

# Hashing for Similarity Search: A Survey

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**Abstract**—Similarity search (nearest neighbor search) is a problem of pursuing the data items whose distances to a query item are the smallest from a large database. Various methods have been developed to address this problem, and recently a lot of efforts have been devoted to approximate search. In this paper, we present a survey on one of the main solutions, hashing, which has been widely studied since the pioneering work locality sensitive hashing. We divide the hashing algorithms two main categories: locality sensitive hashing, which designs hash functions without exploring the data distribution and learning to hash, which learns hash functions according the data distribution, and review them from various aspects, including hash function design and distance measure and search scheme in the hash coding space.

**Index Terms**—Approximate Nearest Neighbor Search, Similarity Search, Hashing, Locality Sensitive Hashing, Learning to Hash, Quantization.

## 1 INTRODUCTION

The problem of similarity search, also known as nearest neighbor search, proximity search, or close item search, is to find an item that is the nearest to a query item, called nearest neighbor, under some distance measure from a search (reference) database. In the case that the reference database is very large or that the distance computation between the query item and the database item is costly, it is often computationally infeasible to find the exact nearest neighbor. Thus, a lot of research efforts have been devoted to approximate nearest neighbor search that is shown to be enough and useful for many practical problems.

Hashing is one of the popular solutions for approximate nearest neighbor search. In general, hashing is an approach of transforming the data item to a low-dimensional representation, or equivalently a short code consisting of a sequence of bits. The application of hashing to approximate nearest neighbor search includes two ways: indexing data items using hash tables that is formed by storing the items with the same code in a hash bucket, and approximating the distance using the one computed with short codes.

The former way regards the items lying the buckets corresponding to the codes of the query as the nearest neighbor candidates, which exploits the locality sensitive property that similar items have larger probability to be mapped to the same code than dissimilar items. The main research efforts along this direction consist of designing hash functions satisfying the locality sensitive

property and designing efficient search schemes using and beyond hash tables.

The latter way ranks the items according to the distances computed using the short codes, which exploits the property that the distance computation using the short codes is efficient. The main research effort along this direction is to design the effective ways to compute the short codes and design the distance measure using the short codes guaranteeing the computational efficiency and preserving the similarity.

## 2 OVERVIEW

### 2.1 The Nearest Neighbor Search Problem

#### 2.1.1 Exact nearest neighbor search

Nearest neighbor search, also known as similarity search, proximity search, or close item search, is defined as: Given a query item  $\mathbf{q}$ , the goal is to find an item  $\text{NN}(\mathbf{q})$ , called nearest neighbor, from a set of items  $\mathcal{X} = \{\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_N\}$  so that  $\text{NN}(\mathbf{q}) = \arg \min_{\mathbf{x} \in \mathcal{X}} \text{dist}(\mathbf{q}, \mathbf{x})$ , where  $\text{dist}(\mathbf{q}, \mathbf{x})$  is a distance computed between  $\mathbf{q}$  and  $\mathbf{x}$ . A straightforward generalization is a  $K$ -NN search, where  $K$ -nearest neighbors ( $\text{KNN}(\mathbf{q})$ ) are needed to be found.

The problem is not fully specified without the distance between an arbitrary pair of items  $\mathbf{x}$  and  $\mathbf{q}$ . As a typical example, the search (reference) database  $\mathcal{X}$  lies in a  $d$ -dimensional space  $\mathbb{R}^d$  and the distance is induced by an  $\ell_s$  norm,  $\|\mathbf{x} - \mathbf{q}\|_s = (\sum_{i=1}^d |x_i - q_i|^s)^{1/s}$ . The search problem under the Euclidean distance, i.e., the  $\ell_2$  norm, is widely studied. Other notions of search database, such as each item formed by a set, and distance measure, such as  $\ell_1$  distance, cosine similarity and so on are also possible.

The fixed-radius near neighbor ( $R$ -near neighbor) problem, an alternative of nearest neighbor search, is defined as: Given a query item  $\mathbf{q}$ , the goal is to find

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the items  $\mathcal{R}$  that are within the distance  $C$  of  $\mathbf{q}$ ,  $\mathcal{R} = \{\mathbf{x} | \text{dist}(\mathbf{q}, \mathbf{x}) \leq R, \mathbf{x} \in \mathcal{X}\}$ .

### 2.1.2 Approximate nearest neighbor search

There exists efficient algorithms for exact nearest neighbor and  $R$ -near neighbor search problems in low-dimensional cases. It turns out that the problems become hard in the large scale high-dimensional case and even most algorithms take higher computational cost than the naive solution, linear scan. Therefore, a lot of recent efforts are moved to approximate nearest neighbor search problems. The  $(1 + \epsilon)$ -approximate nearest neighbor search problem,  $\epsilon > 0$ , is defined as: Given a query  $\mathbf{x}$ , the goal is to find an item  $\mathbf{x}$  so that  $\text{dist}(\mathbf{q}, \mathbf{x}) \leq (1 + \epsilon) \text{dist}(\mathbf{q}, \mathbf{x}^*)$ , where  $\mathbf{x}^*$  is the true nearest neighbor. The  $c$ -approximate  $R$ -near neighbor search problem is defined as: Given a query  $\mathbf{x}$ , the goal is to find some item  $\mathbf{x}$ , called  $cR$ -near neighbor, so that  $\text{dist}(\mathbf{q}, \mathbf{x}) \leq cR$ , where  $\mathbf{x}^*$  is the true nearest neighbor.

### 2.1.3 Randomized nearest neighbor search

The randomized search problem aims to report the (approximate) nearest (or near) neighbors with probability instead of deterministically. There are two widely-studied randomized search problems: randomized  $c$ -approximate  $R$ -near neighbor search and randomized  $R$ -near neighbor search. The former one is defined as: Given a query  $\mathbf{x}$ , the goal is to report some  $cR$ -near neighbor of the query  $\mathbf{q}$  with probability  $1 - \delta$ , where  $0 < \delta < 1$ . The latter one is defined as: Given a query  $\mathbf{x}$ , the goal is to report some  $R$ -near neighbor of the query  $\mathbf{q}$  with probability  $1 - \delta$ .

## 2.2 The Hashing Approach

The hashing approach aims to map the reference and/or query items to the target items so that approximate nearest neighbor search can be efficiently and accurately performed using the target items and possibly a small subset of the raw reference items. The target items are called hash codes (also known as hash values, simply hashes). In this paper, we may also call it short/compact code interchangeably.

Formally, the hash function is defined as:  $y = h(\mathbf{x})$ , where  $y$  is the hash code and  $h(\cdot)$  is the function. In the application to approximate nearest neighbor search, usually several hash functions are used together to compute the hash code:  $\mathbf{y} = \mathbf{h}(\mathbf{x})$ , where  $\mathbf{y} = [y_1 \ y_2 \ \dots \ y_M]^T$  and  $[h_1(\mathbf{x}) \ h_2(\mathbf{x}) \ \dots \ h_M(\mathbf{x})]^T$ . Here we use a vector  $\mathbf{y}$  to represent the hash code for presentation convenience.

There are two basic strategies for using hash codes to perform nearest (near) neighbor search: hash table lookup and Fast distance approximation.

### 2.2.1 Hash table lookup.

The hash table is a data structure that is composed of buckets, each of which is indexed by a hash code. Each reference item  $\mathbf{x}$  is placed into a bucket  $h(\mathbf{x})$ . Different

from the conventional hashing algorithm in computer science that avoids collisions (i.e., avoids mapping two items into some same bucket), the hashing approach using a hash table aims to maximize the probability of collision of near items. Given the query  $\mathbf{q}$ , the items lying in the bucket  $h(\mathbf{q})$  are retrieved as near items of  $\mathbf{q}$ .

To improve the recall,  $L$  hash tables are constructed, and the items lying in the  $L$  ( $L', L' < L$ ) hash buckets  $h_1(\mathbf{q}), \dots, h_L(\mathbf{q})$  are retrieved as near items of  $\mathbf{q}$  for randomized  $R$ -near neighbor search (or randomized  $c$ -approximate  $R$ -near neighbor search). To guarantee the precision, each of the  $L$  hash codes,  $y_i$ , needs to be a long code, which means that the total number of the buckets is too large to index directly. Thus, only the nonempty buckets are retained by resorting to conventional hashing of the hash codes  $h_l(\mathbf{x})$ .

### 2.2.2 Fast distance approximation.

The direct way is to perform an exhaustive search: compare the query with each reference item by fast computing the distance between the query and the hash code of the reference item and retrieve the reference items with the smallest distances as the candidates of nearest neighbors, which is usually followed by a reranking step: rerank the nearest neighbor candidates retrieved with hash codes according to the true distances computed using the original features and attain the  $K$  nearest neighbors or  $R$ -near neighbor.

This strategy exploits two advantages of hash codes. The first one is that the distance using hash codes can be efficiently computed and the cost is much smaller than that of the computation in the input space. The second one is that the size of the hash codes is much smaller than the input features and hence can be loaded into memory, resulting the disk I/O cost reduction in the case the original features are too large to be loaded into memory.

One practical way of speeding up the search is to perform a non-exhaustive search: first retrieve a set of candidates using inverted index and then compute the distances of the query with the candidates using the short codes. Other research efforts includes organizing the hash codes with a data structure, such as a tree or a graph structure, to avoid exhaustive search.

## 2.3 Organization of This Paper

The organization of the remaining part is given as follows. Section 3 presents the definition of the locality sensitive hashing (LSH) family and the instances of LSH with various distances. Section 4 presents some research works on how to perform efficient search given LSH codes and model and analyze LSH in aspects Sections 5, 6, and 7 review the learning-to-hash algorithms. Finally, Section 9 concludes this survey.

### 3 LOCALITY SENSITIVE HASHING: DEFINITION AND INSTANCES

The term “locality-sensitive hashing” (LSH) was introduced in 1998 [42], to name a randomized hashing framework for efficient approximate nearest neighbor (ANN) search in high dimensional space. It is based on the definition of LSH family  $\mathcal{H}$ , a family of hash functions mapping similar input items to the same hash code with higher probability than dissimilar items. However, the first specific LSH family, min-hash, was invented in 1997 by Andrei Broder [11], for near-duplicate web page detection and clustering, and it is one of the most popular LSH method that is extensively-studied in theory and widely-used in practice.

Locality-sensitive hashing was first studied by the theoretical computer science community. The theoretical research mainly focuses on three aspects. The first one is on developing different LSH families for various distances or similarities, for example, p-stable distribution LSH for  $\ell_p$  distance [20], sign-random-projection (or sim-hash) for angle-based distance [13], min-hash for Jaccard coefficient [11], [12] and so on, and many variants are developed based on these basic LSH families [19]. The second one is on exploring the theoretical boundary of the LSH framework, including the bound on the search efficiency (both time and space) that the best possible LSH family can achieve for certain distances and similarities [20], [94], [105], the tight characteristics for a similarity measure to admit an LSH family [13], [16], and so on. The third one focuses on improving the search scheme of the LSH methods, to achieve theoretically provable better search efficiency [107], [19].

Shortly after it was proposed by the theoretical computer science community, the database and related communities began to study LSH, aiming at building real database systems for high dimensional similarity search. Research from this side mainly focuses on developing better data structures and search schemes that lead to better search quality and efficiency in practice [91], [25]. The quality criteria include precision and recall, and the efficiency criteria are commonly the query time, storage requirement, I/O consumption and so on. Some of these work also provide theoretical guarantees on the search quality of their algorithms [25].

In recent years, LSH has attracted extensive attention from other communities including computer vision (CV), machine learning, statistics, natural language processing (NLP) and so on. For example, in computer vision, high dimensional features are often required for various tasks, such as image matching, classification. LSH, as a probabilistic dimension reduction method, has been used in various CV applications which often reduce to approximate nearest neighbor search [17], [18]. However, the performance of LSH is limited due to the fact that it is totally probabilistic and data-independent, and thus it does not take the data distribution into account. On the other hand, as an inspiration of LSH, the concept of

“small code” or “compact code” has become the focus of many researchers from the CV community, and many learning-based hashing methods have come in to being [135][125][126][30][83][139][127][29][82][130][31]. These methods aim at learning the hash functions for better fitting the data distribution and labeling information, and thus overcoming the drawback of LSH. This part of the research often takes LSH as the baseline for comparison.

The machine learning and statistics community also contribute to the study of LSH. Research from this side often view LSH as a probabilistic similarity-preserving dimensionality reduction method, from which the hash codes that are produced can provide estimations to some pairwise distance or similarity. This part of the study mainly focuses on developing variants of LSH functions that provide an (unbiased) estimator of certain distance or similarity, with smaller variance [68], [52], [73], [51], or smaller storage requirement of the hash codes [70], [71], or faster computation of hash functions [69], [73], [51], [118]. Besides, the machine learning community also devotes to developing learning-based hashing methods.

In practice, LSH is widely and successfully used in the IT industry, for near-duplicate web page and image detection, clustering and so on. Specifically, The Altavista search engine uses min-hash to detect near-duplicate web pages [11], [12], while Google uses sim-hash to fulfill the same goal [92].

In the subsequent sections, we will first introduce different LSH families for various kinds of distances or similarities, and then we review the study focusing on the search scheme and the work devoted to modeling LSH and ANN problem.

#### 3.1 The Family

The locality-sensitive hashing (LSH) algorithm is introduced in [42], [27], to solve the  $(R, c)$ -near neighbor problem. It is based on the definition of LSH family  $\mathcal{H}$ , a family of hash functions mapping similar input items to the same hash code with higher probability than dissimilar items. Formally, an LSH family is defined as follows:

*Definition 1 (Locality-sensitive hashing):* A family of  $\mathcal{H}$  is called  $(R, cR, P_1, P_2)$ -sensitive if for any two items  $\mathbf{p}$  and  $\mathbf{q}$ ,

- if  $\text{dist}(\mathbf{p}, \mathbf{q}) \leq R$ , then  $\text{Prob}[h(\mathbf{p}) = h(\mathbf{q})] \geq P_1$ ,
- if  $\text{dist}(\mathbf{p}, \mathbf{q}) \geq cR$ , then  $\text{Prob}[h(\mathbf{p}) = h(\mathbf{q})] \leq P_2$ .

Here  $c > 1$ , and  $P_1 > P_2$ . The parameter  $\rho = \frac{\log(1/P_1)}{\log(1/P_2)}$  governs the search performance, the smaller  $\rho$ , the better search performance. Given such an LSH family for distance measure  $\text{dist}$ , there exists an algorithm for  $(R, c)$ -near neighbor problem which uses  $O(dn + n^{1+\rho})$  space, with query time dominated by  $O(n^\rho)$  distance computations and  $O(n^\rho \log_{1/P_2} n)$  evaluations of hash functions [20].

The LSH scheme indexes all items in hash tables and searches for near items via hash table lookup. The hash

table is a data structure that is composed of buckets, each of which is indexed by a hash code. Each reference item  $\mathbf{x}$  is placed into a bucket  $h(\mathbf{x})$ . Different from the conventional hashing algorithm in computer science that avoids collisions (i.e., avoids mapping two items into some same bucket), the LSH approach aims to maximize the probability of collision of near items. Given the query  $\mathbf{q}$ , the items lying in the bucket  $h(\mathbf{q})$  are considered as near items of  $h(\mathbf{q})$ .

Given an LSH family  $\mathcal{H}$ , the LSH scheme amplifies the gap between the high probability  $P_1$  and the low probability  $P_2$  by concatenating several functions. In particular, for parameter  $K$ ,  $K$  functions  $h_1(\mathbf{x}), \dots, h_K(\mathbf{x})$ , where  $h_k$  ( $1 \leq k \leq K$ ) are chosen independently and uniformly at random from  $\mathcal{H}$ , form a compound hash function  $g(\mathbf{x}) = (h_1(\mathbf{x}), \dots, h_K(\mathbf{x}))$ . The output of this compound hash function identifies a bucket id in a hash table. However, the concatenation of  $K$  functions also reduces the chance of collision between similar items. To improve the recall,  $L$  such compound hash functions  $g_1, g_2, \dots, g_L$  are sampled independently, each of which corresponds to a hash table. These functions are used to hash each data point into  $L$  hash codes, and  $L$  hash tables are constructed to index the buckets corresponding to these hash codes respectively. The items lying in the  $L$  hash buckets are retrieved as near items of  $h(\mathbf{q})$  for randomized  $R$ -near neighbor search (or randomized  $c$ -approximate  $R$ -near neighbor search).

In practice, to guarantee the precision, each of the  $L$  hash codes,  $g_i(\mathbf{x})$ , needs to be a long code (or  $K$  is large), and thus the total number of the buckets is too large to index directly. Therefore, only the nonempty buckets are retained by resorting to conventional hashing of the hash codes  $g_i(\mathbf{x})$ .

There are different kinds of LSH families for different distances or similarities, including  $\ell_p$  distance, *arccos* or angular distance, Hamming distance, Jaccard coefficient and so on.

## 3.2 $\ell_p$ Distance

### 3.2.1 LSH with $p$ -stable distributions

The LSH scheme based on the  $p$ -stable distributions, presented in [20], is designed to solve the search problem under the  $\ell_p$  distance  $\|\mathbf{x}_i - \mathbf{x}_j\|_p$ , where  $p \in (0, 2]$ . The  $p$ -stable distribution is defined as: A distribution  $\mathcal{D}$  is called  $p$ -stable, where  $p \geq 0$ , if for any  $n$  real numbers  $v_1 \cdots v_n$  and i.i.d. variables  $X_1 \cdots X_n$  with distribution  $\mathcal{D}$ , the random variable  $\sum_{i=1}^n v_i X_i$  has the same distribution as the variable  $(\sum_{i=1}^n |v_i|^p)^{1/p} X$ , where  $X$  is a random variable with distribution  $\mathcal{D}$ . The well-known Gaussian distribution  $\mathcal{D}_G$ , defined by the density function  $g(x) = \frac{1}{\sqrt{2\pi}} e^{-x^2/2}$ , is 2-stable.

In the case that  $p = 1$ , the exponent  $\rho$  is equal to  $\frac{1}{c} + O(R/r)$ , and later it is shown in [94] that it is impossible to achieve  $\rho \leq \frac{1}{2c}$ . Recent study in [105] provides more lower bound analysis for Hamming distance, Euclidean distance, and Jaccard distance.

The LSH scheme using the  $p$ -stable distribution to generate hash codes is described as follows. The hash function is formulated as  $h_{\mathbf{w},b}(\mathbf{x}) = \lfloor \frac{\mathbf{w}^T \mathbf{x} + b}{r} \rfloor$ . Here,  $\mathbf{w}$  is a  $d$ -dimensional vector with entries chosen independently from a  $p$ -stable distribution.  $b$  is a real number chosen uniformly from the range  $[0, r]$ .  $r$  is the window size, thus a positive real number.

The following equation can be proved

$$P(h_{\mathbf{w},b}(\mathbf{x}_1) = h_{\mathbf{w},b}(\mathbf{x}_2)) = \int_0^r \frac{1}{c} f_p\left(\frac{t}{c}\right) \left(1 - \frac{t}{r}\right) dt, \quad (1)$$

where  $c = \|\mathbf{x}_1 - \mathbf{x}_2\|_p$ , which means that such a hash function belongs to the LSH family under the  $\ell_p$  distance.

Specifically, to solve the search problem under the Euclidean distance, the 2-stable distribution, i.e., the Gaussian distribution, is chosen to generate the random projection  $\mathbf{w}$ . In this case ( $p = 2$ ), the exponent  $\rho$  drops strictly below  $1/c$  for some (carefully chosen) finite value of  $r$ .

It is claimed that uniform quantization [72] without the offset  $b$ ,  $h_{\mathbf{w}}(\mathbf{x}) = \lfloor \frac{\mathbf{w}^T \mathbf{x}}{r} \rfloor$  is more accurate and uses fewer bits than the scheme with the offset.

### 3.2.2 Leech lattice LSH

Leech lattice LSH [1] is an LSH algorithm for the search in the Euclidean space. It is a multi-dimensional version of the aforementioned approach. The approach firstly randomly projects the data points into  $\mathbb{R}^t$ ,  $t$  is a small super-constant ( $= 1$  in the aforementioned approach). The space  $\mathbb{R}^t$  is partitioned into cells, using Leech lattice, which is a constellation in 24 dimensions. The nearest point in Leech lattice can be found using a (bounded) decoder which performs only 519 floating point operations per decoded point. On the other hand, the exponent  $\rho(c)$  is quite attractive:  $\rho(2)$  is less than 0.37.  $E_8$  lattice is used because its decoding is much cheaper than Leech lattice (its quantization performance is slightly worse) A comparison of LSH methods for the Euclidean distance is given in [108].

### 3.2.3 Spherical LSH

Spherical LSH [123] is an LSH algorithm designed for points that are on a unit hypersphere in the Euclidean space. The idea is to consider the regular polytope, simplex, orthoplex, and hypercube, for example, that are inscribed into the hypersphere and rotated at random. The hash function maps a vector on the hypersphere into the closest polytope vertex lying on the hypersphere. It means that the buckets of the hash function are the Voronoi cells of the polytope vertices. Though there is no theoretic analysis about exponent  $\rho$ , the Monte Carlo simulation shows that it is an improvement over the Leech lattice approach [1].

### 3.2.4 Beyond LSH

Beyond LSH [3] improves the ANN search in the Euclidean space, specifically solving  $(c, 1)$ -ANN. It consists

of two-level hashing structures: outer hash table and inner hash table. The outer hash scheme aims to partition the data into buckets with a filtered out process such that all the pairs of points in the bucket are not more than a threshold, and find a  $(1 + 1/c)$ -approximation to the minimum enclosing ball for the remaining points. The inner hash tables are constructed by first computing the center of the ball corresponding to a non-empty bucket in outer hash tables and partitioning the points belonging to the ball into a set of over-lapped subsets, for each of which the differences of the distance of the points to the center is within  $[-1, 1]$  and the distance of the overlapped area to the center is within  $[0, 1]$ . For the subset, an LSH scheme is conducted. The query process first locates a bucket from outer hash tables for a query. If the bucket is empty, the algorithm stops. If the distance of the query to the bucket center is not larger than  $c$ , then the points in the bucket are output as the results. Otherwise, the process further checks the subsets in the bucket whose distances to the query lie in a specific range and then does the LSH query in those subsets.

### 3.3 Angle-Based Distance

#### 3.3.1 Random projection

The LSH algorithm based on random projection [2], [13] is developed to solve the near neighbor search problem under the angle between vectors,  $\theta(\mathbf{x}_i, \mathbf{x}_j) = \arccos \frac{\mathbf{x}_i^T \mathbf{x}_j}{\|\mathbf{x}_i\|_2 \|\mathbf{x}_j\|_2}$ . The hash function is formulated as  $h(\mathbf{x}) = \text{sign}(\mathbf{w}^T \mathbf{x})$ , where  $\mathbf{w}$  follows the standard Gaussian distribution. It is easily shown that  $P(h(\mathbf{x}_i) = h(\mathbf{x}_j)) = 1 - \frac{\theta(\mathbf{x}_i, \mathbf{x}_j)}{\pi}$ , where  $\theta(\mathbf{x}_i, \mathbf{x}_j)$  is the angle between  $\mathbf{x}_i$  and  $\mathbf{x}_j$ , thus such a hash function belongs to the LSH family with the angle-based distance.

#### 3.3.2 Super-bit LSH

Super-bit LSH [52] aims to improve the above hashing functions for arccos (angular) similarity, by dividing the random projections into  $G$  groups then orthogonalizing  $B$  random projections for each group, obtaining new  $GB$  random projections and thus  $G$   $B$ -super bits. It is shown that the Hamming distance over the super bits is an unbiased estimation for the angular distance and the variance is smaller than the above random projection algorithm.

#### 3.3.3 Kernel LSH

Kernel LSH [64], [65] aims to build LSH functions with the angle defined in the kernel space,  $\theta(\mathbf{x}_i, \mathbf{x}_j) = \arccos \frac{\phi(\mathbf{x}_i)^T \phi(\mathbf{x}_j)}{\|\phi(\mathbf{x}_i)\|_2 \|\phi(\mathbf{x}_j)\|_2}$ . The key challenge is in constructing a projection vector  $\mathbf{w}$  from the Gaussian distribution. Define  $\mathbf{z}_t = \frac{1}{t} \sum_{i \in S_t} \phi(\mathbf{x}_i)$  where  $t$  is a natural number, and  $S$  is a set of  $t$  database items chosen i.i.d.. The central limit theorem shows that for sufficiently large  $t$ , the random variables  $\tilde{\mathbf{z}}_t = \sqrt{t} \Sigma^{-1/2} (\mathbf{z}_t - \boldsymbol{\mu})$  follows a

Normal distribution  $N(\mathbf{0}, \mathbf{I})$ . Then the hash function is given as

$$h(\phi(\mathbf{x})) = \begin{cases} 1 & \text{if } \phi(\mathbf{x}) \Sigma^{-1/2} \tilde{\mathbf{z}}_t \geq 0 \\ 0 & \text{otherwise.} \end{cases} \quad (2)$$

The covariance matrix  $\Sigma$  and the mean  $\boldsymbol{\mu}$  are estimated over a set of randomly chosen  $p$  database items, using a technique similar to that used in kernel principal component analysis.

Multi-kernel LSH [133], [132], uses multiple kernels instead of a single kernel to form the hash functions with assigning the same number of bits to each kernel hash function. A boosted version of multi-kernel LSH is presented in [137], which adopts the boosting scheme to automatically assign various number of bits to each kernel hash function.

#### 3.3.4 LSH with learnt metric

Semi-supervised LSH [45], [46], [66] first learns a Mahalanobis metric from the semi-supervised information and then form the hash function according to the pairwise similarity  $\theta(\mathbf{x}_i, \mathbf{x}_j) = \arccos \frac{\mathbf{x}_i^T \mathbf{A} \mathbf{x}_j}{\|\mathbf{G} \mathbf{x}_i\|_2 \|\mathbf{G} \mathbf{x}_j\|_2}$ , where  $\mathbf{G}^T \mathbf{G} = \mathbf{A}$  and  $\mathbf{A}$  is the learnt metric from the semi-supervised information. An extension, distribution aware LSH [146], is proposed, which, however, partitions the data along each projection direction into multiple parts instead of only two parts.

#### 3.3.5 Concomitant LSH

Concomitant LSH [23] is an LSH algorithm that uses concomitant rank order statistics to form the hash functions for cosine similarity. There are two schemes: concomitant min hash and concomitant min  $L$ -multi-hash.

Concomitant min hash is formulated as follows: generate  $2^K$  random projections  $\{\mathbf{w}_1, \mathbf{w}_2, \dots, \mathbf{w}_{2^K}\}$ , each of which is drawn independently from the standard normal distribution  $\mathcal{N}(\mathbf{0}, \mathbf{I})$ . The hash code is computed in two steps: compute the  $2^K$  projections along the  $2^K$  projection directions, and output the index of the projection direction along which the projection value is the smallest, formally written by  $h_c(\mathbf{x}) = \arg \min_{k=1}^{2^K} \mathbf{w}_k^T \mathbf{x}$ . It is shown that the probability  $\text{Prob}[h_c(\mathbf{x}_1) = h_c(\mathbf{x}_2)]$  is a monotonically increasing function with respect to  $\frac{\mathbf{x}_1^T \mathbf{x}_2}{\|\mathbf{x}_1\|_2 \|\mathbf{x}_2\|_2}$ .

Concomitant min  $L$ -multi-hash instead generates  $L$  hash codes: the indices of the projection directions along which the projection values are the top  $L$  smallest. It can be shown that the collision probability is similar to that of Concomitant min hash.

Generating a hash code of length  $K = 20$  means that it requires 1,048,576 random projections and vector multiplications, which is too high. To solve this problem, a cascading scheme is adopted: e.g., generate two concomitant hash functions, each of which generates a code of length 10, and compose them together, yielding a code of 20 bits, which only requires  $2 \times 2^{10}$  random projections and vector multiplications. There are two schemes proposed in [23]:

cascade concomitant min & max hash that composes the two codes  $[\arg \min_{k=1}^{2^K} \mathbf{w}_k^T \mathbf{x}, \arg \max_{k=1}^{2^K} \mathbf{w}_k^T \mathbf{x}]$ , and cascade concomitant  $L^2$  min & max hash multi-hash which is formed using the indices of the top smallest and largest projection values.

### 3.3.6 Hyperplane hashing

The goal of searching nearest neighbors to a query hyperplane is to retrieve the points from the database  $\mathcal{X}$  that are closest to a query hyperplane whose normal is given by  $\mathbf{n} \in \mathbb{R}^d$ . The Euclidean distance of a point  $\mathbf{x}$  to a hyperplane with the normal  $\mathbf{n}$  is:

$$d(P_{\mathbf{n}}, \mathbf{x}) = \|\mathbf{n}^T \mathbf{x}\|. \quad (3)$$

The hyperplane hashing family [47], [124], under the assumption that the hyperplane passes through origin and the data points and the normal are unit norm (which indicates that hyperplane hashing corresponds to search with absolute cosine similarity), is defined as follows,

$$h(\mathbf{z}) = \begin{cases} h_{\mathbf{u}, \mathbf{v}}(\mathbf{z}, \mathbf{z}) & \text{if } \mathbf{z} \text{ is a database vector} \\ h_{\mathbf{u}, \mathbf{v}}(\mathbf{z}, -\mathbf{z}) & \text{if } \mathbf{z} \text{ is a query hyperplane normal.} \end{cases} \quad (4)$$

Here  $h_{\mathbf{u}, \mathbf{v}}(\mathbf{a}, \mathbf{b}) = [h_{\mathbf{u}}(\mathbf{a}) h_{\mathbf{v}}(\mathbf{b})] = [\text{sign}(\mathbf{u}^T \mathbf{a}) \text{sign}(\mathbf{v}^T \mathbf{b})]$ , where  $\mathbf{u}$  and  $\mathbf{v}$  are sampled independently from a standard Gaussian distribution.

It is shown that the above hashing family belongs to LSH: it is  $(r, r(1+\epsilon), \frac{1}{4} - \frac{1}{\pi^2}r, \frac{1}{4} - \frac{1}{\pi^2}r(1+\epsilon))$ -sensitive for the angle distance  $d_{\theta}(\mathbf{x}, \mathbf{n}) = (\theta_{\mathbf{x}, \mathbf{n}} - \frac{\pi}{2})^2$ , where  $r, \epsilon > 0$ . The angle distance is equivalent to the distance of a point to the query hyperplane.

The below family, called XOR 1-bit hyperplane hashing,

$$h(\mathbf{z}) = \begin{cases} h_{\mathbf{u}}(\mathbf{z}) \oplus h_{\mathbf{v}}(\mathbf{z}) & \text{if } \mathbf{z} \text{ is a database vector} \\ h_{\mathbf{u}}(\mathbf{z}) \oplus h_{\mathbf{v}}(-\mathbf{z}) & \text{if } \mathbf{z} \text{ is a hyperplane normal,} \end{cases} \quad (5)$$

is shown to be  $(r, r(1+\epsilon), \frac{1}{2} - \frac{1}{\pi^2}r, \frac{1}{2} - \frac{1}{\pi^2}r(1+\epsilon))$ -sensitive for the angle distance  $d_{\theta}(\mathbf{x}, \mathbf{n}) = (\theta_{\mathbf{x}, \mathbf{n}} - \frac{\pi}{2})^2$ , where  $r, \epsilon > 0$ .

Embedded hyperplane hashing transforms the database vector (the normal of the query hyperplane) into a high-dimensional vector,

$$\bar{\mathbf{a}} = \text{vec}(\mathbf{a}\mathbf{a}^T)[a_1^2, a_1a_2, \dots, a_1a_d, a_2a_1, a_2^2, a_2a_3, \dots, a_d^2]. \quad (6)$$

Assuming  $\mathbf{a}$  and  $\mathbf{b}$  to be unit vectors, the Euclidean distance between the embeddings  $\bar{\mathbf{a}}$  and  $-\bar{\mathbf{b}}$  is given  $\|\bar{\mathbf{a}} - (-\bar{\mathbf{b}})\|_2^2 = 2 + 2(\mathbf{a}^T \mathbf{b})^2$ , which means that minimizing the distance between the two embeddings is equivalent to minimizing  $|\mathbf{a}^T \mathbf{b}|$ .

The embedded hyperplane hash function family is defined as

$$h(\mathbf{z}) = \begin{cases} h_{\mathbf{u}}(\bar{\mathbf{z}}) & \text{if } \mathbf{z} \text{ is a database vector} \\ h_{\mathbf{u}}(-\bar{\mathbf{z}}) & \text{if } \mathbf{z} \text{ is a query hyperplane normal.} \end{cases} \quad (7)$$

It is shown to be  $(r, r(1+\epsilon), \frac{1}{\pi} \cos^{-1} \sin^2(\sqrt{r}), \frac{1}{\pi} \cos^{-1} \sin^2(\sqrt{r(1+\epsilon)}))$  for the angle distance  $d_{\theta}(\mathbf{x}, \mathbf{n}) = (\theta_{\mathbf{x}, \mathbf{n}} - \frac{\pi}{2})^2$ , where  $r, \epsilon > 0$ .

It is also shown that the exponent for embedded hyperplane hashing is similar to that for XOR 1-bit hyperplane hashing and stronger than that for hyperplane hashing.

## 3.4 Hamming Distance

One LSH function for the Hamming distance with binary vectors  $\mathbf{y} \in \{0, 1\}^d$  is proposed in [42],  $h(\mathbf{y}) = y_k$ , where  $k \in \{1, 2, \dots, d\}$  is a randomly-sampled index. It can be shown that  $P(h(\mathbf{y}_i) = h(\mathbf{y}_j)) = 1 - \frac{\|\mathbf{y}_i - \mathbf{y}_j\|_h}{d}$ . It is proven that the exponent  $\rho$  is  $1/c$ .

## 3.5 Jaccard Coefficient

### 3.5.1 Min-hash

The Jaccard coefficient, a similarity measure between two sets,  $\mathcal{A}, \mathcal{B} \in \mathcal{U}$ , is defined as  $\text{sim}(\mathcal{A}, \mathcal{B}) = \frac{|\mathcal{A} \cap \mathcal{B}|}{|\mathcal{A} \cup \mathcal{B}|}$ . Its corresponding distance is taken as  $1 - \text{sim}(\mathcal{A}, \mathcal{B})$ . Min-hash [11], [12] is an LSH function for the Jaccard similarity. Min-hash is defined as follows: pick a random permutation  $\pi$  from the ground universe  $\mathcal{U}$ , and define  $h(\mathcal{A}) = \min_{a \in \mathcal{A}} \pi(a)$ . It is easily shown that  $P(h(\mathcal{A}) = h(\mathcal{B})) = \text{sim}(\mathcal{A}, \mathcal{B})$ . Given the  $K$  hash values of two sets, the Jaccard similarity is estimated as  $\frac{1}{K} \sum_{k=1}^K \delta[h_k(\mathcal{A}) = h_k(\mathcal{B})]$ , where each  $h_k$  corresponds to a random permutation that is independently generated.

### 3.5.2 $K$ -min sketch

$K$ -min sketch [11], [12] is a generalization of min-wise sketch (forming the hash values using the  $K$  smallest nonzeros from one permutation) used for min-hash. It also provides an unbiased estimator of the Jaccard coefficient but with a smaller variance, which however cannot be used for approximate nearest neighbor search using hash tables like min-hash. Conditional random sampling [68], [67] also takes the  $k$  smallest nonzeros from one permutation, and is shown to be a more accurate similarity estimator. One-permutation hashing [73], also uses one permutation, but breaks the space into  $K$  bins, and stores the smallest nonzero position in each bin and concatenates them together to generate a sketch. However, it is not directly applicable to nearest neighbor search by building hash tables due to empty bins. This issue is solved by performing rotation over one permutation hashing [118]. Specifically, if one bin is empty, the hashed value from the first non-empty bin on the right (circular) is borrowed as the key of this bin, which supplies an unbiased estimate of the resemblance unlike [73].

### 3.5.3 Min-max hash

Min-max hash [51], instead of keeping the smallest hash value of each random permutation, keeps both the smallest and largest values of each random permutation. Min-max hash can generate  $K$  hash values, using  $\frac{K}{2}$  random permutations, while still providing an unbiased estimator of the Jaccard coefficient, with a slightly smaller variance than min-hash.

### 3.5.4 B-bit minwise hashing

B-bit minwise hashing [71], [70] only uses the lowest b-bits of the min-hash value as a short hash value, which gains substantial advantages in terms of storage space while still leading to an unbiased estimator of the resemblance (the Jaccard coefficient).

### 3.5.5 Sim-min-hash

Sim-min-hash [149] extends min-hash to compare sets of real-valued vectors. This approach first quantizes the real-valued vectors and assigns an index (word) for each real-valued vector. Then, like the conventional min-hash, several random permutations are used to generate the hash keys. The different thing is that the similarity is estimated as  $\frac{1}{K} \sum_{k=1}^K \text{sim}(\mathbf{x}_k^A, \mathbf{x}_k^B)$ , where  $\mathbf{x}_k^A$  ( $\mathbf{x}_k^B$ ) is the real-valued vector (or Hamming embedding) that is assigned to the word  $h_k(\mathcal{A})$  ( $h_k(\mathcal{B})$ ), and  $\text{sim}(\cdot, \cdot)$  is the similarity measure.

## 3.6 $\chi^2$ Distance

$\chi^2$ -LSH [33] is a locality sensitive hashing function for the  $\chi^2$  distance. The  $\chi^2$  distance over two vectors  $\mathbf{x}_i$  and  $\mathbf{x}_j$  is defined as

$$\chi^2(\mathbf{x}_i, \mathbf{x}_j) = \sqrt{\sum_{t=1}^d \frac{(x_{it} - x_{jt})^2}{x_{it} - x_{jt}}}. \quad (8)$$

The  $\chi^2$  distance can also be defined without the square-root, and the below developments still hold by substituting  $r$  to  $r^2$  in all the equations.

The  $\chi^2$ -LSH function is defined as

$$h_{\mathbf{w},b}(\mathbf{x}) = \lfloor g_r(\mathbf{w}^T \mathbf{x}) + b \rfloor, \quad (9)$$

where  $g_r(x) = \frac{1}{2}(\sqrt{\frac{8x}{r^2} + 1} - 1)$ , each entry of  $\mathbf{w}$  is drawn from a 2-stable distribution, and  $b$  is drawn from a uniform distribution over  $[0, 1]$ .

It can be shown that

$$\begin{aligned} P(h_{\mathbf{w},b}(\mathbf{x}_i) = h_{\mathbf{w},b}(\mathbf{x}_j)) \\ = \int_0^{r^{(n+1)r^2}} \frac{1}{c} f\left(\frac{t}{c}\right) \left(1 - \frac{t}{(n+1)r^2}\right) dt, \end{aligned} \quad (10)$$

where  $f(t)$  denotes the probability density function of the absolute value of the 2-stable distribution,  $c = \|\mathbf{x}_i - \mathbf{x}_j\|_2$ .

Let  $c' = \chi^2(\mathbf{x}_i, \mathbf{x}_j)$ . It can be shown that  $P(h_{\mathbf{w},b}(\mathbf{x}_i) = h_{\mathbf{w},b}(\mathbf{x}_j))$  decreases monotonically with respect to  $c$  and  $c'$ . Thus, we can show it belongs to the LSH family.

## 3.7 Other Similarities

### 3.7.1 Rank similarity

Winner Take All (WTA) hash [140] is a sparse embedding method that transforms the input feature space into binary codes such that the Hamming distance in the resulting space closely correlates with rank similarity measure. The rank similarity measure is shown to be

more useful for high-dimensional features than the Euclidean distance, in particular in the case of normalized feature vectors (e.g., the  $\ell_2$  norm is equal to 1). The used similarity measure is a pairwise-order function, defined as

$$\text{sim}_{po}(\mathbf{x}_1, \mathbf{x}_2) = \sum_{i=0}^{d-1} \sum_{j=1}^i \delta[(x_{1i} - x_{1j})(x_{2i} - x_{2j}) > 0] \quad (11)$$

$$= \sum_{i=1}^d R_i(\mathbf{x}_1, \mathbf{x}_2), \quad (12)$$

where  $R_i(\mathbf{x}_1, \mathbf{x}_2) = |L(\mathbf{x}_1, i) \cap L(\mathbf{x}_2, i)|$  and  $L(\mathbf{x}_1, i) = \{j | x_{1i} > x_{1j}\}$ .

WTA hash generates a set of  $K$  random permutations  $\{\pi_k\}$ . Each permutation  $\pi_k$  is used to reorder the elements of  $\mathbf{x}$ , yielding a new vector  $\bar{\mathbf{x}}$ . The  $k$ th hash code is computed as  $\arg \max_{i=1}^T \bar{x}_i$ , taking a value between 0 and  $T - 1$ . The final hash code is a concatenation of  $T$  values each corresponding to a permutation. It is shown that WTA hash codes satisfy the LSH property and min-hash is a special case of WTA hash.

### 3.7.2 Shift invariant kernels

Locality sensitive binary coding using shift invariant kernel hashing [109] exploits the property that the binary mapping of the original data is guaranteed to preserve the value of a shift-invariant kernel, the random Fourier features (RFF) [110]. The RFF is defined as

$$\phi_{\mathbf{w},b}(\mathbf{x}) = \sqrt{2} \cos(\mathbf{w}^T \mathbf{x} + b), \quad (13)$$

where  $\mathbf{w} \sim P_K$  and  $b \sim \text{Unif}[0, 2\pi]$ . For example, for the Gaussian Kernel  $K(s) = e^{-\gamma \|s\|^2/2}$ ,  $\mathbf{w} \sim \text{Normal}(\mathbf{0}, \gamma \mathbf{I})$ . It can be shown that  $\mathbb{E}_{\mathbf{w},b}[\phi_{\mathbf{w},b}(\mathbf{x})\phi_{\mathbf{w},b}(\mathbf{y})] = K(\mathbf{x}, \mathbf{y})$ .

The binary code is computed as

$$\text{sign}(\phi_{\mathbf{w},b}(\mathbf{x}) + t), \quad (14)$$

where  $t$  is a random threshold,  $t \sim \text{Unif}[-1, 1]$ . It is shown that the normalized Hamming distance (i.e., the Hamming distance divided by the number of bits in the code string) are both lower bounded and upper bounded and that the codes preserve the similarity in a probabilistic way.

### 3.7.3 Non-metric distance

Non-metric LSH [98] extends LSH to non-metric data by embedding the data in the original space into an implicit reproducing kernel Krein space where the hash function is defined. The krein space with the indefinite inner product  $\langle \cdot, \cdot \rangle_{\mathcal{K}}$  admits an orthogonal decomposition as a direct sum  $\mathcal{K} = \mathcal{K}_+ \oplus \mathcal{K}_-$ , where  $(\mathcal{K}_+, \kappa_+(\cdot, \cdot))$  and  $(\mathcal{K}_-, \kappa_-(\cdot, \cdot))$  are separable Hilbert spaces with their corresponding positive definite inner products. The inner product  $\mathcal{K}$  is then computed as

$$\langle \xi_+ + \xi_-, \xi'_+ + \xi'_- \rangle_{\mathcal{K}} = \kappa_+(\xi_+, \xi'_+) - \kappa_-(\xi_-, \xi'_-). \quad (15)$$

Given the orthogonality of  $\mathcal{K}_+$  and  $\mathcal{K}_-$  of, the pairwise  $\ell_2$  distance in  $\mathcal{K}$  is compute as

$$\|\xi - \xi'\|_{\mathcal{K}}^2 = \|\xi_+ - \xi'_+\|_{\mathcal{K}_+}^2 - \|\xi_- - \xi'_-\|_{\mathcal{K}_-}^2. \quad (16)$$

The projections with the definite inner product  $\mathcal{K}_+$  and  $\mathcal{K}_-$  can be computed using the technology in kernel LSH, denoted by  $p_+$  and  $p_-$ , respectively. The hash function with the input being  $(p_+(\xi) - p_+(\xi), p_+(\xi) + p_+(\xi)) = (a_1(\xi), a_2(\xi))$  and the output being two binary bits is defined as,

$$\mathbf{h}(\xi) = [\delta[a_1(\xi) > \theta], \delta[a_2(\xi) > \theta]], \quad (17)$$

where  $a_1(\xi)$  and  $a_2(\xi)$  are assumed to be normalized to  $[0, 1]$  and  $\theta$  is a real number uniformly drawn from  $[0, 1]$ . It can be shown that  $P(\mathbf{h}(\xi) = \mathbf{h}(\xi')) = (1 - |a_1(\xi) - a_1(\xi')|)(1 - |a_2(\xi) - a_2(\xi')|)$ , which indicates that the hash function belongs to the LSH family.

### 3.7.4 Arbitrary distance measures

The basic idea of distance-based hashing [4] uses a line projection function

$$f(\mathbf{x}; \mathbf{a}_1, \mathbf{a}_2) = \frac{1}{2 \text{dist}(\mathbf{a}_1, \mathbf{a}_2)} (\text{dist}^2(\mathbf{x}, \mathbf{a}_1) + \text{dist}^2(\mathbf{a}_1, \mathbf{a}_2) - \text{dist}^2(\mathbf{x}, \mathbf{a}_2)), \quad (18)$$

to formulate a hash function,

$$h(\mathbf{x}; \mathbf{a}_1, \mathbf{a}_2) = \begin{cases} 1 & \text{if } f(\mathbf{x}; \mathbf{a}_1, \mathbf{a}_2) \in [t_1, t_2] \\ 0 & \text{otherwise.} \end{cases} \quad (19)$$

Here,  $\mathbf{a}_1$  and  $\mathbf{a}_2$  are randomly selected data items,  $\text{dist}(\cdot, \cdot)$  is the distance measure, and  $t_1$  and  $t_2$  are two thresholds, selected so that half of the data items are hashed to 1 and the other half to 0.

Similar to LSH, distance-based hashing generates a compound hash function using  $K$  distance-based hash functions and accordingly  $L$  compound hash functions, yielding  $L$  hash tables. However, it cannot be shown that the theoretic guarantee in LSH holds for DBH. There are some other schemes discussed in [4], including optimizing  $L$  and  $K$  from the dataset, applying DBH hierarchically so that different set of queries use different parameters  $L$  and  $K$ , and so on.

## 4 LOCALITY SENSITIVE HASHING: SEARCH, MODELING, AND ANALYSIS

### 4.1 Search

#### 4.1.1 Entropy-based search

The entropy-based search algorithm [107], given a query point  $\mathbf{q}$ , picks a set of  $(O(N^\rho))$  random points  $\mathbf{v}$  from  $B(q, R)$ , a ball centered at  $\mathbf{q}$  with the radius  $r$  and searches in the buckets  $H(\mathbf{v})$ , to find  $cR$ -near neighbors. Here  $N$  is the number of the database items,  $\rho = \frac{E}{\log(1/g)}$ ,  $M$  is the entropy  $I(h(\mathbf{p})|\mathbf{q}, R)$  where  $\mathbf{p}$  is a random point in  $B(q, R)$ , and  $g$  denotes the upper bound on the probability that two points that are at least distance  $cr$

apart will be hashed to the same bucket. In addition, the search algorithm suggests to build a single hash table with  $K = \frac{N}{\log(1/g)}$  hash bits.

The paper [107] presents the theoretic evidence theoretically guaranteeing the search quality.

#### 4.1.2 LSH forest

LSH forest [9] represents each hash table, built from LSH, using a tree, by pruning subtrees (nodes) that do not contain any database points and also restricting the depth of each leaf node not larger than a threshold. Different from the conventional scheme that finds the candidates from the hash buckets corresponding to the hash codes of the query point, the search algorithm finds the points contained in subtrees over LSH forest having the largest prefix match by a two-phase approach: the first top-down phase descends each LSH tree to find the leaf having the largest prefix match with the hash code of the query, the second bottom-up phase back-tracks each tree from the discovered leaf nodes in the first phase in the largest-prefix-match-first manner to find subtrees having the largest prefix match with the hash code of the query.

#### 4.1.3 Adaptive LSH

The basic idea of adaptive LSH [48] is to select the most relevant hash codes based on the relevance value. The relevance value is computed by accumulating the differences between the projection value and the mean of the corresponding line segment along the projection direction (or equivalently the difference of the projection values along the projection directions and the center of the corresponding bucket).

#### 4.1.4 Multi-probe LSH

The basic idea of multi-probe LSH [91] is to intelligently probe multiple buckets that are likely to contain query results in a hash table, whose hash values may not necessarily be the same to the hash value of the query vector. Given a query  $\mathbf{q}$ , with its hash code denoted by  $g(\mathbf{q}) = (h_1(\mathbf{q}), h_2(\mathbf{q}), \dots, h_K(\mathbf{q}))$ , multi-probe LSH finds a sequence of hash perturbation vector,  $\{\delta_i = \{\delta_{i1}, \delta_{i2}, \dots, \delta_{iK}\}\}$  and sequentially probe the hash buckets  $\{g(\mathbf{q}) + \delta_{o(i)}\}$ . A score, computed as  $\sum_{j=1}^K x_j^2(\delta_{ij})$ , where  $x_j(\delta_{ij})$  is the distance of  $\mathbf{q}$  from the boundary of the slot  $h_j(\mathbf{q}) + \delta_j$ , is used to sort the perturbation vectors, so that the buckets are accessed in order of increasing the scores. The paper [91] also proposes to use the expectation  $E(x_j^2(\delta_{ij}))$ , which is estimated with the assumption that  $\delta_{ij}$  is uniformly distributed in  $[0, r]$  ( $r$  is the width of the hash function used for Euclidean LSH), to replace  $x_j^2(\delta_{ij})$  for sorting the perturbation vectors. Compared with conventional LSH, to achieve the same search quality, multi-probe LSH has a similar time efficiency while reducing the number of hash tables by an order of magnitude.

The posteriori multi-probe LSH algorithm presented in [56] gives a probabilistic interpretation of multi-probe



LSH and presents a probabilistic score, to sort the perturbation vectors. The basic ideas of the probabilistic score computation include the property (likelihood) that the difference of the projections of two vectors along a random projection direction drawn from a Gaussian distribution follows a Gaussian distribution, as well as estimating the distribution (prior) of the neighboring points of a point from the train query points and their neighboring points with assuming that the neighbor points of a query point follow a Gaussian distribution.

#### 4.1.5 Dynamic collision counting for search

The collision counting LSH scheme introduced in [25] uses a base of  $m$  single hash functions to construct dynamic compound hash functions, instead of  $L$  static compound hash functions each of which is composed of  $K$  hash functions. This scheme regards a data vector that collides with the query vector over at least  $K$  hash functions out of the base of  $m$  single hash functions as a good cR-NN candidate. The theoretical analysis shows that such a scheme by appropriately choosing  $m$  and  $K$  can have a guarantee on search quality. In case that there is no data returned for a query (i.e., no data vector has at least  $K$  collisions with the query), a virtual reranking scheme is presented with the essential idea of expanding the window width gradually in the hash function for E2LSH, to increase the collision chance, until finding enough number of data vectors that have at least  $K$  collisions with the query.

#### 4.1.6 Bayesian LSH

The goal of Bayesian LSH [113] is to estimate the probability distribution,  $p(s|M(m, k))$ , of the true similarity  $s$  in the case that  $m$  matches out of  $k$  hash bits for a pair of hash codes  $(g(\mathbf{q}), g(\mathbf{p}))$  of the query vector  $\mathbf{q}$  and a NN candidate  $\mathbf{p}$ , which is denoted by  $M(m, k)$ , and prune the candidate  $\mathbf{p}$  if the probability for the case  $s \geq t$  with  $t$  being a threshold is less than  $\epsilon$ . In addition, if the concentration probability  $P(|s - s^*| \leq \delta | M(m, k)) \geq \lambda$ , or intuitively the true similarity  $s$  under the distribution  $p(s|M(m, k))$  is almost located near the mode,  $s^* = \arg \max_s p(s|M(m, k))$ , the similarity evaluation is early stopped and such a pair is regarded as similar enough, which is an alternative of computing the exact similarity of such a pair in the original space. The paper [113] gives two examples of Bayesian LSH for the Jaccard similarity and the arccos similarity for which  $p(s|M(m, k))$  are instantiated.

#### 4.1.7 Fast LSH

Fast LSH [19] presents two algorithms, ACHash and DHHash, that formulate  $L$   $K$ -bits compound hash functions. ACHash pre-conditions the input vector using a random diagonal matrix and a Hadamard transform, and then applies a sparse Gaussian matrix followed by a rounding. DHHash does the same pre-conditioning process and then applies a random permutation, followed by a random diagonal Gaussian matrix and an

another Hadamard transform. It is shown that it takes only  $O(d \log d + KL)$  for both ACHash and DHHash to compute hash codes instead of  $O(dKL)$ . The algorithms are also extended to the angle-based similarity, where the query time to  $\epsilon$ -approximate the angle between two vectors is reduced from  $O(d/\epsilon^2)$  to  $O(d \log 1/\epsilon + 1/\epsilon^2)$ .

#### 4.1.8 Bi-level LSH

The first level of bi-level LSH [106] uses a random-projection tree to divide the dataset into subgroups with bounded aspect ratios. The second level is an LSH table, which is basically implemented by randomly projecting data points into a low-dimensional space and then partitioning the low-dimensional space into cells. The table is enhanced using a hierarchical structure. The hierarchy, implemented using the space filling Morton curve (a.k.a., the Lebesgue or Z-order curve), is useful when there are not enough candidates retrieved for the multi-probe LSH algorithm. In addition, the  $E_8$  lattice is used for partitioning the low-dimensional space to overcome the curse of dimensionality caused by the basic  $Z^M$  lattice.

## 4.2 SortingKeys-LSH

SortingKeys LSH [88] aims at improving the search scheme of LSH by reducing random I/O operations when retrieving candidate data points. The paper defines a distance measure between compound hash keys to estimate the true distance between data points, and introduces a linear order on the set of compound hash keys. The method sorts all the compound hash keys in ascending order and stores the corresponding data points on disk according to this order, then close data points are likely to be stored locally. During ANN search, a limited number of pages on the disk, which are “close” to the query in terms of the distance defined between compound hash keys, are needed to be accessed for sufficient candidate generation, leading to much shorter response time due to the reduction of random I/O operations, yet with higher search accuracy.

## 4.3 Analysis and Modeling

### 4.3.1 Modeling LSH

The purpose [21] is to model the recall and the selectivity and apply it to determine the optimal parameters, the window size  $r$ , the number of hash functions  $K$  forming the compound hash function, the number of tables  $L$ , and the number of bins  $T$  probed in each table for E2LSH. The recall is defined as the percentage of the true NNs in the retrieved NN candidates. The selectivity is defined as the ratio of the number of the retrieved candidates to the number of the database points. The two factors are formulated as a function of the data distribution, for which the squared  $L_2$  distance is assumed to follow a Gamma distribution that is estimated from the real data. The estimated distributions of 1-NN, 2-NNs, and so on are used to compute the recall and

selectivity. Finally, the optimal parameters are computed to minimize the selectivity with the constraint that the recall is not less than a required value. A similar and more complete analysis for parameter optimization is given in [119]

### 4.3.2 The difficulty of nearest neighbor search

[36] introduces a new measure, relative contrast for analyzing the meaningfulness and difficulty of nearest neighbor search. The relative contrast for a query  $\mathbf{q}$ , given a dataset  $\mathbf{X}$  is defined as  $C_r^q = \frac{E_{\mathbf{x}}[d(\mathbf{q}, \mathbf{x})]}{\min_{\mathbf{x}}(d(\mathbf{q}, \mathbf{x}))}$ . The relative contrast expectation with respect to the queries is given as follows,  $C_r = \frac{E_{\mathbf{x}, \mathbf{q}}[d(\mathbf{q}, \mathbf{x})]}{E_{\mathbf{q}}[\min_{\mathbf{x}}(d(\mathbf{q}, \mathbf{x}))]}$ .

Define a random variable  $R = \sum_{j=1}^d R_j = \sum_{j=1}^d E_{\mathbf{q}}[\|x_j - q_j\|_p^2]$ , and let the mean be  $\mu$  and the variance be  $\sigma^2$ . Define the normalized variance:  $\sigma'^2 = \frac{\sigma^2}{\mu^2}$ . It is shown that if  $\{R_1, R_2, \dots, R_d\}$  are independent and satisfy Lindeberg's condition, the expected relative contrast is approximated as,

$$C_r \approx \frac{1}{[1 + \phi^{-1}(\frac{1}{N} + \phi(\frac{-1}{\sigma'}))\sigma']^{\frac{1}{p}}}, \quad (20)$$

where  $N$  is the number of database points,  $\phi(\cdot)$  is the cumulative density function of standard Gaussian,  $\sigma'$  is the normalized standard deviation, and  $p$  is the distance metric norm. It can also be generalized to the relative contrast for the  $k$ th nearest neighbor,

$$C_r^k = \frac{E_{\mathbf{x}, \mathbf{q}}[d(\mathbf{q}, \mathbf{x})]}{E_{\mathbf{q}}[k\text{-min}_{\mathbf{x}}(d(\mathbf{q}, \mathbf{x}))]} \approx \frac{1}{[1 + \phi^{-1}(\frac{k}{N} + \phi(\frac{-1}{\sigma'}))\sigma']^{\frac{1}{p}}}, \quad (21)$$

where  $k\text{-min}_{\mathbf{x}}(d(\mathbf{q}, \mathbf{x}))$  is the distance of the query to the  $k$ th nearest neighbor.

Given the approximate relative contrast, it is clear how the data dimensionality  $d$ , the database size  $N$ , the metric norm  $p$ , and the sparsity of the data vector (determining  $\sigma'$ ) influence the relative contrast.

It is shown that LSH, under the  $\ell_p$ -norm distance, can find the exact nearest neighbor with probability  $1 - \delta$  by returning  $O(\log \frac{1}{\delta} n^{g(C_r)})$  candidate points, where  $g(C_r)$  is a function monotonically decreasing with  $C_r$ , and that, in the context of linear hashing  $\text{sign}(\mathbf{w}^T \mathbf{x} + b)$ , the optimal projection that maximizes the relative contrast is  $\mathbf{w}^* = \arg \max_{\mathbf{w}} \frac{\mathbf{w}^T \Sigma_x \mathbf{w}}{\mathbf{w}^T \mathbf{S}_{NN} \mathbf{w}}$ , where  $\Sigma_x = \frac{1}{N} \sum_{i=1}^N \mathbf{x}_i \mathbf{x}_i^T$  and  $\mathbf{S}_{NN} = E_{\mathbf{q}}[(\mathbf{q} - \text{NN}(\mathbf{q}))(\mathbf{q} - \text{NN}(\mathbf{q}))^T]$ , subject to  $\mathbf{S}_{NN} = \mathbf{I}$ ,  $\mathbf{w}^* = \arg \max_{\mathbf{w}} \mathbf{w}^T \Sigma_x \mathbf{w}$ .

The LSH scheme has very nice theoretic properties. However, as the hash functions are data-independent, the practical performance is not as good as expected in certain applications. Therefore, there are a lot of followups that learn hash functions from the data.

## 5 LEARNING TO HASH: HAMMING EMBEDDING AND EXTENSIONS

Learning to hash is a task of learning a compound hash function,  $\mathbf{y} = \mathbf{h}(\mathbf{x})$ , mapping an input item  $\mathbf{x}$

to a compact code  $\mathbf{y}$ , such that the nearest neighbor search in the coding space is efficient and the result is an effective approximation of the true nearest search result in the input space. An instance of the learning-to-hash approach includes three elements: hash function, similarity measure in the coding space, and optimization criterion. Here The similarity in similarity measure is a general concept, and may mean distance or other forms of similarity.

**Hash function.** The hash function can be based on linear projection, spherical function, kernels, and neural network, even a non-parametric function, and so on. One popular hash function is a linear hash function:  $\mathbf{y} = \text{sign}(\mathbf{w}^T \mathbf{x}) \in \{0, 1\}$ , where  $\text{sign}(\mathbf{w}^T \mathbf{x}) = 1$  if  $\mathbf{w}^T \mathbf{x} \geq 0$  and  $\text{sign}(\mathbf{w}^T \mathbf{x}) = 0$  otherwise. Another widely-used hash function is a function based on nearest vector assignment:  $\mathbf{y} = \arg \min_{k \in \{1, \dots, K\}} \|\mathbf{x} - \mathbf{c}_k\|_2 \in \mathbb{Z}$ , where  $\{\mathbf{c}_1, \dots, \mathbf{c}_K\}$  is a set of centers, computed by some algorithm, e.g.,  $K$ -means.

The choice of hash function types influences the efficiency of computing hash codes and the flexibility of the hash codes, or the flexibility of partitioning the space. The optimization of hash function parameters is dependent to both distance measure and distance preserving.

**Similarity measure.** There are two main distance measure schemes in the coding space. Hamming distance with its variants, and Euclidean distance. Hamming distance is widely used when the hashing function maps the data point into a Hamming code  $\mathbf{y}$  for which each entry is either 1 or 0, and is defined as the number of bits at which the corresponding values are different. There are some other variants, such as weighted Hamming distance, distance table lookup, and so on. Euclidean distance is used in the approaches based on nearest vector assignment and evaluated between the vectors corresponding to the hash codes, i.e., the nearest vectors assigned to the data vectors, which is efficiently computed by looking up a precomputed distance table. There is a variant, asymmetric Euclidean distance, for which only one vector is approximated by its nearest vector while the other vector is not approximated. There are also some works learning a distance table between hash codes by assuming the hash codes are already given.

**Optimization criterion.** The approximate nearest neighbor search result is evaluated by comparing it with the true search result, that is the result according to the distance computed in the input space. Most similarity preserving criteria design various forms as the surrogate of such an evaluation.

The straightforward form is to directly compare the order of the ANN search result with that of the true result (using the reference data points as queries), which called the order-preserving criterion. The empirical results show that the ANN search result usually has higher probability to approach the true search result if the distance computed in the coding space accurately approximates the distance computed in the input space.

TABLE 1  
Hash functions

type	abbreviation
linear	LI
bilinear	BILI
Laplacian eigenfunction	LE
kernel	KE
quantizer	QU
1D quantizer	OQ
spline	SP
neural network	NN
spherical function	SF
classifier	CL

TABLE 2  
Distance measures in the coding space

type	abbreviation
Hamming distance	HD
normalized Hamming distance	NHD
asymmetric Hamming distance	AHD
weighted Hamming distance	WHD
query-dependent weighted Hamming distance	QWHD
normalized Hamming affinity	NHA
Manhattan	MD
asymmetric Euclidean distance	AED
symmetric Euclidean distance	SED
lower bound	LB

This motivates the so-called similarity alignment criterion, which directly minimizes the differences between the distances (similarities) computed in the coding and input space. An alternative surrogate is coding consistent hashing, which penalizes the larger distances in the coding space but with the larger similarities in the input space (called coding consistent to similarity, shorted as coding consistent as a major of algorithms use it) and encourages the smaller (larger) distances in the coding space but with the smaller (larger) distances in the input space (called coding consistent to distance). One typical approach, the space partitioning approach, assumes that space partitioning has already implicitly preserved the similarity to some degree.

Besides similarity preserving, another widely-used criterion is coding balance, which means that the reference vectors should be uniformly distributed in each bucket (corresponding to a hash code). Other related criteria, such as bit balance, bit independence, search efficiency, and so on, are essentially (degraded) forms of coding balance.

In the following, we review Hamming bedding based hashing algorithms. Table 4 presents the summary of the algorithms reviewed from Section 5.1 to Section 5.5, with some concepts given in Tables 1, 1 and 3.

## 5.1 Coding Consistent Hashing

Coding consistent hashing refers to a category of hashing functions based on minimizing the similarity weighted distance,  $s_{ij}d(\mathbf{y}_i, \mathbf{y}_j)$  (and possibly maximizing  $d_{ij}d(\mathbf{y}_i, \mathbf{y}_j)$ ), to formulate the objective function. Here,

TABLE 3  
Optimization criterion.

type	abbreviation
Hamming embedding	
coding consistent	CC
coding consistent to distance	CCD
code balance	CB
bit balance	BB
bit uncorrelation	BU
projection uncorrelation	PU
mutual information maximization	MIM
minimizing differences between distances	MDD
minimizing differences between similarities	MDS
minimizing differences between similarity distribution	MDSD
hinge-like loss	HL
rank order loss	ROL
triplet loss	TL
classification error	CE
space partitioning	SP
complementary partitioning	CP
pair-wise bit balance	PBB
maximum margin	MM
Quantization	
bit allocation	BA
quantization error	QE
equal variance	EV
maximum cosine similarity	MCS

$s_{ij}$  is the similarity between  $\mathbf{x}_i$  and  $\mathbf{x}_j$  computed from the input space or given from the semantic meaning.

### 5.1.1 Spectral hashing

Spectral hashing [135], the pioneering coding consistency hashing algorithm, aims to find an easy-evaluated hash function so that (1) similar items are mapped to similar hash codes based on the Hamming distance (coding consistency) and (2) a small number of hash bits are required. The second requirement is a form similar to coding balance, which is transformed to two requirements: bit balance and bit uncorrelation. The balance means that each bit has around 50% chance of being 1 or 0 (-1). The uncorrelation means that different bits are uncorrelated.

Let  $\{\mathbf{y}_n\}_{n=1}^N$  be the hash codes of the  $N$  data items, each  $\mathbf{y}_n$  be a binary vector of length  $M$ . Let  $s_{ij}$  be the similarity that correlates with the Euclidean distance. The formulation is given as follows:

$$\min_{\mathbf{Y}} \text{Trace}(\mathbf{Y}(\mathbf{D} - \mathbf{S})\mathbf{Y}^T) \quad (22)$$

$$\text{s. t. } \mathbf{Y}\mathbf{1} = \mathbf{0} \quad (23)$$

$$\mathbf{Y}\mathbf{Y}^T = \mathbf{I} \quad (24)$$

$$y_{im} \in \{-1, 1\}, \quad (25)$$

where  $\mathbf{Y} = [\mathbf{y}_1\mathbf{y}_2 \cdots \mathbf{y}_N]$ ,  $\mathbf{S}$  is a matrix  $[s_{ij}]$  of size  $N \times N$ ,  $\mathbf{D}$  is a diagonal matrix  $\text{Diag}(d_{11}, \cdots, d_{NN})$ , and  $d_{nn} = \sum_{i=1}^N s_{ni}$ .  $\mathbf{D} - \mathbf{S}$  is called Laplacian matrix and  $\text{Trace}(\mathbf{Y}(\mathbf{D} - \mathbf{S})\mathbf{Y}^T) = \sum_{i=1}^N \sum_{j=1}^N w_{ij} \|\mathbf{y}_i - \mathbf{y}_j\|_2^2$ .  $\mathbf{Y}\mathbf{1} = \mathbf{0}$  corresponds to the bit balance requirement.  $\mathbf{Y}\mathbf{Y}^T = \mathbf{I}$  corresponds to the bit uncorrelation requirement.

Rather than solving the problem Equation 25 directly, a simple approximate solution with the assumption of

TABLE 4

A summary of hashing algorithms. \* means that hash function does not explicitly rely on the distance measure in the coding space. S = semantic similarity. E = Euclidean distance. sim. = similarity. dist. = distance.

method	input sim.	hash function	dist. measure	optimization criteria
spectral hashing [135]	E	LE	HD	CC + BB + BU
kernelized spectral hashing [37]	S, E	KE	HD	CC + BB + BU
Hypergraph spectral hashing [153], [89]	S	CL	HD	CC + BB + BU
Topology preserving hashing [145]	E	LI	HD	CC + CCD + BB + BU
hashing with graphs [83]	S	KE	HD	CC + BB
ICA Hashing [35]	E	LI, KE	HD	CC + BB + BU + MIM
Semi-supervised hashing [125], [126], [127]	S, E	LI	HD	CC + BB + PU
LDA hash [122]	S	LI	HD	CC + PU
binary reconstructive embedding [63]	E	LI, KE	HD	MDD
supervised hashing with kernels [82]	E, S	LI, KE	HD	MDS
spec hashing [78]	S	CL	HD	MDS
bilinear hyperplane hashing [84]	ACS	BILI	HD	MDS
minimal loss hashing [101]	E, S	LI	HD	HL
order preserving hashing [130]	E	LI	HD	ROL
Triplet loss hashing [103]	E, S	Any	HD, AHD	TL
listwise supervision hashing [128]	E, S	LI	HD	TL
Similarity sensitive coding (SSC) [114]	S	CL	WHD	CE
parameter sensitive hashing [115]	S	CL	WHD	CE
column generation hashing [75]	S	CL	WHD	CE
complementary projection hashing [55]*	E	LI, KE	HD	SP + CP + PBB
label-regularized maximum margin hashing [96]*	E, S	KE	HD	SP + MM + BB
Random maximum margin hashing [57]*	E	LI, KE	HD	SP + MM + BB
spherical hashing [38]*	E	SF	NHD	SP + PBB
density sensitive hashing [79]*	E	LI	HD	SP + BB
multi-dimensional spectral hashing [134]	E	LE	WHD	CC + BB + BU
Weighted hashing [131]	E	LI	WHD	CC + BB + BU
Query-adaptive bit weights [53], [54]	S	LI (all)	QWHD	CE
Query adaptive hashing [81]	S	LI	QWHD	CE

uniform data distribution is presented in [135]. The algorithm is given as follows:

- 1) Find the principal components of the  $N$   $d$ -dimensional reference data items using principal component analysis (PCA).
- 2) Compute the  $M$  1D Laplacian eigenfunctions with the smallest eigenvalues along each PCA direction.
- 3) Pick the  $M$  eigenfunctions with the smallest eigenvalues among  $Md$  eigenfunctions.
- 4) Threshold the eigenfunction at zero, obtaining the binary codes.

The 1D Laplacian eigenfunction for the case of uniform distribution on  $[r_l, r_r]$  is  $\phi_f(x) = \sin(\frac{\pi}{2} + \frac{f\pi}{r_r - r_l}x)$  and the corresponding eigenvalue is  $\lambda_f = 1 - \exp(-\frac{\epsilon^2}{2}|\frac{f\pi}{r_r - r_l}|^2)$ , where  $f = 1, 2, \dots$  is the frequency and  $\epsilon$  is a fixed small value.

The assumption that the data is uniformly distributed does not hold in real cases, resulting in that the performance of spectral hashing is deteriorated. Second, the eigenvalue monotonously increases with respect to  $|\frac{f}{r_r - r_l}|^2$ , which means that the PCA direction with a large spread ( $|r_r - r_l|$ ) and a lower frequency ( $f$ ) is preferred. This means that there might be more than one eigenfunctions picked along a single PCA direction, which breaks the uncorrelation requirement, and thus the performance is influenced. Last, thresholding the eigenfunction  $\phi_f(x) = \sin(\frac{\pi}{2} + \frac{f\pi}{r_r - r_l}x)$  at zero leads to that near points are mapped to different values and even far points are mapped to the same value. It turns out

that the hamming distance is not well consistent to the Euclidean distance.

In the case that the spreads along the top  $M$  PCA direction are the same, the spectral hashing algorithm actually partitions each direction into two parts using the median (due to the bit balance requirement) as the threshold. It is noted that, in the case of uniform distributions, the solution is equivalent to thresholding at the mean value. In the case that the true data distribution is a multi-dimensional isotropic Gaussian distribution, it is equivalent to iterative quantization [30], [31] and isotropic hashing [60].

Principal component hashing [93] also uses the principal direction to formulate the hash function. Specifically, it partitions the data points into  $K$  buckets so that the projected points along the principal direction are uniformly distributed in the  $K$  buckets. In addition, bucket overlapping is adopted to deal with the boundary issue (neighboring points around the partitioning position are assigned to different buckets). Different from spectral hashing, principal component hashing aims at constructing hash tables rather than compact codes.

The approach in [74], spectral hashing with semantically consistent graph first learns a linear transform matrix such that the similarities computed over the transformed space is consistent to the semantic similarity as well as the Euclidean distance-based similarity, then applies spectral hashing to learn hash codes.

### 5.1.2 Kernelized spectral hashing

The approach introduced in [37] extends spectral hashing by explicitly defining the hash function using kernels. The  $m$ th hash function is given as follows,

$$y_m = h_m(\mathbf{x}) \quad (26)$$

$$= \text{sign}\left(\sum_{t=1}^{T_m} w_{mt} K(\mathbf{s}_{mt}, \mathbf{x}) - b_m\right) \quad (27)$$

$$= \text{sign}\left(\sum_{t=1}^{T_m} w_{mt} \langle \phi(\mathbf{s}_{mt}), \phi(\mathbf{x}) \rangle - b_m\right) \quad (28)$$

$$= \text{sign}(\langle \mathbf{v}_m, \phi(\mathbf{x}) \rangle - b_m). \quad (29)$$

Here  $\{\mathbf{s}_{mt}\}_{t=1}^{T_m}$  is the set of randomly-sampled anchor items for forming the hash function, and its size  $T_m$  is usually the same for all  $M$  hash functions.  $K(\cdot, \cdot)$  is a kernel function, and  $\phi(\cdot)$  is its corresponding mapping function.  $\mathbf{v}_m = [w_{m1}\phi(\mathbf{s}_{m1}) \cdots w_{mT_m}\phi(\mathbf{s}_{mT_m})]^T$ .

The objective function is written as:

$$\min_{\{\mathbf{v}_m\}} \text{Trace}(\mathbf{Y}(\mathbf{D} - \mathbf{S})\mathbf{Y}^T) + \sum_{m=1}^M \|\mathbf{v}_m\|_2^2, \quad (30)$$

The constraints are the same to those of spectral hashing, and differently the hash function is given in Equation 29. To efficiently solve the problem, the sparse similarity matrix  $\mathbf{W}$  and the Nyström algorithm are used to reduce the computation cost.

### 5.1.3 Hypergraph spectral hashing

Hypergraph spectral hashing [153], [89] extends spectral hashing from an ordinary (pair-wise) graph to a hypergraph (multi-wise graph), formulates the problem using the hypergraph Laplacian (replace the graph Laplacian [135], [134]) to form the objective function, with the same constraints to spectral hashing. The algorithm in [153], [89] solves the optimization problem, by relaxing the binary constraint eigen-decomposing the the hypergraph Laplacian matrix, and thresholding the eigenvectors at zero. It computes the code for an out-of-sample vector, by regarding each hash bit as a class label of the data vector and learning a classifier for each bit. In essence, this approach is a two-step approach that separates the optimization of coding and hash functions. The remaining challenge lies in how to extend the algorithm to large scale because the eigen-decomposition step is quite time-consuming.

### 5.1.4 Sparse spectral hashing

Sparse spectral hashing [116] combines sparse principal component analysis (Sparse PCA) and Boosting Similarity Sensitive Hashing (Boosting SSC) into traditional spectral hashing. The problem is formulated as as thresholding a subset of eigenvectors of the Laplacian graph by constraining the number of nonzero features. The convex relaxation makes the learnt codes globally optimal and the out-of-sample extension is achieved by learning the eigenfunctions.

### 5.1.5 ICA hashing

The idea of independent component analysis (ICA) Hashing [35] starts from coding balance. Intuitively coding balance means that the average number of data items mapped to each hash code is the same. The coding balance requirement is formulated as maximizing the entropy  $\text{entropy}(y_1, y_2, \dots, y_M)$ , and subsequently formulated as bit balance:  $E(y_m) = 0$  and mutual information minimization:  $I(y_1, y_2, \dots, y_M)$ .

The approach approximates the mutual information using the scheme similar to the one widely used independent component analysis. The mutual information is relaxed:  $I(y_1, y_2, \dots, y_M) = I(\mathbf{w}_1^T \mathbf{x}, \mathbf{w}_2^T \mathbf{x}, \dots, \mathbf{w}_M^T \mathbf{x})$  and is approximated as maximizing

$$\sum_{m=1}^M \|c - \frac{1}{N} \sum_{n=1}^N g(\mathbf{W}^T \mathbf{x}_n)\|_2^2, \quad (31)$$

under the constraint of whiten condition (which can be derived from bit uncorrelation),  $\mathbf{w}_i^T E(\mathbf{x}\mathbf{x}^T)\mathbf{w}_j = \delta[i = j]$ ,  $c$  is a constant,  $g(u)$  is some non-quadratic functions, such that  $g(u) = -\exp(-\frac{u^2}{2})$  or  $g(u) = \log \cosh(u)$ .

The whole objective function together preserving the similarities as done in spectral hashing is written as follows,

$$\max_{\mathbf{W}} \sum_{m=1}^M \|c - \frac{1}{N} \sum_{n=1}^N g(\mathbf{W}^T \mathbf{x}_n)\|_2^2 \quad (32)$$

$$s.t. \mathbf{w}_i^T E(\mathbf{x}\mathbf{x}^T)\mathbf{w}_j = \delta[i = j] \quad (33)$$

$$\text{trace}(\mathbf{W}^T \mathbf{\Sigma} \mathbf{W}) \leq \eta. \quad (34)$$

The paper [35] also presents a kernelized version by using the kernel hash function.

### 5.1.6 Semi-supervised hashing

Semi-supervised hashing [125], [126], [127] extends spectral hashing into the semi-supervised case, in which some pairs of data items are labeled as belonging to the same semantic concept, some pairs are labeled as belonging to different semantic concepts. Specifically, the similarity weight  $s_{ij}$  is assigned to 1 and  $-1$  if the corresponding pair of data items,  $(\mathbf{x}_i, \mathbf{x}_j)$ , belong to the same concept, and different concepts, and 0 if no labeling information is given. This leads to a formulation maximizing the empirical fitness,

$$\sum_{i,j \in \{1, \dots, N\}} s_{ij} \sum_{m=1}^M h_m(\mathbf{x}_i) h_m(\mathbf{x}_j), \quad (35)$$

where  $h_k(\cdot) \in \{1, -1\}$ . It is easily shown that this objective function 35 is equivalent to minimizing  $\sum_{i,j \in \{1, \dots, N\}} s_{ij} \sum_{m=1}^M \frac{(h_m(\mathbf{x}_i) - h_m(\mathbf{x}_j))^2}{2} = \frac{1}{2} \sum_{i,j \in \{1, \dots, N\}} s_{ij} \|\mathbf{y}_i - \mathbf{y}_j\|_2^2$ .

In addition, the bit balance requirement (over each hash bit) is explained as maximizing the variance over the hash bits. Assuming the hash function is a sign function,  $h(\mathbf{x}) = \text{sign}(\mathbf{w}^T \mathbf{x})$ , variance maximization is

relaxed as maximizing the variance of the projected data  $\mathbf{w}^T \mathbf{x}$ . In summary, the formulation is given as

$$\text{trace}[\mathbf{W}^T \mathbf{X}_l \mathbf{S} \mathbf{X}_l^T \mathbf{W}] + \eta \text{trace}[\mathbf{W}^T \mathbf{X} \mathbf{X}^T \mathbf{W}], \quad (36)$$

where  $\mathbf{S}$  is the similarity matrix over the labeled data  $\mathbf{X}_l$ ,  $\mathbf{X}$  is the data matrix with each column corresponding to one data item, and  $\eta$  is a balance variable.

In the case that  $\mathbf{W}$  is an orthogonal matrix (the columns are orthogonal to each other,  $\mathbf{W}^T \mathbf{W} = \mathbf{I}$ , which is called projection uncorrelation) (equivalent to the independence requirement in spectral hashing), it is solved by eigen-decomposition. The authors present a sequential projection learning algorithm by embedding  $\mathbf{W}^T \mathbf{W} = \mathbf{I}$  into the objective function as a soft constraint

$$\begin{aligned} & \text{trace}[\mathbf{W}^T \mathbf{X}_l \mathbf{S} \mathbf{X}_l^T \mathbf{W}] + \eta \text{trace}[\mathbf{W}^T \mathbf{X} \mathbf{X}^T \mathbf{W}] \\ & + \rho \|\mathbf{W}^T \mathbf{W} - \mathbf{I}\|_F^2, \end{aligned} \quad (37)$$

where  $\rho$  is a tradeoff variable. An extension of semi-supervised hashing to nonlinear hash functions is presented in [136], where the kernel hash function,  $h(\mathbf{x}) = \text{sign}(\sum_{t=1}^T w_t \langle \mathbf{x}, \phi(\mathbf{s}_t) \rangle - b)$ , is used.

### 5.1.7 LDA hash

LDA (linear discriminant analysis) hash [122] aims to find the binary codes by minimizing the following objective function,

$$\alpha \mathbb{E}\{\|\mathbf{y}_i - \mathbf{y}_j\|^2 | (i, j) \in \mathcal{P}\} - \mathbb{E}\{\|\mathbf{y}_i - \mathbf{y}_j\|^2 | (i, j) \in \mathcal{N}\}, \quad (38)$$

where  $\mathbf{y} = \text{sign}(\mathbf{W}^T \mathbf{x} + \mathbf{b})$ ,  $\mathcal{P}$  is the set of positive (similar) pairs, and  $\mathcal{N}$  is the set of negative (dissimilar) pairs.

LDA hash consists of two steps: (1) finding the projection matrix that best discriminates the nearer pairs from the farther pairs, which is a form of coding consistency, and (2) finding the threshold to generate binary hash codes. The first step relaxes the problem, by removing the sign and minimizes a related function,

$$\begin{aligned} & \alpha \mathbb{E}\{\|\mathbf{W}^T \mathbf{x}_i - \mathbf{W}^T \mathbf{x}_j\|^2 | (i, j) \in \mathcal{P}\} \\ & - \mathbb{E}\{\|\mathbf{W}^T \mathbf{x}_i - \mathbf{W}^T \mathbf{x}_j\|^2 | (i, j) \in \mathcal{N}\}. \end{aligned} \quad (39)$$

This formulation is then transformed to an equivalent form,

$$\alpha \text{trace}\{\mathbf{W}^T \boldsymbol{\Sigma}_p \mathbf{W}\} - \text{trace}\{\mathbf{W}^T \boldsymbol{\Sigma}_n \mathbf{W}\}, \quad (40)$$

where  $\boldsymbol{\Sigma}_p = \mathbb{E}\{(\mathbf{x}_i - \mathbf{x}_j)(\mathbf{x}_i - \mathbf{x}_j)^T | (i, j) \in \mathcal{P}\}$  and  $\boldsymbol{\Sigma}_n = \mathbb{E}\{(\mathbf{x}_i - \mathbf{x}_j)(\mathbf{x}_i - \mathbf{x}_j)^T | (i, j) \in \mathcal{N}\}$ . There are two solutions given in [122]: minimizing  $\text{trace}\{\mathbf{W}^T \boldsymbol{\Sigma}_p \boldsymbol{\Sigma}_n^{-1} \mathbf{W}\}$ , which does not need to specify  $\alpha$ , and minimizing  $\text{trace}\{\mathbf{W}^T (\alpha \boldsymbol{\Sigma}_p - \boldsymbol{\Sigma}_n)\}$ .

The second step aims to find the threshold by minimizing

$$\alpha \mathbb{E}\{\text{sign}\{\mathbf{W}^T \mathbf{x}_i - \mathbf{b}\} - \text{sign}\{\mathbf{W}^T \mathbf{x}_j - \mathbf{b}\} | (i, j) \in \mathcal{P}\} \quad (41)$$

$$- \mathbb{E}\{\text{sign}\{\mathbf{W}^T \mathbf{x}_i - \mathbf{b}\} - \text{sign}\{\mathbf{W}^T \mathbf{x}_j - \mathbf{b}\} | (i, j) \in \mathcal{N}\}, \quad (42)$$

which is then decomposed into  $K$  subproblems each of which finds  $b_k$  for each hash function  $\mathbf{w}_k^T \mathbf{x} - b_k$ . The subproblem can be exactly solved using simple 1D search.

### 5.1.8 Topology preserving hashing

Topology preserving hashing [145] formulates the hashing problem by considering two forms of coding consistency: preserving the neighborhood ranking and preserving the data topology.

The first coding consistency form is presented as a maximization problem,

$$\frac{1}{2} \sum_{i,j,s,t} \text{sign}(d_{i,j}^o - d_{s,t}^o) \text{sign}(d_{i,j}^h - d_{s,t}^h) \quad (43)$$

$$\approx \frac{1}{2} \sum_{i,j,s,t} (d_{i,j}^o - d_{s,t}^o)(d_{i,j}^h - d_{s,t}^h) \quad (44)$$

where  $d^o$  and  $d^h$  are the distances in the original space and the Hamming space. This ranking preserving formulation, based on the rearrangement inequality, is transformed to

$$\frac{1}{2} \sum_{i,j} d_{i,j}^o d_{i,j}^h \quad (45)$$

$$= \frac{1}{2} \sum_{i,j} d_{i,j}^o \|\mathbf{y}_i - \mathbf{y}_j\|_2^2 \quad (46)$$

$$= \text{trace}(\mathbf{Y} \mathbf{L}_t \mathbf{Y}^T), \quad (47)$$

where  $\mathbf{L}_t = \mathbf{D}_t - \mathbf{S}_t$ ,  $\mathbf{D}_t = \text{diag}(\mathbf{S}_t \mathbf{1})$  and  $s_t(i, j) = f(d_{ij}^o)$  with  $f(\cdot)$  is monotonically non-decreasing.

Data topology preserving is formulated in a way similar to spectral hashing, by minimizing the following function

$$\frac{1}{2} \sum_{ij} s_{ij} \|\mathbf{y}_i - \mathbf{y}_j\|_2^2 \quad (48)$$

$$= \text{trace}(\mathbf{Y} \mathbf{L}_s \mathbf{Y}^T), \quad (49)$$

where  $\mathbf{L}_s = \mathbf{D}_s - \mathbf{S}_s$ ,  $\mathbf{D}_s = \text{diag}(\mathbf{S}_s \mathbf{1})$ , and  $s_s(i, j)$  is the similarity between  $\mathbf{x}_i$  and  $\mathbf{x}_j$  in the original space.

Assume the hash function is in the form of  $\text{sign}(\mathbf{W}^T \mathbf{x})$  (the following formulation can also be extended to the kernel hash function), the overall formulation, by a relaxation step  $\text{sign}(\mathbf{W}^T \mathbf{x}) \approx \mathbf{W}^T \mathbf{x}$ , is given as follows,

$$\max \frac{\text{trace}(\mathbf{W}^T \mathbf{X} (\mathbf{L}_t + \alpha \mathbf{I}) \mathbf{X}^T \mathbf{W})}{\text{trace}(\mathbf{W}^T \mathbf{X} \mathbf{L}_s \mathbf{X}^T \mathbf{W})}, \quad (50)$$

where  $\alpha \mathbf{I}$  introduces a regularization term,  $\text{trace}(\mathbf{W}^T \mathbf{X} \mathbf{X}^T \mathbf{W})$ , similar to the bit balance condition in semi-supervised hashing [125], [126], [127].

### 5.1.9 Hashing with graphs

The key ideas of hashing with graphs [83] consist of using the anchor graph to approximate the neighborhood graph, (accordingly using the graph Laplacian over the anchor graph to approximate the graph Laplacian of the original graph) for fast computing the eigenvectors and

using a hierarchical hashing to address the boundary issue for which the points around the hash plane are assigned different hash bits. The first idea aims to solve the same problem in spectral hashing [135], present an approximate solution using the anchor graph rather than the PCA-based solution with the assumption that the data points are uniformly distributed. The second idea breaks the independence constraint over hash bits.

Compressed hashing [80] borrows the idea about anchor graph in [83] uses the anchors to generate a sparse representation of data items by computing the kernels with the nearest anchors and normalizing it so that the summation is 1. Then it uses  $M$  random projections and the median of the projections of the sparse projections along each random projection as the bias to generate the hash functions.

## 5.2 Similarity Alignment Hashing

Similarity alignment hashing is a category of hashing algorithms that directly compare the similarities (distances) computed from the input space and the coding space. In addition, the approach aligning the distance distribution is also discussed in this section. Other algorithms, such as quantization, can also be interpreted as similarity alignment, and for clarity, are described in separate paragraphs.

### 5.2.1 Binary reconstructive embedding

The key idea of binary reconstructive embedding [63] is to learn the hash codes such that the difference between the Euclidean distance in the input space and the Hamming distance in the hash codes is minimized. The objective function is formulated as follows,

$$\min \sum_{(i,j) \in \mathcal{N}} \left( \frac{1}{2} \|\mathbf{x}_i - \mathbf{x}_j\|_f^2 - \frac{1}{M} \|\mathbf{y}_i - \mathbf{y}_j\|_2^2 \right)^2. \quad (51)$$

The set  $\mathcal{N}$  is composed of point pairs, which includes both the nearest neighbors and other pairs.

The hash function is parameterized as:

$$y_{nm} = h_m(\mathbf{x}) = \text{sign} \left( \sum_{t=1}^{T_m} w_{mt} K(\mathbf{s}_{mt}, \mathbf{x}) \right), \quad (52)$$

where  $\{\mathbf{s}_{mt}\}_{t=1}^{T_m}$  are sampled data items forming the hashing function  $h_m(\cdot) \in \{h_1(\cdot), \dots, h_M(\cdot)\}$ ,  $K(\cdot, \cdot)$  is a kernel function, and  $\{w_{mt}\}$  are the weights to be learnt.

Instead of relaxing the sign function to a continuous function, an alternative optimization scheme is presented in [63]: fixing all but one weight  $w_{mt}$  and optimizing the problem 51 with respect to  $w_{mt}$ . It is shown that an exact, optimal update to this weight  $w_{mt}$  (fixing all the other weights) can be achieved in time  $O(N \log N + n|\mathcal{N}|)$ .

### 5.2.2 Supervised hashing with kernels

The idea of supervised hashing with kernels [82] consists of two aspects: (1) using the kernels to form the hash functions, which is similar to binary reconstructive

embedding [63], and (2) minimizing the differences between the Hamming affinity over the hash codes and the similarity over the data items, which has two types, similar ( $s = 1$ ) or dissimilar ( $s = -1$ ) e.g., given by the Euclidean distance or the labeling information.

The hash function is given as follows,

$$y_{nm} = h_m(\mathbf{x}_n) = \text{sign} \left( \sum_{t=1}^{T_m} w_{mt} K(\mathbf{s}_{mt}, \mathbf{x}) + b \right), \quad (53)$$

where  $b$  is the bias. The objective function is given as the following,

$$\min \sum_{(i,j) \in \mathcal{L}} (s_{ij} - \text{affinity}(\mathbf{y}_i, \mathbf{y}_j))^2, \quad (54)$$

where  $\mathcal{L}$  is the set of labeled pairs,  $\text{affinity}(\mathbf{y}_i, \mathbf{y}_j) = M - \|\mathbf{y}_i - \mathbf{y}_j\|_1$  is the Hamming affinity, and  $\mathbf{y} \in \{1, -1\}^M$ .

Kernel reconstructive hashing [141] extends this technique using a normalized Gaussian kernel similarity.

### 5.2.3 Spec hashing

The idea of spec hashing [78] is to view each pair of data items as a sample and their (normalized) similarity as the probability, and to find the hash functions so that the probability distributions from the input space and the Hamming space are well aligned. Let  $s_{ij}^i$  be the normalized similarity ( $\sum_{ij} s_{ij}^i = 1$ ) given in the input space, and  $s_{ij}^h$  be the normalized similarity computed in the Hamming space,  $s_{ij}^h = \frac{1}{Z} \exp(-\lambda \text{dist}_h(i, j))$ , where  $Z$  is a normalization variable  $Z = \sum_{ij} \exp(-\lambda \text{dist}_h(i, j))$ . Then, the objective function is given as follows,

$$\begin{aligned} \min \quad & \text{KL}(\{s_{ij}^i\} \| \{s_{ij}^h\}) \\ & = - \sum_{ij} \lambda s_{ij}^i \log s_{ij}^h \\ & = \lambda \sum_{ij} s_{ij}^i \text{dist}_h(i, j) + \log \sum_{ij} \exp(-\lambda \text{dist}_h(i, j)). \end{aligned} \quad (56)$$

Supervised binary hash code learning [24] presents a supervised binary hash code learning algorithm using Jensen Shannon Divergence which is derived from minimizing an upper bound of the probability of Bayes decision errors.

### 5.2.4 Bilinear hyperplane hashing

Bilinear hyperplane hashing [84] transforms the database vector (the normal of the query hyperplane) into a high-dimensional vector,

$$\bar{\mathbf{a}} = \text{vec}(\mathbf{a}\mathbf{a}^T) [a_1^2, a_1 a_2, \dots, a_1 a_d, a_2 a_1, a_2^2, a_2 a_3, \dots, a_d^2]. \quad (57)$$

The bilinear hyperplane hashing family is defined as follows,

$$h(\mathbf{z}) = \begin{cases} \text{sign}(\mathbf{u}^T \mathbf{z} \mathbf{z}^T \mathbf{v}) & \text{if } \mathbf{z} \text{ is a database vector} \\ \text{sign}(-\mathbf{u}^T \mathbf{z} \mathbf{z}^T \mathbf{v}) & \text{if } \mathbf{z} \text{ is a hyperplane normal.} \end{cases} \quad (58)$$

Here  $\mathbf{u}$  and  $\mathbf{v}$  are sampled independently from a standard Gaussian distribution. It is shown to be  $r, r(1 + \epsilon), \frac{1}{2} - \frac{2r}{\pi^2}, \frac{1}{2} - \frac{2r(1+\epsilon)}{\pi^2}$ -sensitive to the angle distance  $d_\theta(\mathbf{x}, \mathbf{n}) = (\theta_{\mathbf{x}, \mathbf{n}} - \frac{\pi}{2})^2$ , where  $r, \epsilon > 0$ .

Rather than randomly drawn,  $\mathbf{u}$  and  $\mathbf{u}$  can be also learnt according to the similarity information. A formulation is given in [84] as the below,

$$\min_{\{\mathbf{u}_k, \mathbf{v}_k\}_{k=1}^K} \left\| \frac{1}{K} \mathbf{Y}^T \mathbf{Y} - \mathbf{S} \right\|, \quad (59)$$

where  $\mathbf{Y} = [\mathbf{y}_1, \mathbf{y}_2, \dots, \mathbf{y}_N]$  and  $\mathbf{S}$  is the similarity matrix,

$$s_{ij} = \begin{cases} 1 & \text{if } \cos(\theta_{\mathbf{x}_i, \mathbf{x}_j}) \geq t_1 \\ -1 & \text{if } \cos(\theta_{\mathbf{x}_i, \mathbf{x}_j}) \leq t_2 \\ 2|\cos(\theta_{\mathbf{x}_i, \mathbf{x}_j})| - 1 & \text{otherwise,} \end{cases} \quad (60)$$

The above problem is solved by relaxing sign with the sigmoid-shaped function and finding the solution with the gradient descent algorithm.

### 5.3 Order Preserving Hashing

This section reviews the category of hashing algorithms that depend on various forms of maximizing the alignment between the orders of the reference data items computed from the input space and the coding space.

#### 5.3.1 Minimal loss hashing

The key point of minimal loss hashing [101] is to use a hinge-like loss function to assign penalties for similar (or dissimilar) points when they are too far apart (or too close). The formulation is given as follows,

$$\min \sum_{(i,j) \in \mathcal{L}} I[s_{ij} = 1] \max(\|\mathbf{y}_i - \mathbf{y}_j\|_1 - \rho + 1, 0) + I[s_{ij} = 0] \lambda \max(\rho - \|\mathbf{y}_i - \mathbf{y}_j\|_1 + 1, 0), \quad (61)$$

where  $\rho$  is a hyper-parameter and is used as a threshold in the Hamming space that differentiates neighbors from non-neighbors,  $\lambda$  is also a hyper-parameter that controls the ratio of the slopes for the penalties incurred for similar (or dissimilar) points. Both the two hyper-parameters are selected using the validation set.

Minimal loss hashing [101] solves the problem by building the convex-concave upper bound of the above objective function and optimizing it using the perceptron-like learning procedure.

#### 5.3.2 Rank order loss

The idea of order preserving hashing [130] is to learn hash functions by maximizing the alignment between the similarity orders computed from the original space and the ones in the Hamming space. To formulate the problem, given a data point  $\mathbf{x}_n$ , the database points  $\mathcal{X}$  are divided into  $M$  categories,  $(\mathcal{C}_{n0}^e, \mathcal{C}_{n1}^e, \dots, \mathcal{C}_{nM}^e)$  and  $(\mathcal{C}_{n0}^h, \mathcal{C}_{n1}^h, \dots, \mathcal{C}_{nM}^h)$ , using the distance in the original

space and the distance in the Hamming space, respectively. The objective function maximizing the alignment between the two categories is given as follows,

$$L(\mathbf{h}(\cdot); \mathcal{X}) \quad (62)$$

$$= \sum_{n=1}^N L(\mathbf{h}(\cdot); \mathbf{x}_n) \quad (63)$$

$$= \sum_{n=1}^N \sum_{m=0}^{M-1} L(\mathbf{h}(\cdot); \mathbf{x}_n, m) \quad (64)$$

$$= \sum_{n=1}^N \sum_{m=0}^{M-1} (|\mathcal{N}_{nm}^e - \mathcal{N}_{nm}^h| + \lambda |\mathcal{N}_{nm}^h - \mathcal{N}_{nm}^e|), \quad (65)$$

where  $\mathcal{N}_{nm}^e = \cup_{j=0}^m \mathcal{C}_{nj}^e$  and  $\mathcal{N}_{nm}^h = \cup_{j=0}^m \mathcal{C}_{nj}^h$ .

Given the compound hash function defined as below,

$$\mathbf{h}(\mathbf{x}) = \text{sign}(\mathbf{W}^T \mathbf{x} + \mathbf{b}) = [\text{sign}(\mathbf{w}_1^T \mathbf{x} + b_1) \cdots \text{sign}(\mathbf{w}_m^T \mathbf{x} + b_m)]^T, \quad (66)$$

the loss is transformed to:

$$L(\mathbf{W}; \mathbf{x}_n, i) = \sum_{\mathbf{x}' \in \mathcal{N}_{ni}^e} \text{sign}(\|\mathbf{h}(\mathbf{x}_n) - \mathbf{h}(\mathbf{x}')\|_2^2 - i) + \lambda \sum_{\mathbf{x}' \notin \mathcal{N}_{ni}^e} \text{sign}(i + 1 - \|\mathbf{h}(\mathbf{x}_n) - \mathbf{h}(\mathbf{x}')\|_2^2). \quad (67)$$

This problem is solved by dropping the sign function and using the quadratic penalty algorithm [130].

#### 5.3.3 Triplet loss hashing

Triplet loss hashing [103] formulates the hashing problem by preserving the relative similarity defined over triplets of items,  $(\mathbf{x}, \mathbf{x}^+, \mathbf{x}^-)$ , where the pair  $(\mathbf{x}, \mathbf{x}^+)$  is more similar than the pair  $(\mathbf{x}, \mathbf{x}^-)$ . The triplet loss is defined as

$$\ell_{\text{triplet}}(\mathbf{y}, \mathbf{y}^+, \mathbf{y}^-) = \max(\|\mathbf{y} - \mathbf{y}^+\|_1 - \|\mathbf{y} - \mathbf{y}^-\|_1 + 1, 0). \quad (68)$$

Suppose the compound hash function is defined as  $\mathbf{h}(\mathbf{x}; \mathbf{W})$ , the objective function is given as follows,

$$\sum_{(\mathbf{x}, \mathbf{x}^+, \mathbf{x}^-) \in \mathcal{D}} \ell_{\text{triplet}}(\mathbf{h}(\mathbf{x}; \mathbf{W}), \mathbf{h}(\mathbf{x}^+; \mathbf{W}), \mathbf{h}(\mathbf{x}^-; \mathbf{W})) + \frac{\lambda}{2} \text{trace}(\mathbf{W}^T \mathbf{W}). \quad (69)$$

The problem is optimized using the algorithm similar to minimal loss hashing [101]. The extension to asymmetric Hamming distance is also discussed in [101].

#### 5.3.4 Listwise supervision hashing

Similar to [101], listwise supervision hashing [128] also uses triplets of items to approximate the listwise loss. The formulation is based on a triplet tensor  $\mathbf{S}$  defined as follows,

$$s(i; j, k) = \begin{cases} 1 & \text{if } \text{sim}(\mathbf{x}_i; \mathbf{i}) > \text{sim}(\mathbf{x}_i; \mathbf{j}) \\ -1 & \text{if } \text{sim}(\mathbf{x}_i; \mathbf{i}) < \text{sim}(\mathbf{x}_i; \mathbf{j}) \\ 0 & \text{if } \text{sim}(\mathbf{x}_i; \mathbf{i}) = \text{sim}(\mathbf{x}_i; \mathbf{j}). \end{cases} \quad (70)$$

The goal is to minimize the following objective function,

$$-\sum_{i,j,k} \mathbf{h}(\mathbf{x}_i)^T (\mathbf{h}(\mathbf{x}_j) - \mathbf{h}(\mathbf{x}_k)) s_{ijk}, \quad (71)$$



where is solved by dropping the sign operator in  $\mathbf{h}(\mathbf{x}; \mathbf{W}) = \text{sign}(\mathbf{W}^T \mathbf{x})$ .

### 5.3.5 Similarity sensitive coding

Similarity sensitive coding (SSC) [114] aims to learn an embedding, which can be called weighted Hamming embedding:  $\mathbf{h}(\mathbf{x}) = [\alpha_1 h(\mathbf{x}_1) \alpha_2 h(\mathbf{x}_2) \cdots \alpha_M h(\mathbf{x}_M)]$  that is faithful to a task-specific similarity. An example algorithm, boosted SSC, uses adaboost to learn a classifier. The output of each weak learner on an input item is a binary code, and the outputs of all the weak learners are aggregated as the hash code. The weight of each weak learner forms the weight in the embedding, and is used to compute the weighted Hamming distance. Parameter sensitive hashing [115] is a simplified version of SSC with the standard LSH search procedure instead of the linear scan with weighted Hamming distance and uses decision stumps to form hash functions with threshold optimally decided according to the information of similar pairs, dissimilar pairs and pairs with undefined similarities. The forgiving hashing approach [6], [7], [8] extends parameter sensitive hashing and does not explicitly create dissimilar pairs, but instead relies on the maximum entropy constraint to provide that separation.

A column generation algorithm, which can be used to solve adaboost, is presented to simultaneously learn the weights and hash functions [75], with the following objective function

$$\min_{\alpha, \zeta} \sum_{i=1}^N \zeta_i + C \|\alpha\|_p \quad (72)$$

$$\text{s. t. } \alpha \geq 0, \zeta \geq 0, \quad (73)$$

$$d_h(\mathbf{x}_i, \mathbf{x}_i^-) - d_h(\mathbf{x}_i, \mathbf{x}_i^+) \geq 1 - \zeta_i \forall i. \quad (74)$$

Here  $\|\cdot\|_l$  is a  $l_p$  norm, e.g.,  $l = 1, 2, \infty$ .

## 5.4 Regularized Space Partitioning

Almost all hashing algorithms can be interpreted from the view of partitioning the space. In this section, we review the category of hashing algorithms that focus on pursuing effective space partitioning without explicitly evaluating the distance in the coding space.

### 5.4.1 Complementary projection hashing

Complementary projection hashing [55] computes the  $m$ th hash function according to the previously computed  $(m-1)$  hash functions, using a way similar to complementary hashing [139], checking the distance of the point to the previous  $(m-1)$  partition planes. The penalty weight for  $\mathbf{x}_n$  when learning the  $m$ th hash function is given as

$$u_n^m = 1 + \sum_{j=1}^{m-1} H(\epsilon - |\mathbf{w}_j^T \mathbf{x}_n + b_j|), \quad (75)$$

where  $H(\cdot) = \frac{1}{2}(1 + \text{sign}(\cdot))$  is a unit function.

Besides, it generalizes the bit balance condition, for each hit, half of points are mapped to  $-1$  and the rest mapped to  $1$ , and introduces a pair-wise bit balance condition to approximate the coding balance condition, i.e. every two hyperplanes spit the space into four subspaces, and each subspace contains  $N/4$  data points. The condition is guaranteed by

$$\sum_{n=1}^N h_1(\mathbf{x}_n) = 0, \quad (76)$$

$$\sum_{n=1}^N h_2(\mathbf{x}_n) = 0, \quad (77)$$

$$\sum_{n=1}^N h_1(\mathbf{x}_n) h_2(\mathbf{x}_n) = 0. \quad (78)$$

The whole formulation for updating the  $m$ th hash function is written as the following

$$\begin{aligned} \min \quad & \sum_{n=1}^N u_n^m H(\epsilon - |\mathbf{w}_m^T \mathbf{x}_n + b|) + \alpha \left( \sum_{n=1}^N h_m(\mathbf{x}_n) \right)^2 \\ & + \sum_{j=1}^{m-1} \left( \sum_{n=1}^N h_j(\mathbf{x}_n) h_m(\mathbf{x}_n) \right)^2, \end{aligned} \quad (79)$$

where  $h_m(\mathbf{x}) = (\mathbf{w}_m^T \mathbf{x} + b)$ .

The paper [55] also extends the linear hash function the kernel function, and presents the gradient descent algorithm to optimize the continuous-relaxed objective function which is formed by dropping the sign function.

### 5.4.2 Label-regularized maximum margin hashing

The idea of label-regularized maximum margin hashing [96] is to use the side information to find the hash function with the maximum margin criterion. Specifically, the hash function is computed so that ideally one pair of similar points are mapped to the same hash bit and one pair of dissimilar points are mapped to different hash bits. Let  $\mathcal{P}$  be a set of pairs  $\{(i, j)\}$  labeled to be similar. The formulation is given as follows,

$$\min_{\{y_i\}, \mathbf{w}, b, \{\xi_i\}, \{\zeta\}} \|\mathbf{w}\|_2^2 + \frac{\lambda_1}{N} \sum_{n=1}^N \xi_n + \frac{\lambda_2}{N} \sum_{(i,j) \in \mathcal{S}} \zeta_{ij} \quad (80)$$

$$\text{s. t. } y_i(\mathbf{w}^T \mathbf{x}_i + b) + \xi_i \geq 1, \xi_i \geq 0, \forall i, \quad (81)$$

$$y_i y_j + \zeta_{ij} \geq 0, \forall (i, j) \in \mathcal{P}, \quad (82)$$

$$-l \leq \mathbf{w}^T \mathbf{x}_i + b \leq l. \quad (83)$$

Here,  $\|\mathbf{w}\|_2^2$  corresponds to the maximum margin criterion. The second constraint comes from the side information for similar pairs, and its extension to dissimilar pairs is straightforward. The last constraint comes from the bit balance constraint, half of data items mapped to  $-1$  or  $1$ .

Similar to the BRE, the hash function is defined as  $h(\mathbf{x}) = \text{sign}(\sum_{t=1}^T v_t < \phi(\mathbf{s}_t), \phi(\mathbf{x}) > -b)$ , which means that  $w = \sum_{t=1}^T v_t \phi(\mathbf{s}_t)$ . This definition reduces the optimization cost. Constrained-concave-convex-procedure (CCCP) and cutting plane are used for the optimization.

### 5.4.3 Random maximum margin hashing

Random maximum margin hashing [57] learns a hash function with the maximum margin criterion, where the positive and negative labels are randomly generated, by randomly sampling  $N$  data items and randomly labeling half of the items with  $-1$  and the other half with  $1$ . The formulation is a standard SVM formulation that is equivalent to the following form,

$$\max \frac{1}{\|\mathbf{w}\|_2} \min \left[ \min_{i=1}^{\frac{N'}{2}} (\mathbf{w}^T \mathbf{x}_i^+ + b), \min_{i=1}^{\frac{N'}{2}} (-\mathbf{w}^T \mathbf{x}_i^- - b) \right], \quad (84)$$

where  $\{\mathbf{x}_i^+\}$  are the positive samples and  $\{\mathbf{x}_i^-\}$  are the negative samples. Using the kernel trick, the hash function can be a kernel-based function,  $h(\mathbf{x} = \text{sign}(\sum_{i=1}^v \alpha_i \langle \phi(\mathbf{x}), \phi(\mathbf{s}_i) \rangle) + b)$ , where  $\{\mathbf{s}_i\}$  are the selected  $v$  support vectors.

### 5.4.4 Spherical hashing

The basic idea of spherical hashing [38] is to use a hypersphere to formulate a spherical hash function,

$$h(\mathbf{x}) = \begin{cases} +1 & \text{if } d(\mathbf{p}, \mathbf{x}) \leq t \\ 0 & \text{otherwise.} \end{cases} \quad (85)$$

The compound hash function consists of  $K$  spherical functions, depending on  $K$  pivots  $\{\mathbf{p}_1, \dots, \mathbf{p}_K\}$  and  $K$  thresholds  $\{t_1, \dots, t_K\}$ . Given two hash codes,  $\mathbf{y}_1$  and  $\mathbf{y}_2$ , the distance is computed as

$$\frac{\|\mathbf{y}_1 - \mathbf{y}_2\|_1}{\mathbf{y}_1^T \mathbf{y}_2}, \quad (86)$$

where  $\|\mathbf{y}_1 - \mathbf{y}_2\|_1$  is similar to the Hamming distance, i.e., the frequency that both the two points lie inside (or outside) the hypersphere, and  $\mathbf{y}_1^T \mathbf{y}_2$  is equivalent to the number of common 1 bits between two binary codes, i.e., the frequency that both the two points lie inside the hypersphere.

The paper [38] proposes an iterative optimization algorithm to learn  $K$  pivots and thresholds such that it satisfies a pairwise bit balanced condition:

$$\|\{\mathbf{x} | h_k(\mathbf{x}) = 1\}\| = \|\{\mathbf{x} | h_k(\mathbf{x}) = 0\}\|,$$

and

$$\|\{\mathbf{x} | h_i(\mathbf{x}) = b_1, h_j(\mathbf{x}) = b_2\}\| = \frac{1}{4} \|\mathcal{X}\|, b_1, b_2 \in \{0, 1\}.$$

### 5.4.5 Density sensitive hashing

The idea of density sensitive hashing [79] is to exploit the clustering results to generate a set of candidate hash functions and to select the hash functions which can split the data most equally. First, the  $k$ -means algorithm is run over the data set, yielding  $K$  clusters with centers being  $\{\boldsymbol{\mu}_1, \boldsymbol{\mu}_2, \dots, \boldsymbol{\mu}_K\}$ . Second, a hash function is defined over two clusters  $(\boldsymbol{\mu}_i, \boldsymbol{\mu}_j)$  if the center is one of the  $r$  nearest neighbors of the other,  $h(\mathbf{x}) = \text{sign}(\mathbf{w}^T \mathbf{x} - b)$ , where  $\mathbf{w} = \boldsymbol{\mu}_i - \boldsymbol{\mu}_j$  and  $b = \frac{1}{2}(\boldsymbol{\mu}_i + \boldsymbol{\mu}_j)^T (\boldsymbol{\mu}_i - \boldsymbol{\mu}_j)$ . The third step aims to evaluate if the hash function  $(\mathbf{w}_m, b_m)$  can split the data most equally, which is evaluated by the

entropy,  $-P_{m0} \log P_{m0} - P_{m1} \log P_{m1}$ , where  $P_{m0} = \frac{n_0}{n}$  and  $P_{m1} = 1 - P_{m0}$ .  $n$  is the number of the data points, and  $n_0$  is the number of the data points lying one partition formed by the hyperplane of the corresponding hash function. Lastly,  $L$  hash functions with the greatest entropy scores are selected to form the compound hash function.

## 5.5 Hashing with Weighted Hamming Distance

This section presents the hashing algorithms which evaluate the distance in the coding space using the query-dependent and query-independent weighted Hamming distance scheme.

### 5.5.1 Multi-dimensional spectral hashing

Multi-dimensional spectral hashing [134] seeks hash codes such that the weighted Hamming affinity is equal to the original affinity,

$$\min \sum_{(i,j) \in \mathcal{N}} (w_{ij} - \mathbf{y}_i^T \boldsymbol{\Lambda} \mathbf{y}_j)^2 = \|\mathbf{W} - \mathbf{Y}^T \boldsymbol{\Lambda} \mathbf{Y}\|_F^2, \quad (87)$$

where  $\boldsymbol{\Lambda}$  is a diagonal matrix, and both  $\boldsymbol{\Lambda}$  and hash codes  $\{\mathbf{y}_i\}$  are needed to be optimized.

The algorithm for solving the problem 87 to compute hash codes is exactly the same to that given in [135]. Differently, the affinity over hash codes for multi-dimensional spectral hashing is the weighted Hamming affinity rather than the ordinary (isotropically weighted) Hamming affinity. Let  $(d, l)$  correspond to the index of one selected eigenfunction for computing the hash bit, the  $l$  eigenfunction along the PC direction  $d$ ,  $\mathcal{I} = \{(d, l)\}$  be the set of the indices of all the selected eigenfunctions. The weighted Hamming affinity using pure eigenfunctions along (PC) dimension  $d$  is computed as

$$\text{affinity}_d(i, j) = \sum_{(d,l) \in \mathcal{I}} \lambda_{dl} \text{sign}(\phi_{dl}(x_{id})) \text{sign}(\phi_{dl}(x_{jd})), \quad (88)$$

where  $x_{id}$  is the projection of  $\mathbf{x}_i$  along dimension  $d$ ,  $\phi_{dl}(\cdot)$  is the  $l$ th eigenfunction along dimension  $d$ ,  $\lambda_{dl}$  is the corresponding eigenvalue. The weighted Hamming affinity using all the hash codes is then computed as follows,

$$\text{affinity}(\mathbf{y}_i, \mathbf{y}_j) = \prod_d (1 + \text{affinity}_d(i, j)) - 1. \quad (89)$$

The computation can be accelerated using lookup tables.

### 5.5.2 Weighted hashing

Weighted hashing [131] uses the weighted Hamming distance to evaluate the distance between hash codes,  $\|\boldsymbol{\alpha}^T (\mathbf{y}_i - \mathbf{y}_j)\|_2^2$ . It optimizes the following problem,

$$\min \text{trace}(\text{diag}(\boldsymbol{\alpha}) \mathbf{Y} \mathbf{L} \mathbf{Y}^T) + \lambda \left\| \frac{1}{n} \mathbf{Y} \mathbf{Y}^T - \mathbf{I} \right\|_F^2 \quad (90)$$

$$\text{s. t. } \mathbf{Y} \in \{-1, 1\}^{M \times N}, \mathbf{Y}^T \mathbf{1} = \mathbf{0} \quad (91)$$

$$\|\boldsymbol{\alpha}\|_1 = 1 \quad (92)$$

$$\frac{\alpha_1}{\text{var}(y_1)} = \frac{\alpha_2}{\text{var}(y_2)} = \dots = \frac{\alpha_M}{\text{var}(y_M)}, \quad (93)$$

where  $\mathbf{L} = \mathbf{D} - \mathbf{S}$  is the Laplacian matrix. The formulation is essentially similar to spectral hashing [135], and the difference lies in including the weights for weighed Hamming distance.

The above problem is solved by discarding the first constraint and then binarizing  $\mathbf{y}$  at the  $M$  medians. The hash function  $\mathbf{w}_m^T \mathbf{x} + b$  is learnt by mapping the input  $\mathbf{x}$  to a hash bit  $y_m$ .

### 5.5.3 Query-adaptive bit weights

[53], [54] presents a weighted Hamming distance measure by learning the weights from the query information. Specifically, the approach learns class-specific bit weights so that the weighted Hamming distance between the hash codes belong to the class and the center, the mean of those hash codes is minimized. The weight for a specific query is the average weight of the weights of the classes that the query most likely belong to and that are discovered using the top similar images (each of which is associated with a semantic label).

### 5.5.4 Query-adaptive hashing

Query adaptive hashing [81] aims to select the hash bits (thus hash functions forming the hash bits) according to the query vector (image). The approach consists of two steps: offline hash functions  $\mathbf{h}(\mathbf{x}) = \text{sign}(\mathbf{W}^T \mathbf{x})$  ( $\{h_b(\mathbf{x}) = \text{sign}(\mathbf{w}_b^T \mathbf{x})\}$ ) and online hash function selection. The online hash function selection, given the query  $\mathbf{q}$ , is formulated as the following,

$$\min_{\alpha} \|\mathbf{q} - \mathbf{W}\alpha\|_2^2 + \rho \|\alpha\|_1. \quad (94)$$

Given the optimal solution  $\alpha^*$ ,  $\alpha_i^* = 0$  means the  $i$ th hash function is not selected, and the hash function corresponding to the nonzero entries in  $\alpha^*$ . A solution based on biased discriminant analysis is given to find  $\mathbf{W}$ , for which more details can be found from [81].

## 5.6 Other Hash Learning Algorithms

### 5.6.1 Semantic hashing

Semantic hashing [111], [112] generate the hash codes, which can be used to reconstruct the input data, using the deep generative model (based on the pretraining technique and the fine-tuning scheme originally designed for the restricted Boltzmann machines). This algorithm does not use any similarity information. The binary codes can be used for finding similarity data as they can be used to well reconstruct the input data.

### 5.6.2 Spline regression hashing

Spline regression hashing [90] aims to find a global hash function in the kernel form,  $h(\mathbf{x}) = \mathbf{v}^T \phi(\mathbf{x})$ , such that the hash value from the global hash function is consistent to those from the local hash functions that corresponds to its neighborhood points. Each data point corresponds to a local hash function in the form of spline regression,  $h_n(\mathbf{x}) = \sum_{i=1}^t \beta_{ni} p_i(\mathbf{x}) + \sum_{i=1}^k \alpha_{ni} g_{ni}(\mathbf{x})$ , where  $\{p_i(\mathbf{x})\}$

are the set of primitive polynomials which can span the polynomial space with a degree less than  $s$ ,  $\{g_{ni}(\mathbf{x})\}$  are the green functions, and  $\{\alpha_{ni}\}$  and  $\{\beta_{ni}\}$  are the corresponding coefficients. The whole formulation is given as follows,

$$\min_{\mathbf{v}, \{h_i\}, \{y_n\}} \sum_{n=1}^N \left( \sum_{\mathbf{x}_i \in \mathcal{N}_n} \|\mathbf{h}_n(\mathbf{x}_i) - \mathbf{y}_i\|_2^2 + \gamma \psi_n(\mathbf{h}_n) \right) + \lambda \left( \sum_{n=1}^N \|\mathbf{h}(\mathbf{x}_n) - \mathbf{y}_n\|_2^2 + \gamma \|\mathbf{v}\|_2^2 \right). \quad (95)$$

### 5.6.3 Inductive manifold hashing

Inductive manifold hashing [117] consists of three steps: cluster the data items into  $K$  clusters, whose centers are  $\{\mathbf{c}_1, \mathbf{c}_2, \dots, \mathbf{c}_K\}$ , embed the cluster centers into a low-dimensional space,  $\{\mathbf{y}_1, \mathbf{y}_2, \dots, \mathbf{y}_K\}$ , using existing manifold embedding technologies, and finally the hash function is given as follows,

$$\mathbf{h}(\mathbf{x}) = \text{sign} \left( \frac{\sum_{k=1}^K w(\mathbf{x}, \mathbf{c}_k) \mathbf{y}_k}{\sum_{k=1}^K w(\mathbf{x}, \mathbf{c}_k)} \right). \quad (96)$$

### 5.6.4 Nonlinear embedding

The approach introduced in [41] is an exact nearest neighbor approach, which relies on a key inequality,

$$\|\mathbf{x}_1 - \mathbf{x}_2\|_2^2 \geq d((\mu_1 - \mu_2)^2 + (\sigma_1 - \sigma_2)^2), \quad (97)$$

where  $\mu = \frac{1}{d} \sum_{i=1}^d x_i$  is the mean of all the entries of the vector  $\mathbf{x}$ , and  $\sigma = \frac{1}{d} \sum_{i=1}^d (x_i - \mu)^2$  is the standard deviation. The above inequality is generalized by dividing the vector into  $M$  subvectors, with the length of each subvector being  $d_m$ , and the resulting inequality is formulated as follows,

$$\|\mathbf{x}_1 - \mathbf{x}_2\|_2^2 \geq \sum_{m=1}^M d_m ((\mu_{1m} - \mu_{2m})^2 + (\sigma_{1m} - \sigma_{2m})^2). \quad (98)$$

In the search strategy, before computing the exact Euclidean distance between the query and the database point, the lower bound is first computed and is compared with the current minimal Euclidean distance, to determine if the exact distance is necessary to be computed.

### 5.6.5 Anti-sparse coding

The idea of anti-sparse coding [50] is to learn a hash code so that *non-zero elements in the hash code as many as possible*. The binarization process is as follows. First, it solves the following problem,

$$\mathbf{z}^* = \arg \min_{\mathbf{z}: \mathbf{W}\mathbf{z}=\mathbf{x}} \|\mathbf{z}\|_{\infty}, \quad (99)$$

where  $\|\mathbf{z}\|_{\infty} = \max_{i \in \{1, 2, \dots, K\}} |z_i|$ , and  $\mathbf{W}$  is a projection matrix. It is proved that in the optimal solution (minimizing the range of the components),  $K - d + 1$  of the components are stuck to the limit, i.e.,  $z_i = \pm \|\mathbf{z}\|_{\infty}$ . The binary code (of the length  $K$ ) is computed as  $\mathbf{y} = \text{sign}(\mathbf{z})$ .

The distance between the query  $\mathbf{q}$  and a vector  $\mathbf{x}$  can be evaluated based on the similarity in the Hamming space,  $\mathbf{y}_q^\top \mathbf{y}_x$  or the asymmetric similarity  $\mathbf{z}_q^\top \mathbf{y}_x$ . The nice property is that the anti-sparse code allows, up to a scaling factor, the explicit reconstruction of the original vector  $\mathbf{x} \propto \mathbf{W}\mathbf{y}$ .

### 5.6.6 Two-Step Hashing

The paper [77] presents a general two-step approach to learning-based hashing: learn binary embedding (codes) and then learn the hash function mapping the input item to the learnt binary codes. An instance algorithm [76] uses an efficient GraphCut based block search method for inferring binary codes for large databases and trains boosted decision trees fit the binary codes.

Self-taught hashing [144] optimizes an objective function, similar to the spectral hashing,

$$\min \text{trace}(\mathbf{Y}\mathbf{L}\mathbf{Y}^T) \quad (100)$$

$$\text{s. t. } \mathbf{Y}\mathbf{D}\mathbf{Y}^T = \mathbf{I} \quad (101)$$

$$\mathbf{Y}\mathbf{D}\mathbf{1} = \mathbf{0}, \quad (102)$$

where  $\mathbf{Y}$  is a real-valued matrix, relaxed from the binary matrix),  $\mathbf{L}$  is the Laplacian matrix and  $\mathbf{D}$  is the degree matrix. The solution is the  $M$  eigenvectors corresponding to the smallest  $M$  eigenvalues (except the trivial eigenvalue 0),  $\mathbf{L}\mathbf{v} = \lambda\mathbf{D}\mathbf{v}$ . To get the binary code, each row of  $\mathbf{Y}$  is thresholded using the median value of the column. To form the hash function, mapping the vector to a single hash bit is regarded as a classification problem, which is solved by linear SVM,  $\text{sign}(\mathbf{w}^T \mathbf{x} + b)$ . The linear SVM is then regarded as the hash function.

Sparse hashing [151] also is a two step approach. The first step learns a sparse nonnegative embedding, in which the positive embedding is encoded as 1 and the zero embedding is encoded as 0. The formulation is as follows,

$$\sum_{n=1}^N \|\mathbf{x}_n - \mathbf{P}^T \mathbf{z}_n\|_2^2 + \alpha \sum_{i=1}^N \sum_{j=1}^N s_{ij} \|\mathbf{z}_i - \mathbf{z}_j\|_2^2 + \lambda \sum_{n=1}^N \|\mathbf{z}_n\|_1, \quad (103)$$

where  $s_{ij} = \exp(-\frac{\|\mathbf{x}_i - \mathbf{x}_j\|_2^2}{\sigma^2})$  is the similarity between  $\mathbf{x}_i$  and  $\mathbf{x}_j$ .

The second step is to learn a linear hash function for each hash bit, which is optimized based on the elastic net estimator (for the  $m$ th hash function),

$$\min_{\mathbf{w}} \sum_{n=1}^N \|\mathbf{y}_n - \mathbf{w}_m^T \mathbf{x}_n\|_2^2 + \lambda_1 \|\mathbf{w}_m\|_1 + \lambda_2 \|\mathbf{w}_m\|_2^2. \quad (104)$$

Locally linear hashing [43] first learns binary codes that preserves the locally linear structures and then introduces a locally linear extension algorithm for out-of-sample extension. The objective function of the first step to obtain the binary embedding  $\mathbf{Y}$  is given as

$$\min_{\mathbf{Z}, \mathbf{R}, \mathbf{Y}} \text{trace}(\mathbf{Z}^T \mathbf{M} \mathbf{Z}) + \eta \|\mathbf{Y} - \mathbf{Z}\mathbf{R}\|_F^2 \quad (105)$$

$$\text{s. t. } \mathbf{Y} \in \{1, -1\}^{N \times M}, \mathbf{R}^T \mathbf{R} = \mathbf{I}. \quad (106)$$

Here  $\mathbf{Z}$  is a nonlinear embedding, similar to locally linear embedding and  $\mathbf{M}$  is a sparse matrix,  $\mathbf{M} = (\mathbf{I} - \mathbf{W})^T (\mathbf{I} - \mathbf{W})$ .  $\mathbf{W}$  is the locally linear reconstruction weight matrix, which is computed by solving the following optimization problem for each database item,

$$\min_{\mathbf{w}_n} \lambda \|\mathbf{s}_n^T \mathbf{w}_n\|_1 + \frac{1}{2} \|\mathbf{x}_n - \sum_{j \in \mathcal{N}(\mathbf{x}_n)} w_{ij} \mathbf{x}_j\|_2^2 \quad (107)$$

$$\text{s. t. } \mathbf{w}_n^T \mathbf{1} = 1, \quad (108)$$

where  $\mathbf{w}_n = [w_{n1}, w_{n2}, \dots, w_{nn}]^T$ , and  $w_{nj} = 0$  if  $j \notin \mathcal{N}(\mathbf{x}_n)$ .  $\mathbf{s}_n = [s_{n1}, s_{n2}, \dots, s_{nn}]^T$  is a vector and  $s_{nj} = \frac{\|\mathbf{x}_n - \mathbf{x}_j\|_2}{\sum_{t \in \mathcal{N}(\mathbf{x}_n)} \|\mathbf{x}_n - \mathbf{x}_t\|_2}$ .

Out-of-sample extension computes the binary embedding of a query  $\mathbf{q}$  as  $\mathbf{y}_q = \text{sign}(\mathbf{Y}^T \mathbf{w}_q)$ . Here  $\mathbf{w}_q$  is a locally linear reconstruction weight, and computed similarly to the above optimization problem. Differently,  $\mathbf{Y}$  and  $\mathbf{w}_q$  correspond to the cluster centers, computed using  $k$ -means, of the database  $\mathbf{X}$ .

## 5.7 Beyond Hamming Distances in the Coding Space

This section reviews the algorithms focusing on designing effective distance measures given the binary codes and possibly the hash functions. The summary is given in Table 5.

### 5.7.1 Manhattan distance

When assigning multiple bits into a projection direction, the Hamming distance breaks the neighborhood structure, thus the points with smaller Hamming distance along the projection direction might have large Euclidean distance along the projection direction. Manhattan hashing [61] introduces a scheme to address this issue, the Hamming codes along the projection direction are in turn (e.g., from the left to the right) transformed integers, and the difference of the integers is used to replace the Hamming distance. The aggregation of the differences along all the projection directions is used as the distance of the hash codes.

### 5.7.2 Asymmetric distance

Let the compound hash function consist of  $K$  hash functions  $\{h_k(\mathbf{x}) = b_k(g_k(\mathbf{x}))\}$ , where  $g_k()$  is a real-valued embedding function and  $b_k()$  is a binarization function. Asymmetric distance [32] presents two schemes. The first one (Asymmetric distance I) is based on the expectation  $\bar{g}_{kb} = \mathbb{E}(g_k(\mathbf{x}) | h_k(\mathbf{x}) = b_k(g_k(\mathbf{x})) = b)$ , where  $b = 0$  and  $b = 1$ . When performing an online search, a distance lookup table is precomputed:

$$\{d_e(g_1(\mathbf{q}), \bar{g}_{10}), d_e(g_1(\mathbf{q}), \bar{g}_{11}), d_e(g_2(\mathbf{q}), \bar{g}_{20}), \\ d_e(g_2(\mathbf{q}), \bar{g}_{21}), \dots, d_e(g_K(\mathbf{q}), \bar{g}_{K0}), d_e(g_K(\mathbf{q}), \bar{g}_{K1}), \quad (109)$$

where  $d_e(\cdot, \cdot)$  is an Euclidean distance operation. Then the distance is computed as  $d_{ah}(\mathbf{q}, \mathbf{x}) =$

TABLE 5  
A summary of algorithms beyond Hamming distances in the coding space.

method	input similarity	distance measure
Manhattan hashing [61]	E	MD
Asymmetric distance I [61]	E	AED, SED
Asymmetric distance II [61]	E	LB
asymmetric Hamming embedding [44]	E	LB

$\sum_{k=1}^K d_e(g_k(\mathbf{q}), \bar{g}_{kh_k(\mathbf{x})})$ , which can be speeded up e.g., by grouping the hash functions in blocks of 8 bits and have one 256-dimensional look-up table per block (rather than one 2-dimensional look-up table per hash function.) This reduces the number of summations as well as the number of lookup operations.

The second scheme (Asymmetric distance II) is under the assumption that  $b_k(g_k(\mathbf{x})) = \delta[g_k(\mathbf{x}) > t_k]$ , and computes the distance lower bound (similar way also adopted in asymmetric Hamming embedding [44]) over the  $k$ -th hash function,

$$d(g_k(\mathbf{q}), b_k(g_k(\mathbf{x}))) = \begin{cases} |g_k(\mathbf{q})| & \text{if } h_k(\mathbf{x}) \neq h_k(\mathbf{q}) \\ 0 & \text{otherwise.} \end{cases} \quad (110)$$

Similar to the first one, the distance is computed as  $d_{ah}(\mathbf{q}, \mathbf{x}) = \sum_{k=1}^K d(g_k(\mathbf{q}), b_k(g_k(\mathbf{x})))$ . Similar hash function grouping scheme is used to speed up the search efficiency.

### 5.7.3 Query sensitive hash code ranking

Query sensitive hash code ranking [148] presented a similar asymmetric scheme for  $R$ -neighbor search. This method uses the PCA projection  $\mathbf{W}$  to formulate the hash functions  $\text{sign}(\mathbf{W}^T \mathbf{x}) = \text{sign}(\mathbf{z})$ . The similarity along the  $k$  projection is computed as

$$s_k(q_k, y_k, R) = \frac{P(z_k y_k > 0, |q_k - z_k| \leq R)}{P(|q_k - z_k| \leq R)}, \quad (111)$$

which intuitively means that the fraction of the points that lie in the range  $|q_k - z_k| \leq R$  and are mapped to  $y_k$  over the points that lie in the range  $|q_k - z_k| \leq R$ . The similarity is computed with the assumption that  $p(z_k)$  is a Gaussian distribution. The whole similarity is then computed as  $\prod_{k=1}^K s_k(q_k, y_k, R)$ , equivalently  $\sum_{k=1}^K \log s_k(q_k, y_k, R)$ . The lookup table is also used to speed up the distance computation.

### 5.7.4 Bit reconfiguration

The goal of bits reconfiguration [95] is to learn a good distance measure over the hash codes precomputed from a pool of hash functions. Given the hash codes  $\{\mathbf{y}_n\}_{n=1}^N$  with length  $M$ , the similar pairs  $\mathcal{M} = \{(i, j)\}$  and the dissimilar pairs  $\mathcal{C} = \{(i, j)\}$ , compute the difference matrix  $\mathbf{D}_m$  ( $\mathbf{D}_c$ ) over  $\mathcal{M}$  ( $\mathcal{C}$ ) each column of which corresponds to  $\mathbf{y}_i - \mathbf{y}_j$ ,  $(i, j) \in \mathcal{M}$  ( $(i, j) \in \mathcal{C}$ ). The formulation

is given as the following maximization problem,

$$\max_{\mathbf{W}} \frac{1}{n_c} \text{trace}(\mathbf{W}^T \mathbf{D}_c \mathbf{D}_c^T \mathbf{W}) - \frac{1}{n_m} \text{trace}(\mathbf{W}^T \mathbf{D}_m \mathbf{D}_m^T \mathbf{W}) + \frac{\eta}{n_s} \text{trace}(\mathbf{W}^T \mathbf{Y}_s \mathbf{Y}_s^T \mathbf{W}) - \eta \text{trace}(\mathbf{W}^T \boldsymbol{\mu} \boldsymbol{\mu}^T \mathbf{W}), \quad (112)$$

where  $\mathbf{W}$  is a projection matrix of size  $b \times t$ . The first term aims to maximize the differences between dissimilar pairs, and the second term aims to minimize the differences between similar pairs. The last two terms are maximized so that the bit distribution is balanced, which is derived by maximizing  $E[\|\mathbf{W}^T(\mathbf{y} - \boldsymbol{\mu})\|_2^2]$ , where  $\boldsymbol{\mu}$  represents the mean of the hash vectors, and  $\mathbf{Y}_s$  is a subset of input hash vectors with cardinality  $n_s$ . [95] furthermore refines the hash vectors using the idea of supervised locality-preserving method based on graph Laplacian.

## 6 LEARNING TO HASH: QUANTIZATION

This section focuses on the algorithms that are based on quantization. The representative algorithms are summarized in Table 6.

### 6.1 1D Quantization

This section reviews the hashing algorithms that focuses on how to do the quantization along a projection direction (partitioning the projection values of the reference data items along the direction into multiple parts).

#### 6.1.1 Transform coding

Similar to spectral hashing, transform coding [10] first transforms the data using PCA and then assigns several bits to each principal direction. Different from spectral hashing that uses Laplacian eigenvalues computed along each direction to select Laplacian eigenfunctions to form hash functions, transform coding first adopts bit allocation to determine which principal direction is used and how many bits are assigned to such a direction.

The bit allocation algorithm is given as follows in Algorithm 1. To form the hash function, each selected principal direction  $i$  is quantized into  $2^{m_i}$  clusters with the centers as  $\{c_{i1}, c_{i2}, \dots, c_{i2^{m_i}}\}$ , where each center is represented by a binary code of length  $m_i$ . Encoding an item consists of PCA projection followed by quantization of the components. the hash function can be formulated. The distance between a query item and the hash code is evaluated as the aggregation of the distance between the

TABLE 6  
A summary of quantization algorithms. sim. = similarity. dist. = distance.

method	input sim.	hash function	dist. measure	optimization criteria
transform coding [10]	E	OQ	AED, SED	BA
double-bit quantization [59]	E	OQ	HD	3 partitions
iterative quantization [30], [31]	E	LI	HD	QE
isotropic hashing [60]	E	LI	HD	EV
harmonious hashing [138]	E	LI	HD	QE + EV
Angular quantization [29]	CS	LI	NHA	MCS
product quantization [49]	E	QU	(A)ED	QE
Cartesian $k$ -means [102]	E	QU	(A)ED	QE
composite quantization [147]	E	QU	(A)ED	QE

---

**Algorithm 1** Distribute  $M$  bits into the principal directions

---

1. Initialization:  $e_i \leftarrow \log_2 \sigma_i$ ,  $m_i \leftarrow 0$ .
  2. **for**  $j = 1$  to  $b$  **do**
  3.    $i \leftarrow \arg \max e_i$ .
  4.    $m_i \leftarrow m_i + 1$ .
  5.    $e_i \leftarrow e_i - 1$ .
  6. **end for**
- 

centers of the query and the database item along each selected principal direction, or the aggregation of the distance between the center of the database item and the projection of the query of the corresponding principal direction along all the selected principal direction.

### 6.1.2 Double-bit quantization

The double-bit quantization-based hashing algorithm [59] distributes two bits into each projection direction instead of one bit in ITQ or hierarchical hashing [83]. Unlike transform coding quantizing the points into  $2^b$  clusters along each direction, double-bit quantization conducts 3-cluster quantization, and then assigns 01, 00, and 11 to each cluster so that the Hamming distance between the points belonging to neighboring clusters is 1, and the Hamming distance between the points not belonging to neighboring clusters is 2.

Local digit coding [62] represents each dimension of a point by a single bit, which is set to 1 if the value of the dimension it corresponds to is larger than a threshold (derived from the mean of the corresponding data points), and 0 otherwise.

## 6.2 Hypercubic Quantization

Hypercubic quantization refers to a category of algorithms that quantize a data item to a vertex in a hypercubic, i.e., a vector belonging to  $\{[y_1, y_2, \dots, y_M] | y_m \in \{-1, 1\}\}$ .

### 6.2.1 Iterative quantization

Iterative quantization [30], [31] aims to find the hash codes such that the difference between the hash codes and the data items, by viewing each bit as the quantization value along the corresponding dimension, is minimized. It consists of two steps: (1) reduce the dimension using PCA to  $M$  dimensions,  $\mathbf{v} = \mathbf{P}^T \mathbf{x}$ , where  $\mathbf{P}$  is a

matrix of size  $d \times M$  ( $M \leq d$ ) computed using PCA, and (2) find the hash codes as well as an optimal rotation  $\mathbf{R}$ , by solving the following optimization problem,

$$\min \|\mathbf{Y} - \mathbf{R}^T \mathbf{V}\|_F^2, \quad (113)$$

where  $\mathbf{V} = [\mathbf{v}_1 \mathbf{v}_2 \dots \mathbf{v}_M]$  and  $\mathbf{Y} = [\mathbf{y}_1 \mathbf{y}_2 \dots \mathbf{y}_N]$ .

The problem is solved via alternative optimization. There are two alternative steps. Fixing  $\mathbf{R}$ ,  $\mathbf{Y} = \text{sign}(\mathbf{R}^T \mathbf{V})$ . Fixing  $\mathbf{B}$ , the problem becomes the classic orthogonal Procrustes problem, and the solution is  $\mathbf{R} = \hat{\mathbf{S}} \mathbf{S}^T$ , where  $\mathbf{S}$  and  $\hat{\mathbf{S}}$  is obtained from the SVD of  $\mathbf{Y} \mathbf{V}^T$ ,  $\mathbf{Y} \mathbf{V}^T = \mathbf{S} \hat{\mathbf{S}}^T$ .

We present an integrated objective function that is able to explain the necessity of the first step. Let  $\bar{\mathbf{y}}$  be a  $d$ -dimensional vector, which is a concatenated vector from  $\mathbf{y}$  and an all-zero subvector:  $\bar{\mathbf{y}} = [\mathbf{y}^T 0 \dots 0]^T$ . The integrated objective function is written as follows:

$$\min \|\bar{\mathbf{Y}} - \bar{\mathbf{R}}^T \mathbf{X}\|_F^2, \quad (114)$$

where  $\bar{\mathbf{Y}} = [\bar{\mathbf{y}}_1 \bar{\mathbf{y}}_2 \dots \bar{\mathbf{y}}_N]$ ,  $\mathbf{X} = [\mathbf{x}_1 \mathbf{x}_2 \dots \mathbf{x}_N]$ , and  $\bar{\mathbf{R}}$  is a rotation matrix.

Let  $\bar{\mathbf{P}}$  be the projection matrix of  $d \times d$ , computed using PCA,  $\bar{\mathbf{P}} = [\mathbf{P} \mathbf{P}_-]$ . It can be seen that, the solutions for  $\bar{\mathbf{y}}$  of the two problems in 114 and 113 are the same, if  $\bar{\mathbf{R}} = \bar{\mathbf{P}} \text{Diag}(\mathbf{R}, \mathbf{I})$ .

### 6.2.2 Isotropic hashing

The idea of isotropic hashing [60] is to rotate the space so that the variance along each dimension is the same. It consists of three steps: (1) reduce the dimension using PCA to  $M$  dimensions,  $\mathbf{v} = \mathbf{P}^T \mathbf{x}$ , where  $\mathbf{P}$  is a matrix of size  $d \times M$  ( $M \leq d$ ) computed using PCA, and (2) find an optimal rotation  $\mathbf{R}$ , so that  $\mathbf{R}^T \mathbf{V} \mathbf{V}^T \mathbf{R} = \mathbf{\Sigma}$  becomes a matrix with equal diagonal values, i.e.,  $[\mathbf{\Sigma}]_{11} = [\mathbf{\Sigma}]_{22} = \dots = [\mathbf{\Sigma}]_{MM}$ .

Let  $\sigma = \frac{1}{M} \text{Trace} \mathbf{V} \mathbf{V}^T$ . The isotropic hashing algorithm then aims to find an rotation matrix, by solving the following problem:

$$\|\mathbf{R}^T \mathbf{V} \mathbf{V}^T \mathbf{R} - \mathbf{Z}\|_F = 0, \quad (115)$$

where  $\mathbf{Z}$  is a matrix with all the diagonal entries equal to  $\sigma$ . The problem can be solved by two algorithms: lift and projection and gradient flow.

The goal of making the variances along the  $M$  directions same is to make the bits in the hash codes equally

contributed to the distance evaluation. In the case that the data items satisfy the isotropic Gaussian distribution, the solution from isotropic hashing is equivalent to iterative quantization.

Similar to generalized iterative quantization, the PCA preprocess in isotropic hashing is also interpretable: finding a global rotation matrix  $\bar{\mathbf{R}}$  such that the first  $M$  diagonal entries of  $\bar{\Sigma}\bar{\mathbf{R}}^T\mathbf{X}\mathbf{X}^T\bar{\mathbf{R}}$  are equal, and their sum is as large as possible, which is formally written as follows,

$$\max \sum_{m=1}^M [\Sigma]_{mm} \quad (116)$$

$$\text{s. t. } [\Sigma] = \sigma, m = 1, \dots, M \quad (117)$$

$$\mathbf{R}^T \mathbf{R} = \mathbf{I}. \quad (118)$$

### 6.2.3 Harmonious hashing

Harmonious hashing [138] can be viewed as a combination of ITQ and Isotropic hashing. The formulation is given as follows,

$$\min_{\mathbf{Y}, \mathbf{R}} \|\mathbf{Y} - \mathbf{R}^T \mathbf{V}\|_F^2 \quad (119)$$

$$\text{s. t. } \mathbf{Y}\mathbf{Y}^T = \sigma \mathbf{I} \quad (120)$$

$$\mathbf{R}^T \mathbf{R} = \mathbf{I}. \quad (121)$$

It is different from ITQ in that the formulation does not require  $\mathbf{Y}$  to be a binary matrix. An iterative algorithm is presented to optimize the above problem. Fixing  $\mathbf{R}$ , let  $\mathbf{R}^T \mathbf{V} = \mathbf{U}\mathbf{A}\mathbf{V}^T$ , then  $\mathbf{Y} = \sigma^{1/2}\mathbf{U}\mathbf{V}^T$ . Fixing  $\mathbf{Y}$ ,  $\mathbf{R} = \hat{\mathbf{S}}\mathbf{S}^T$ , where  $\mathbf{S}$  and  $\hat{\mathbf{S}}$  is obtained from the SVD of  $\mathbf{Y}\mathbf{V}^T$ ,  $\mathbf{Y}\mathbf{V}^T = \mathbf{S}\mathbf{A}\hat{\mathbf{S}}^T$ . Finally,  $\mathbf{Y}$  is cut at zero, attaining binary codes.

### 6.2.4 Angular quantization

Angular quantization [29] addresses the ANN search problem under the cosine similarity. The basic idea is to use the nearest vertex from the vertices of the binary hypercube  $\{0, 1\}^d$  to approximate the data vector  $\mathbf{x}$ ,  $\arg \max_{\mathbf{y}} \frac{\mathbf{y}^T \mathbf{x}}{\|\mathbf{y}\|_2}$ , subject to  $\mathbf{y} \in \{0, 1\}^d$ , which is shown to be solved in  $O(d \log d)$  time, and then to evaluate the similarity  $\frac{\mathbf{b}_x^T \mathbf{b}_q}{\|\mathbf{b}_q\|_2 \|\mathbf{b}_x\|_2}$  in the Hamming space.

The objective function of finding the binary codes, similar to iterative quantization [30], is formulated as below,

$$\max_{\mathbf{R}, \{\mathbf{y}_n\}} \sum_{n=1}^N \frac{\mathbf{y}_n^T}{\|\mathbf{y}_n\|_2} \frac{\mathbf{R}^T \mathbf{x}_n}{\|\mathbf{R}^T \mathbf{x}_n\|_2} \quad (122)$$

$$\text{s. t. } \mathbf{y}_n \in \{0, 1\}^M, \quad (123)$$

$$\mathbf{R}^T \mathbf{R} = \mathbf{I}_M. \quad (124)$$

Here  $\mathbf{R}$  is a projection matrix of  $d \times M$ . This is transformed to an easily-solved problem by discarding the

denominator  $\|\mathbf{R}^T \mathbf{x}_n\|_2$ :

$$\max_{\mathbf{R}, \{\mathbf{y}_n\}} \sum_{n=1}^N \frac{\mathbf{y}_n^T}{\|\mathbf{y}_n\|_2} \mathbf{R}^T \mathbf{x}_n \quad (125)$$

$$\text{s. t. } \mathbf{y}_n \in \{0, 1\}^M, \quad (126)$$

$$\mathbf{R}^T \mathbf{R} = \mathbf{I}_M. \quad (127)$$

The above problem is solved using alternative optimization.

## 6.3 Cartesian Quantization

### 6.3.1 Product quantization

The basic idea of product quantization [49] is to divide the feature space into ( $P$ ) disjoint subspaces, thus the database is divided into  $P$  sets, each set consisting of  $N$  subvectors  $\{\mathbf{x}_{p1}, \dots, \mathbf{x}_{pN}\}$ , and then to quantize each subspace separately into ( $K$ ) clusters. Let  $\{\mathbf{c}_{p1}, \mathbf{c}_{p2}, \dots, \mathbf{c}_{pK}\}$  be the cluster centers of the  $p$  subspace, each of which can be encoded as a code of length  $\log_2 K$ .

A data item  $\mathbf{x}_n$  is divided into  $P$  subvectors  $\{\mathbf{x}_{pn}\}$ , and each subvector is assigned to the nearest center  $\mathbf{c}_{pk_{pn}}$  among the cluster centers of the  $p$ th subspace. Then the data item  $\mathbf{x}_n$  is represent by  $P$  subvectors  $\{\mathbf{c}_{pk_{pn}}\}_{p=1}^P$ , thus represented by a code of length  $P \log_2 K$ ,  $k_{1n}k_{2n} \dots k_{Pn}$ . Product quantization can be viewed as minimizing the following objective function,

$$\min_{\mathbf{C}, \{\mathbf{b}_n\}} \sum_{n=1}^N \|\mathbf{x}_n - \mathbf{C}\mathbf{b}_n\|_2^2. \quad (128)$$

Here  $\mathbf{C}$  is a matrix of  $d \times PK$  in the form of

$$\text{diag}(\mathbf{C}_1, \mathbf{C}_2, \dots, \mathbf{C}_P) = \begin{bmatrix} \mathbf{C}_1 & \mathbf{0} & \dots & \mathbf{0} \\ \mathbf{0} & \mathbf{C}_2 & \dots & \mathbf{0} \\ \vdots & \vdots & \ddots & \vdots \\ \mathbf{0} & \mathbf{0} & \dots & \mathbf{C}_P \end{bmatrix}, \quad (129)$$

where  $\mathbf{C}_p = [\mathbf{c}_{p1}\mathbf{c}_{p2} \dots \mathbf{c}_{pK}]$ .  $\mathbf{b}_n$  is the composition vector, and its subvector  $\mathbf{b}_{np}$  of length  $K$  is an indicator vector with only one entry being 1 and all others being 0, showing which element is selected from the  $p$ th dictionary for quantization.

Given a query vector  $\mathbf{x}_t$ , the distance to a vector  $\mathbf{x}_n$ , represented by a code  $k_{1n}k_{2n} \dots k_{Pn}$  can be evaluated in symmetric and asymmetric ways. The symmetric distance is computed as follows. First, the code of the query  $\mathbf{x}_t$  is computed using the way similar to the database vector, denoted by  $k_{1t}k_{2t} \dots k_{Pt}$ . Second, a distance table is computed. The table consists of  $PK$  distance entries,  $\{d_{pk} = \|\mathbf{c}_{pk_{pt}} - \mathbf{c}_{pk}\|_2^2 | p = 1, \dots, P, k = 1, \dots, K\}$ . Finally, the distance of the query to the vector  $\mathbf{x}_n$  is computed by looking up the distance table and summing up  $P$  distances,  $\sum_{p=1}^P d_{pk_{pn}}$ . The asymmetric distance does not encode the query vector, directly computes the distance table that also includes  $PK$  distance entries,  $\{d_{pk} = \|\mathbf{x}_{pt} - \mathbf{c}_{pk}\|_2^2 | p = 1, \dots, P, k = 1, \dots, K\}$ , and

finally conducts the same step to the symmetric distance evaluation, computing the distance as  $\sum_{p=1}^P d_{pk_{pn}}$ .

Distance-encoded product quantization [39] extends product quantization by encoding both the cluster index and the distance between a point and its cluster center. The way of encoding the cluster index is similar to that in product quantization. The way of encoding the distance between a point and its cluster center is given as follows. Given a set of points belonging to a cluster, those points are partitioned (quantized) according to the distances to the cluster center.

### 6.3.2 Cartesian $k$ -means

Cartesian  $k$ -means [102], [26] extends product quantization and introduces a rotation  $\mathbf{R}$  into the objective function,

$$\min_{\mathbf{R}, \mathbf{C}, \{\mathbf{b}_n\}} \sum_{n=1}^N \|\mathbf{R}^T \mathbf{x}_n - \mathbf{C} \mathbf{b}_n\|_2^2. \quad (130)$$

The introduced rotation does not affect the Euclidean distance as the Euclidean distance is invariant to the rotation, and helps to find an optimized subspace partition for quantization.

The problem is solved by an alternative optimization algorithm. Each iteration alternatively solves  $\mathbf{C}$ ,  $\{\mathbf{b}_n\}$ , and  $\mathbf{R}$ . Fixing  $\mathbf{R}$ ,  $\mathbf{C}$  and  $\{\mathbf{b}_n\}$  are solved using the same way as the one in product quantization but with fewer iterations and the necessity of reaching the converged solution. Fixing  $\mathbf{C}$  and  $\{\mathbf{b}_n\}$ , the problem of optimizing  $\mathbf{R}$  is the classic orthogonal Procrustes problem, also occurring in iterative quantization.

The database vector  $\mathbf{x}_n$  with Cartesian  $k$ -means is represented by  $P$  subvectors  $\{\mathbf{c}_{pk_{pn}}\}_{p=1}^P$ , thus encoded as  $k_{1n}k_{2n} \cdots k_{Pn}$ , with a rotation matrix  $\mathbf{R}$  for all database vector (thus the rotation matrix does not increase the code length). Given a query vector  $\mathbf{x}_t$ , it is first rotated as  $\mathbf{R}^T \mathbf{x}_t$ . Then the distance is computed using the same way to that in production quantization. As rotating the query vector is only done once for a query, its computation cost for a large database is negligible compared with the cost of computing the approximate distances with a large amount of database vectors.

Locally optimized product quantization [58] applies Cartesian  $k$ -means to the search algorithm with the inverted index, where there is a quantizer for each inverted list.

### 6.3.3 Composite quantization

The basic ideas of composite quantization [147] consist of (1) approximating the database vector  $\mathbf{x}_n$  using  $P$  vectors with the same dimension  $d$ ,  $\mathbf{c}_{1k_{1n}}, \mathbf{c}_{1k_{2n}}, \dots, \mathbf{c}_{1k_{Pn}}$ , each selected from  $K$  elements among one of  $P$  source dictionaries  $\{\mathcal{C}_1, \mathcal{C}_2, \dots, \mathcal{C}_P\}$ , respectively, (2) making the summation of the inner products of all pairs of elements that are used to approximate the vector but from different dictionaries,  $\sum_{i=1}^P \sum_{j=1, j \neq i}^P \mathbf{c}_{ik_{in}} \mathbf{c}_{jk_{jn}}$ , be constant.

The problem is formulated as

$$\begin{aligned} \min_{\{\mathbf{C}_p\}, \{\mathbf{b}_n\}, \epsilon} \quad & \sum_{n=1}^N \|\mathbf{x}_n - [\mathbf{C}_1 \mathbf{C}_2 \cdots \mathbf{C}_P] \mathbf{b}_n\|_2^2 \quad (131) \\ \text{s. t.} \quad & \sum_{i=1}^P \sum_{j=1, j \neq i}^P \mathbf{b}_{ni}^T \mathbf{C}_i^T \mathbf{C}_j \mathbf{b}_{nj} = \epsilon \\ & \mathbf{b}_n = [\mathbf{b}_{n1}^T \mathbf{b}_{n2}^T \cdots \mathbf{b}_{nP}^T]^T \\ & \mathbf{b}_{np} \in \{0, 1\}^K, \|\mathbf{b}_{np}\|_1 = 1 \\ & n = 1, 2, \dots, N, p = 1, 2, \dots, P. \end{aligned}$$

Here,  $\mathbf{C}_p$  is a matrix of size  $d \times K$ , and each column corresponds to an element of the  $p$ th dictionary  $\mathcal{C}_p$ .

To get an easily optimization algorithm, the objective function is transformed as

$$\begin{aligned} \phi(\{\mathbf{C}_p\}, \{\mathbf{b}_n\}, \epsilon) = \quad & \sum_{n=1}^N \|\mathbf{x}_n - \mathbf{C} \mathbf{b}_n\|_2^2 \\ & + \mu \sum_{n=1}^N \left( \sum_{i \neq j}^P \mathbf{b}_{ni}^T \mathbf{C}_i^T \mathbf{C}_j \mathbf{b}_{nj} - \epsilon \right)^2, \quad (132) \end{aligned}$$

where  $\mu$  is the penalty parameter,  $\mathbf{C} = [\mathbf{C}_1 \mathbf{C}_2 \cdots \mathbf{C}_P]$  and  $\sum_{i \neq j}^P = \sum_{i=1}^P \sum_{j=1, j \neq i}^P$ . The transformed problem is solved by alternative optimization.

The idea of using the summation of several dictionary items as an approximation of a data item has already been studied in the signal processing area, known as multi-stage vector quantization, residual quantization, or more generally structured vector quantization [34], and recently re-developed for similarity search under the Euclidean distance [5], [129] and inner product [22].

## 7 LEARNING TO HASH: OTHER TOPICS

### 7.1 Multi-Table Hashing

#### 7.1.1 Complementary hashing

The purpose of complementary hashing [139] is to learn multiple hash tables such that nearest neighbors have a large probability to appear in the same bucket at least in one hash table. The algorithm learns the hashing functions for the multiple hash tables in a sequential way. The compound hash function for the first table is learnt by solving the same problem in [125], as formulated below

$$\text{trace}[\mathbf{W}^T \mathbf{X}_i \mathbf{S} \mathbf{X}_i^T \mathbf{W}] + \eta \text{trace}[\mathbf{W}^T \mathbf{X} \mathbf{X}^T \mathbf{W}], \quad (133)$$

where  $s_{ij}$  is initialized as  $K(a_{ij} - \alpha)$ ,  $a_{ij}$  is the similarity between  $\mathbf{x}_i$  and  $\mathbf{x}_j$  and  $\alpha$  is a super-constant.

To compute the second compound hash functions, the same objective function is optimized but with different matrix  $\mathbf{S}$ :

$$s_{ij}^t = \begin{cases} 0 & b_{ij}^a = b_{ij}^{(t-1)} \\ \min(s_{ij}, f_{ij}) & b_{ij}^a = 1, b_{ij}^{(t-1)} = -1 \\ -\min(-s_{ij}, f_{ij}) & b_{ij}^a = -1, b_{ij}^{(t-1)} = 1 \end{cases} \quad (134)$$

where  $f_{ij} = (a_{ij} - \alpha) \left( \frac{1}{4} d_h^{(t-1)}(\mathbf{x}_i, \mathbf{x}_j) - \beta \right)$ ,  $\beta$  is a super-constant, and  $b^{(t-1)ij} = 1 - 2 \text{sign} \left[ \frac{1}{4} d_h^{(t-1)}(\mathbf{x}_i, \mathbf{x}_j) - \beta \right]$ . Some tricks are also given to scale up the problem to large scale databases.



### 7.1.2 Reciprocal hash tables

The reciprocal hash tables [86] extends complementary hashing by building a graph over a pool  $B$  hash functions (with the output being a binary value) and searching the best hash functions over such a graph for building a hashing table, updating the graph weight using a boosting-style algorithm and finding the subsequent hash tables. The vertex in the graph corresponds to a hash function and is associated with a weight showing the degree that similar pairs are mapped to the same binary value and dissimilar pairs are mapped to different binary values. The weight over the edge connecting two hash functions reflects the independence between two hash functions the weight is higher if the difference of the distributions of the binary values  $\{-1, 1\}$  computed from the two hash functions is larger. [87] shows how to formulate the hash bit selection problem into a quadric program, which is derived from organizing the candidate bits in graph.

## 7.2 Active and Online Hashing

### 7.2.1 Active hashing

Active hashing [150] starts with a small set of pairs of points with labeling information and actively selects the most informative labeled pairs for hash function learning. Given the sets of labeled data  $\mathcal{L}$ , unlabeled data  $\mathcal{U}$ , and candidate data  $\mathcal{C}$ , the algorithm first learns the compound hash function  $\mathbf{h} = \text{sign}(\mathbf{W}^T \mathbf{x})$ , and then computes the data certainty score for each point in the candidate set,  $f(\mathbf{x}) = \|\mathbf{W}^T \mathbf{x}\|_2$ , which reflects the distance of a point to the hyperplane forming the hash functions. Points with smaller the data certainty scores should be selected for further labeling. On the other hand, the selected points should not be similar to each other. To this end, the problem of finding the most informative points is formulated as the following,

$$\min_{\mathbf{b}} \mathbf{b}^T \bar{\mathbf{f}} + \frac{\lambda}{M} \mathbf{b}^T \mathbf{K} \mathbf{b} \quad (135)$$

$$\text{s. t. } \mathbf{b} \in \{0, 1\}^{|\mathcal{C}|} \quad (136)$$

$$\|\mathbf{b}^T\|_1 = M, \quad (137)$$

where  $\mathbf{b}$  is an indicator vector in which  $b_i = 1$  when  $\mathbf{x}_i$  is selected and  $b_i = 0$  when  $\mathbf{x}_i$  is not selected,  $M$  is the number of points that need to be selected,  $\bar{\mathbf{f}}$  is a vector of the normalized certainty scores over the candidate set, with each element  $\bar{f}_i = \frac{f_i}{\max_{j=1}^c f_j}$ ,  $\mathbf{K}$  is the similarity matrix computed over  $\mathcal{C}$ , and  $\lambda$  is the trade-off parameter.

### 7.2.2 Online hashing

Online hashing [40] presents an algorithm to learn the hash functions when the similar/dissimilar pairs come sequentially rather than at the beginning, all the similar/dissimilar pairs come together. Smart hashing [142] also addresses the problem when the similar/dissimilar

pairs come sequentially. Unlike the online hash algorithm that updates all hash functions, smart hashing only selects a small subset of hash functions for relearning for a fast response to newly-coming labeled pairs.

## 7.3 Hashing for the Absolute Inner Product Similarity

### 7.3.1 Concomitant hashing

Concomitant hashing [97] aims to find the points with the smallest and largest absolute cosine similarity. The approach is similar to concomitant LSH [23] and formulate a two-bit hash code using a multi-set  $\{h_{\min}(\mathbf{x}), h_{\max}(\mathbf{x})\} = \{\arg \min_{k=1}^{2^K} \mathbf{w}_k^T \mathbf{x}, \arg \max_{k=1}^{2^K} \mathbf{w}_k^T \mathbf{x}\}$ . The two bits are unordered, which is slightly different from concomitant LSH [23]. The collision probability is defined as  $\text{Prob}\{\{h_{\min}(\mathbf{x}), h_{\max}(\mathbf{x})\} = \{h_{\min}(\mathbf{y}), h_{\max}(\mathbf{y})\}\}$ , which is shown to be a monotonically increasing function with respect to  $|\mathbf{x}_1^T \mathbf{x}_2|$ . This, thus, means that the larger hamming distance, the smaller  $|\mathbf{x}_1^T \mathbf{x}_2|$  (min-inner-product) and the smaller hamming distance, the larger  $|\mathbf{x}_1^T \mathbf{x}_2|$  (max-inner-product).

## 7.4 Matrix Hashing

### 7.4.1 Bilinear projection

A bilinear projection algorithm is proposed in [28] to hash a matrix feature to short codes. The (compound) hash function is defined as

$$\text{vec}(\text{sign}(\mathbf{R}_l^T \mathbf{X} \mathbf{R}_r)), \quad (138)$$

where  $\mathbf{X}$  is a matrix of  $d_l \times d_r$ ,  $\mathbf{R}_l$  of size  $d_l \times d_l$  and  $\mathbf{R}_r$  of size  $d_r \times d_r$  are two random orthogonal matrices. It is easy to show that

$$\text{vec}(\mathbf{R}_l^T \mathbf{X} \mathbf{R}_r) = (\mathbf{R}_r^T \otimes \mathbf{R}_l^T) \text{vec}(\mathbf{X}) = \mathbf{R}^T \text{vec}(\mathbf{X}). \quad (139)$$

The objective is to minimize the angle between a rotated feature  $\mathbf{R}^T \text{vec}(\mathbf{X})$  and its binary encoding  $\text{sign}(\mathbf{R}^T \text{vec}(\mathbf{X})) = \text{vec}(\text{sign}(\mathbf{R}_l^T \mathbf{X} \mathbf{R}_r))$ . The formulation is given as follows,

$$\max_{\mathbf{R}_l, \mathbf{R}_r, \{\mathbf{B}_n\}} \sum_{n=1}^N \text{trace}(\mathbf{B}_n \mathbf{R}_r^T \mathbf{X}_n^T \mathbf{R}_l) \quad (140)$$

$$\text{s. t. } \mathbf{B}_n \in \{-1, +1\}^{d_l \times d_r} \quad (141)$$

$$\mathbf{R}_l^T \mathbf{R}_l = \mathbf{I} \quad (142)$$

$$\mathbf{R}_r^T \mathbf{R}_r = \mathbf{I}, \quad (143)$$

where  $\mathbf{B}_n = \text{sign}(\mathbf{R}_l^T \mathbf{X}_n \mathbf{R}_r)$ . The problem is optimized by alternating between  $\{\mathbf{B}_n\}$ ,  $\mathbf{R}_l$  and  $\mathbf{R}_r$ . To reduce the code length, the low-dimensional orthogonal matrices can be used:  $\mathbf{R}_l \in \mathbb{R}^{d_l \times c_l}$  and  $\mathbf{R}_r \in \mathbb{R}^{d_r \times c_r}$ .

## 7.5 Compact Sparse Coding

Compact sparse coding [14], the extension of the early work robust sparse coding [15] adopts sparse codes to represent the database items: the atom indices corresponding to nonzero codes are used to build the inverted index, and the nonzero coefficients are used to reconstruct the database items and compute the approximate distances between the query and the database items.

The sparse coding objective function, with introducing the incoherence constraint of the dictionary, is given as follows,

$$\min_{\mathbf{C}, \{\mathbf{z}_n\}_{n=1}^N} \frac{1}{2} \sum_{i=1}^N \|\mathbf{x}_i - \sum_{j=1}^K z_{ij} \mathbf{c}_j\|_2^2 + \lambda \|\mathbf{z}_i\|_1 \quad (144)$$

$$\text{s. t. } \|\mathbf{C}_{\sim k}^T \mathbf{c}_k\|_\infty \leq \gamma; k = 1, 2, \dots, n, \quad (145)$$

where  $\mathbf{C}$  is the dictionary,  $\mathbf{C}_{\sim k}^T$  is the dictionary  $\mathbf{C}$  with the  $k$ th atom removed,  $\{\mathbf{z}_n\}_{n=1}^N$  are the  $N$  sparse codes.  $\|\mathbf{C}_{\sim k}^T \mathbf{c}_k\|_\infty \leq \gamma$  aims to control the dictionary coherence degree.

The support of  $\mathbf{x}_n$  is defined as the indices corresponding to nonzero coefficients in  $\mathbf{z}_n$ :  $\mathbf{b}_n = \delta.[\mathbf{z}_n \neq 0]$ , where  $\delta.[\cdot]$  is an element-wise operation. The introduced approach uses  $\{\mathbf{b}_n\}_{n=1}^N$  to build the inverted indices, which is similar to min-hash, and also uses the Jaccard similarity to get the search results. Finally, the asymmetric distances between the query and the retrieved results using the Jaccard similarity,  $\|\mathbf{q} - \mathbf{B}\mathbf{z}_n\|_2$  are computed for reranking.

## 7.6 Fast Search in Hamming Space

### 7.6.1 Multi-index hashing

The idea [104] is that binary codes in the reference database are indexed  $M$  times into  $M$  different hash tables, based on  $M$  disjoint binary substrings. Given a query binary code, entries that fall close to the query in at least one substring are considered neighbor candidates. Specifically, each code  $\mathbf{y}$  is split into  $M$  disjoint subcodes  $\{\mathbf{y}^1, \dots, \mathbf{y}^M\}$ . For each subcode,  $\mathbf{y}^m$ , one hash table is built, where each entry corresponds to a list of indices of the binary code whose  $m$ th subcodes is equal to the code associated with this entry.

To find  $R$ -neighbors of a query  $\mathbf{q}$  with substrings  $\{\mathbf{q}^m\}_{m=1}^M$ , the algorithm search  $m$ th hash table for entries that are within a Hamming distance  $\lfloor \frac{R}{M} \rfloor$  of  $\mathbf{q}^m$ , thereby retrieving a set of candidates, denoted by  $\mathcal{N}_m(\mathbf{q})$  and thus a set of final candidates,  $\mathcal{N} = \cup_{m=1}^M \mathcal{N}_m(\mathbf{q})$ . Lastly, the algorithm computes the Hamming distance between  $\mathbf{q}$  and each candidate, retaining only those codes that are true  $R$ -neighbors of  $\mathbf{q}$ . [104] also discussed how to choose the optimal number  $M$  of substrings.

### 7.6.2 FLANN

[100] extends the FLANN algorithm [99] that is initially designed for ANN search over real-value vectors to search over binary vectors. The key idea is to build multiple hierarchical cluster trees to organize the binary

vectors and search for the nearest neighbors simultaneously over the multiple trees.

The tree building process starts with all the points and divides them into  $K$  clusters with cluster centers randomly selected from the input points and each point assigned to the center that is closest to the point. The algorithm is repeated recursively for each of the resulting clusters until the number of points in each cluster is below a certain threshold, in which case that node becomes a leaf node. The whole process is repeated several times, yielding multiple trees.

The search process starts with a single traverse of each of the trees, during which the algorithm always picks the node closest to the query point and recursively explores it, while adding the unexplored nodes to a priority queue. When reaching the leaf node all the points contained within are linearly searched. After each of the trees has been explored once, the search is continued by extracting from the priority queue the closest node to the query point and resuming the tree traversal from there. The search ends when the number of points examined exceeds a maximum limit.

## 8 DISCUSSIONS AND FUTURE TRENDS

### 8.1 Scalable Hash Function Learning

The algorithms depending on the pairwise similarity, such binary reconstructive embedding, usually sample a small subset of pairs to reduce the cost of learning hash functions. It is shown that the search accuracy is increased with a high sampling rate, but the training cost is greatly increased. The algorithms even without relying pairwise similarity are also shown to be slow and even infeasible when handling very large data, e.g.,  $1B$  data items, and usually learn hash functions over a small subset, e.g.,  $1M$  data items. This poses a challenging request to learn the hash function over larger datasets.

### 8.2 Hash Code Computation Speedup

Existing hashing algorithms rarely do not take consideration of the cost of encoding a data item. Such a cost during the query stage becomes significant in the case that only a small number of database items or a small database are compared to the query. The search with combining inverted index and compact codes is such a case. an recent work, circulant binary embedding [143], formulates the projection matrix (the weights in the hash function) using a circular matrix  $\mathbf{R} = \text{circ}(\mathbf{r})$ . The compound hash function is formulated is given as  $\mathbf{h}(\mathbf{x}) = \text{sign}(\mathbf{R}^T \mathbf{x})$ , where the computation is accelerated using fast Fourier transformation with the time cost reduced from  $O(d^2)$  to  $d \log d$ . It expects more research study to speed up the hash code computation for other hashing algorithms, such as composite quantization.

### 8.3 Distance Table Computation Speedup

Product quantization and its variants need to precompute the distance table between the query and the elements of the dictionaries. Existing algorithms claim the cost of distance table computation is negligible. However in practice, the cost becomes bigger when using the codes computed from quantization to rank the candidates retrieved from inverted index. This is a research direction that will attract research interests.

### 8.4 Multiple and Cross Modality Hashing

One important characteristic of big data is the variety of data types and data sources. This is particularly true to multimedia data, where various media types (e.g., video, image, audio and hypertext) can be described by many different low- and high-level features, and relevant multimedia objects may come from different data sources contributed by different users and organizations. This raises a research direction, performing joint-modality hashing learning by exploiting the relation among multiple modalities, for supporting some special applications, such as cross-model search. This topic is attracting a lot of research efforts, such as collaborative hashing [85], and cross-media hashing [120], [121], [152].

## 9 CONCLUSION

In this paper, we review two categories of hashing algorithm developed for similarity search: locality sensitive hashing and learning to hash and show how they are designed to conduct similarity search. We also point out the future trends of hashing for similarity search.

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