively. The learning objective is to minimize the reconstruction error of \( ||x - \tilde{x}||^2 \), and the weights in the encoder and decoder are optimized end-to-end using standard stochastic gradient descent. Following our discussion in Section 3, this is an suboptimal objective in the MIPS settings, and the learning objective given in (9) should be preferred. This implies minimal changes to the algorithm of [22] except the loss function part, while holding everything else unchanged.

5 Experiments

In this section, we show our proposed quantization objective leads to improved performance on MIPS, when applied to binary and product quantization tasks. Other more sophisticated methods can also benefit from the new objective. Our experiments analyze the usefulness of proposed objectives relative to the typical reconstruction loss. Finally, we also discuss the speed-recall trade off in Section 5.5

---

1Random rotation or permutation of the original vectors can be done before doing the Cartesian product.
Figure 1: (a) $\lambda$ in (7) computed analytically as function of $d$ using recursion of (8), quickly approaches its limit. (b) The relative error of inner product estimation for true Top-1 on Glove1.2M dataset, across multiple number of bits settings for $\mu$ at $T = 0.2$. (c) The retrieval Recall1@10 for different $T$.

5.1 Estimation of True Inner Product

In addition to retrieval, many application scenarios also require estimating the value of the inner product $\langle q, x \rangle$. For example, in softmax functions, inner product values are often used to compute the probability directly; In many textual or multimedia retrieval system, $\langle q, x \rangle$ is used as a score for downstream classification. One direct consequence of (9) is that the objective weighs pairs by their importance and thus leads to lower estimation error on top-ranking pairs. We compare the estimation error of true inner product value on the Top-1 pair, under the same bitrate with product quantization on Glove1.2M dataset. Glove1.2M is a collection of 1.2 million 100-dimensional word embeddings trained with the method described in [33]. We measure $|\langle q, x \rangle - \langle q, \tilde{x} \rangle|/\langle q, x \rangle$ as the relative error on true inner product. New objective clearly produces smaller relative error over all bitrate settings (Figure 1b).

5.2 Maximum Inner Product Search Retrieval

Next, we show our MIPS retrieval results, comparing quantization methods that use our proposed loss function and the state-of-the-arts that uses reconstruction loss. The goal of the comparison is to show that the new objective is compatible with common quantization techniques, such as product and binary quantization and can benefit their performance. To evaluate retrieval performance, we use RecallM@N metric, which measures the fraction of the $M$ ground truth MIPS results recalled in first $N$ datapoints returned by the retrieval algorithm.

5.2.1 Product Quantization Retrieval

We follow the formulation in Section 4.2 to evaluate the effect of new objective for MIPS, testing on Glove1.2M dataset, reporting Recall1@1, Recall1@10, Recall10@10, Recall10@100, respectively in Figure 2a. To be compatible with SIMD optimized ADC computation, we set the number of centers in each cluster to 16. The experiments clearly show that the proposed loss function significantly outperforms existing state-of-the-arts methods.

5.2.2 Binary Quantization Retrieval

We use SIFT1M, which is a standard benchmarking dataset with 1 million, 128 dimensional normalized datapoints extracted from image descriptors. We apply the learning algorithm in Section 4.3 using MIPS and report the results in Figure 2b.

5.3 Extreme Classification Inference

Extreme classification with large number of classes requires evaluating the last layer (classification layer) with all possible classes. When there are $O(M)$ classes, this becomes a major computation bottleneck as it involves huge matrix multiplication. Thus this is often solved using Maximum Inner Product Search to speed up the inference. We evaluate our methods on extreme classification using the Amazon-670k dataset [34]. An MLP classifier is trained over 670,091 classes, where the last layer has a dimensionality of 1,024. We evaluate retrieval performance on the classification layer and show the results in Figure 2c, by comparing it against brute force matrix multiplication.
5.4 Sensitivity to choice of $T$

Another interesting question is how the retrieval performance relates to $T$, given $\mu(T)$. Intuitively, if $T$ is set too low, then the objective takes almost all pairs of query and database points into consideration, and becomes similar to the standard reconstruction loss. If $T$ is too high, then very few pairs will be considered and the quantization may be inaccurate for low value inner product pairs. Figure 1c shows the retrieval evaluation of Glove1.2M dataset under different $T$. We use $T = 0.2$ for all of our retrieval experiments.

5.5 Speed benchmark

Although MIPS and $\ell_2$ nearest neighbor search are different problems, they are often asked to be compared, especially in the case of unit norm data, where the problem become equivalent. To evaluate our methods on speed-recall trade-off, we adopted the methodology of public benchmark suite ANN-benchmarks [35], which plots a comprehensive set of algorithms for comparison. The benchmarks are conducted on same platform of Intel Xeon W-2135 with one CPU single thread. Our implementation builds on product quantization in proposed method and SIMD based ADC [17]. This is further combined with a vector quantization based tree [11], and the curve is plotted by varying the number of leaves to search in the tree. Figure 2d shows our performance on Glove1.2M significantly outperforms the competing methods, especially in high recall region, where Recall10 is over 80%.

6 Conclusion

In this paper, we propose a new quantization loss function for inner product search, which replaces traditional reconstruction error. The new loss function is weighted based on the inner product values, giving more weight to the pairs of query and database points with higher inner product values. The proposed loss function is theoretically proven and can be applied to a wide range of quantization methods, for example product and binary quantization. Our experiments show superior performance on retrieval recall and inner product value estimation, compared to methods that use reconstruction error. The speed-recall benchmark on public datasets further indicates that the proposed method outperform state-of-arts baselines which are known to be hard to beat.
References

[1] Paolo Cremonesi, Yehuda Koren, and Roberto Turrin. Performance of recommender algorithms on top-n recommendation tasks. In Proceedings of the Fourth ACM Conference on Recommender Systems, pages 39–46, 2010.

[2] Thomas Dean, Mark Ruzon, Mark Segal, Jonathon Shlens, Sudheendra Vijayanarasimhan, and Jay Yagnik. Fast, accurate detection of 100,000 object classes on a single machine: Technical supplement. In Proceedings of IEEE Conference on Computer Vision and Pattern Recognition, 2013.

[3] Ian En-Hsu Yen, Satyen Kale, Felix Yu, Daniel Holtmann-Rice, Sanjiv Kumar, and Pradeep Ravikumar. Loss decomposition for fast learning in large output spaces. In Proceedings of the 35th International Conference on Machine Learning, volume 80, pages 5640–5649, 2018.

[4] Stephen Mussmann and Stefano Ermon. Learning and inference via maximum inner product search. In Proceedings of The 33rd International Conference on Machine Learning, volume 48, pages 2587–2596, 2016.

[5] Alexander Pritzel, Benigno Uria, Sriram Srinivasan, Adrià Puigdomènech Badia, Oriol Vinyals, Demis Hassabis, Daan Wierstra, and Charles Blundell. Neural episodic control. In Proceedings of the 34th International Conference on Machine Learning, volume 70, pages 2827–2836, 2017.

[6] T. Ge, K. He, Q. Ke, and J. Sun. Optimized product quantization. IEEE Transactions on Pattern Analysis and Machine Intelligence, 36(4):744–755, April 2014. ISSN 0162-8828. doi: 10.1109/TPAMI.2013.240.

[7] Artem Babenko and Victor Lempitsky. Additive quantization for extreme vector compression. In Computer Vision and Pattern Recognition (CVPR), 2014 IEEE Conference on, pages 931–938. IEEE, 2014.

[8] Jeff Johnson, Matthijs Douze, and Hervé Jégou. Billion-scale similarity search with gpus. arXiv preprint arXiv:1702.08734, 2017.

[9] Mohammad Norouzi, Ali Punjani, and David J Fleet. Fast exact search in hamming space with multi-index hashing. IEEE transactions on pattern analysis and machine intelligence, 36(6):1107–1119, 2014.

[10] Herve Jegou, Matthijs Douze, and Cordelia Schmid. Product quantization for nearest neighbor search. IEEE transactions on pattern analysis and machine intelligence, 33(1):117–128, 2011.

[11] Xiang Wu, Ruiqi Guo, Ananda Theertha Suresh, Sanjiv Kumar, Daniel N Holtmann-Rice, David Simcha, and Felix Yu. Multiscale quantization for fast similarity search. In Advances in Neural Information Processing Systems 30, pages 5745–5755. 2017.

[12] Jingdong Wang, Heng Tao Shen, Jingkuan Song, and Jianqiu Ji. Hashing for similarity search: A survey. arXiv preprint arXiv:1408.2927, 2014.

[13] Jun Wang, Wei Liu, Sanjiv Kumar, and Shih-Fu Chang. Learning to hash for indexing big data survey. Proceedings of the IEEE, 104(1):34–57, 2016.

[14] Anshumali Shrivastava and Ping Li. Asymmetric lsh (alsh) for sublinear time maximum inner product search (mips). In Advances in Neural Information Processing Systems, pages 2321–2329, 2014.

[15] Behnam Neyshabur and Nathan Srebro. On symmetric and asymmetric lshs for inner product search. arXiv preprint arXiv:1410.5518, 2014.

[16] Piotr Indyk and Rajeev Motwani. Approximate nearest neighbors: towards removing the curse of dimensionality. In Proceedings of the thirtieth annual ACM symposium on Theory of computing, pages 604–613. ACM, 1998.

[17] Ruiqi Guo, Sanjiv Kumar, Krzysztof Choromanski, and David Simcha. Quantization based fast inner product search. In Proceedings of the 19th International Conference on Artificial Intelligence and Statistics, AISTATS 2016, Cadiz, Spain, May 9-11, 2016, pages 482–490, 2016. URL http://jmlr.org/proceedings/papers/v51/guo16a.html
[18] Julieta Martinez, Joris Clement, Holger H Hoos, and James J Little. Revisiting additive quantization. In European Conference on Computer Vision, pages 137–153. Springer, 2016.

[19] Chenzhuo Zhu, Song Han, Huizi Mao, and William J Dally. Trained ternary quantization. arXiv preprint arXiv:1612.01064, 2016.

[20] Kaiming He, Fang Wen, and Jian Sun. K-means hashing: An affinity-preserving quantization method for learning binary compact codes. In Proceedings of the IEEE conference on computer vision and pattern recognition, pages 2938–2945, 2013.

[21] Venice Erin Liong, Jiwen Lu, Gang Wang, Pierre Moulin, and Jie Zhou. Deep hashing for compact binary codes learning. In The IEEE Conference on Computer Vision and Pattern Recognition (CVPR), June 2015.

[22] Bo Dai, Ruiqi Guo, Sanjiv Kumar, Niao He, and Le Song. Stochastic generative hashing. In Proceedings of the 34th International Conference on Machine Learning-Volume 70, pages 913–922. JMLR. org, 2017.

[23] Ting Zhang, Chao Du, and Jingdong Wang. Composite quantization for approximate nearest neighbor search. In ICML, volume 2, page 3, 2014.

[24] Yunchao Gong, Svetlana Lazebnik, Albert Gordo, and Florent Perronnin. Iterative quantization: A procrustean approach to learning binary codes for large-scale image retrieval. IEEE Transactions on Pattern Analysis and Machine Intelligence, 35(12):2916–2929, 2013.

[25] Marius Muja and David G Lowe. Scalable nearest neighbor algorithms for high dimensional data. IEEE Transactions on Pattern Analysis and Machine Intelligence, 36(11):2227–2240, 2014.

[26] Parikshit Ram and Alexander G Gray. Maximum inner-product search using cone trees. In Proceedings of the 18th ACM SIGKDD international conference on Knowledge discovery and data mining, pages 931–939. ACM, 2012.

[27] Kush Bhatia, Himanshu Jain, Manik Varma, and Prateek Jain. Sparse local embeddings for extreme multi-label classification. In Advances in neural information processing systems, pages 730–738, 2015.

[28] Ben Harwood and Tom Drummond. FANNG: Fast approximate nearest neighbour graphs. In Computer Vision and Pattern Recognition (CVPR), 2016 IEEE Conference on, pages 5713–5722. IEEE, 2016.

[29] Artem Babenko and Victor Lempitsky. The inverted multi-index. In Computer Vision and Pattern Recognition (CVPR), 2012 IEEE Conference on, pages 3069–3076. IEEE, 2012.

[30] Jeffrey Pennington, Richard Socher, and Christopher D. Manning. Glove: Global vectors for word representation. In Empirical Methods in Natural Language Processing (EMNLP), pages 1532–1543, 2014.

[31] Kush Bhatia, Himanshu Jain, Purushottam Kar, Manik Varma, and Prateek Jain. Sparse local embeddings for extreme multi-label classification. In Advances in neural information processing systems, pages 730–738, 2015.

[32] Martin Aumüller, Erik Bernhardsson, and Alexander Faithfull. Ann-benchmarks: A benchmarking tool for approximate nearest neighbor algorithms. Information Systems, 2019.
7 Appendix

7.1 Proof of Theorem 3.3

Proof of Theorem 3.3 First, it is easy to see that because $\sin^{d-2} \alpha < \sin^d \alpha$, $\frac{I_d - 2}{I_d} < 1$. Next, from Cauchy–Schwarz inequality for integrals, we have

$$\left( \int_0^\alpha \sin^{d+2} x \sin^{d-2} x dx \right)^2 \leq \int_0^\alpha \sin^{d+2} x dx \int_0^\alpha \sin^{d-2} x dx$$

Rearranging this we have $\frac{I_d}{I_{d+2}} \leq \frac{I_{d-2}}{I_d}$, which proves that $\frac{I_d - 2}{I_d}$ is monotonically non-increasing. Given that it has a lower bound and is monotonically non-increasing, the limit of $\frac{I_d}{I_{d+2}}$ exists.

Dividing both sides of Equation (8) by $I_d$, we have

$$1 = \frac{-\cos \alpha \sin^d \alpha}{dI_d} + \frac{(d - 1)I_d - 2}{dI_d}$$

Thus $\lim_{d \to \infty} \frac{(d - 1)I_d - 2}{dI_d} = \lim_{d \to \infty} \frac{I_d - 2}{I_d} > 1$ exists. And therefore $\lim_{d \to \infty} \frac{\cos \alpha \sin^{d-1} \alpha}{dI_d} > 0$ also exists. Furthermore,

$$\lim_{d \to \infty} \frac{\cos \alpha \sin^{d-1} \alpha}{(d-2)^d - 2} = 1 \Rightarrow \lim_{d \to \infty} \frac{(d - 2)I_d - 2}{dI_d} = \frac{1}{2 \sin^2 \alpha}$$

Finally we have $\lim_{d \to \infty} \lambda = \frac{1}{\sin^2 \alpha} - 1 = \frac{T}{1 - T^2}$, and this proves Theorem 3.3. \qed
7.2 Proof of Theorem 4.1

Proof of Theorem 4.1 Indeed,

$$g(x_i, \hat{x}) := \mu \|r(\mu T(x_i, \hat{x}))\|^2 + \|r_{\perp}(x_i, \hat{x})\|^2$$

$$= \mu \frac{((\hat{x} - x_i) \cdot x_i)^2}{\|x_i\|^2} + \|\hat{x} - x_i\| - \frac{(\hat{x} - x_i)^T x_i}{\|x_i\|} x_i \|^2$$

$$= (\hat{x} - x_i)^T (\hat{x} - x_i) + (\mu - 1) \frac{(\hat{x} - x_i)^T x_i)^2}{\|x_i\|^2}$$

$$= (\hat{x} - x_i)^T (\hat{x} - x_i) + (\mu - 1) \frac{(\hat{x} T x_i - x_i^T x_i)^2}{\|x_i\|^2}$$

$$= (\hat{x} - x_i)^T (\hat{x} - x_i) + (\mu - 1) \left( \frac{(\hat{x} T x_i)^2}{\|x_i\|^2} + \|x_i\|^2 - 2\hat{x}^T x_i \right)$$

$$= \|\hat{x}\|^2 + (\mu - 1) \frac{(\hat{x} T x_i)^2}{\|x_i\|^2} - 2\hat{x}^T x_i + \mu \|x_i\|^2$$

$$= \hat{x}^T \hat{x} + (\mu - 1) \frac{\hat{x}^T x_i x_i^T \hat{x} - 2\hat{x}^T x_i + \mu \|x_i\|^2}{\|x_i\|^2}.$$

Therefore, the derivative of $g(x_i, \hat{x})$ with respect to $\hat{x}$ is

$$\frac{dg(x_i, \hat{x})}{d\hat{x}} = 2\hat{x} + 2\mu - 1 \frac{1}{\|x_i\|^2} x_i x_i^T \hat{x} - 2\mu x_i.$$

Setting $\sum_{i=1}^{m} \frac{dg(x_i, \hat{x})}{d\hat{x}} = 0$, we have

$$\sum_{i=1}^{m} \frac{dg(x_i, \hat{x})}{d\hat{x}} = 0$$

$$\iff \sum_{i=1}^{m} \left( 2\hat{x} + 2\mu - 1 \frac{1}{\|x_i\|^2} x_i x_i^T \hat{x} - 2\mu x_i \right) = 0$$

$$\iff \left( 1 + \frac{\mu - 1}{m} \sum_{i=1}^{m} \frac{x_i x_i^T}{\|x_i\|^2} \right) \hat{x} = \mu \sum_{i=1}^{m} x_i$$

$$\iff \hat{x} = \mu \left( 1 + \frac{\mu - 1}{m} \sum_{i=1}^{m} \frac{x_i x_i^T}{\|x_i\|^2} \right)^{-1} \sum_{i=1}^{m} x_i.$$

7.3 Algorithm for Vector Quantization with the modified objective

7.4 Codebook Optimization in Product Quantization

For example, consider the first vector $C_{1,1}$ in the codebook $C_1$ for the first subspace, and let $x_i$ be one of the datapoints the first subspace of which is encoded as $C_{1,1}$, i.e., $x_i^{(1)} = C_{1,1}$. Write $x_i$ as
Algorithm 1 Proposed Vector Quantization Algorithm For Minimizing Weighted Quantization Errors

Input:
- A set of $N$ datapoints $x_1, x_2, \ldots, x_N \in \mathbb{R}^d$.
- A scalar $\mu > 0$, the weight for quantization error components tradeoff (selection guided by desired inner product threshold $T$ in Sec[3]).
- A positive integer $k$, the size of the codebook.

Output:
- A set of codebook $c_1, c_2, \ldots, c_k \in \mathbb{R}^d$
- Partition assignment $a_1, a_2, \ldots, a_N \in \{1, 2, \ldots, k\}$ for the $N$ datapoints such that $x_i$ is quantized as $c_{a_i}$.

Algorithm:
Initialize the centroids $c_1, c_2, \ldots, c_k$ by choosing $k$ random datapoints.
Set $\text{new\_error} = +\infty$.

do
old_error $\leftarrow$ new_error.

[Partition Assignment]
for each $i \in \{1, 2, \ldots, N\}$ do
$$a_i \leftarrow \arg\min_j \left( \mu \|r_\parallel(x_i, c_j)\|^2 + \|r_\perp(x_i, c_j)\|^2 \right)$$
end for

[Centroid Update]
for each $i \in \{1, 2, \ldots, k\}$ do
$$S \leftarrow \{x_j | a_j = i, 1 \leq j \leq N\}$$
$$c_i \leftarrow \mu \left( 1 + \frac{\mu - 1}{|S|} \sum_{x \in S} \frac{x x^T}{\|x\|^2} \right)^{-1} \frac{\sum_{x \in S} x}{|S|},$$

where $|S|$ denote the cardinality of the set $S$.
end for

Compute new_error $\leftarrow \sum_{i=1}^N (\|r_\parallel(x_i, c_{a_i})\|^2 + \lambda \|r_\perp(x_i, c_{a_i})\|^2)$
while old_error $< $ new_error

Output the codebook $c_1, c_2, \ldots, c_k$ and the assignment $a_1, a_2, \ldots, a_N$.

$$x_i = (x_i^{(1)}, x_i^{(-1)}), \text{ and } \tilde{x}_i = (C_{1,1}, x_i^{(-1)}).$$ Then
$$\mu \|r_\parallel(x_i, \tilde{x}_i)\|^2 + \|r_\perp(x_i, \tilde{x}_i)\|^2 = \tilde{x}_i^T \tilde{x}_i + (\mu - 1) \frac{\tilde{x}_i^T C_{1,1}^T x_i x_i^T \tilde{x}_i}{\|x_i\|^2} - 2 \mu \tilde{x}_i^T x_i + \mu \|x_i\|^2$$
$$= (C_{1,1}^T x_i^{(-1)} - C_{1,1}^T x_i^{(-1)}) - 2\mu (C_{1,1}^T x_i^{(+1)} + x_i^{(-1)} + x_i^{(-1)} + \mu \|x_i\|^2$$
$$+ (\mu - 1) \frac{C_{1,1}^T x_i^{(+1)} + x_i^{(-1)} + x_i^{(-1)} + x_i^{(-1)} + x_i^{(-1)} + x_i^{(-1)} + x_i^{(-1)} + x_i^{(-1)}}{\|x_i\|^2}.$$}

Let $S$ denote the set of indices $S := \{i | A_{i,1} = 1\}$. Therefore, the partial derivative of (13) with respect to $C_{1,1}$ is
$$\sum_{i \in S} \left( 2C_{1,1} + (\mu - 1) \frac{2x_i^{(+1)} x_i^{(+1)} - C_{1,1}^T + x_i^{(-1)} x_i^{(-1)}}{\|x_i\|^2} \right).$$

Set (14) to be zero, and we have
$$C_{1,1}^* = \mu \left( 1 + \frac{\mu - 1}{|S|} \sum_{i \in S} \frac{x_i^{(+1)} x_i^{(+1)}}{|S|} \right)^{-1} \sum_{i \in S} (x_i^{(+1)} - \frac{(1-\frac{1}{\mu}) x_i^{(+1)} x_i^{(-1)} x_i^{(-1)}}{\|x_i\|^2}) \frac{1}{|S|}. $$

13