Tree-wise Distribution Sensitive hashing: Efficient Maximum likelihood Classification by joint dimensionality reduction in known probabilistic settings

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Abstract

We consider the problem of maximum likelihood classification of a high dimensional data point $y$ to billions of classes $x_1, \cdots, x_N$, where the conditional probability $p(y \mid x)$ is known. In the most general case, the complexity of the brute-force method for this classification grows linearly, $O(N)$, with the number of classes $N$. Efficient multiclass classification methods have been introduced to solve this problem with logarithmic complexity. However, these methods suffer from the curse of dimensionality, i.e., in large dimensions their complexity approaches $O(N)$ per query data point. In the special case where the conditional probability distribution $p(y \mid x)$ is a Gaussian centered at $x$, i.e., $p(y \mid x) \propto \mathcal{N}(x, \sigma)$, the maximum likelihood classification reduces to the nearest neighbor search with the Euclidean norm. Sublinear methods based on locality sensitive hashing (LSH) have been introduced to solve an approximate version of the nearest neighbor search for high dimensional data. Inspired by these advances, here we introduce distribution sensitive hashing (DSH) to solve an approximate version of the maximum likelihood classification problem through joint dimensionality reduction. In the case of discrete probability distributions, we design TreeDSH, a universal family of distribution sensitive hashes based on the decision trees, and show that their complexity grow sub-linearly. Theory and simulation presented in this paper demonstrate that TreeDSH is more efficient than LSH-hamming and Min-Hashing schemes. Finally, we apply TreeDSH to the problem of peptide identification from mass spectrometry data.

1 Introduction

Consider a data point $y$, and a set of classes $X = \{x_1, \cdots, x_N\}$ where $N$ is the number of classes. Assume the conditional probability distribution $p(y \mid x)$ is given, and we can compute $p(y \mid x = x_i)$, the likelihood that data-point $y$ corresponds to the class $x_i$, with complexity $O(1)$. Under uniform prior assumption, the maximum likelihood (ML) classifier assigns each data-point to the class that maximizes its posterior probability\footnote{In Bayesian inference, ML classification is a special case of maximum a posteriori classification (MAP) that assumes a uniform prior distribution of the parameters.}

$$\hat{x}(y) = \arg \max_{x \in X} p(y \mid x)$$

(1)

The brute-force method for computing this optimization problem for each data point $y$ has $O(N)$ running time. Our goal is to provide a solution to this problem with sub-linear complexity. In
many real life applications, including peptide identification from mass spectrometry data, we have millions/billions of data points (mass spectra) and we want to classify them into millions/billions of classes (peptides) \[1, 2\]. In these problems, \( P \) is factorizable into i.i.d. distributions, i.e.,

\[
P(x, y) = \prod_{s=1}^{S} p(x_s, y_s)
\]

and learning \( p(y \mid x) \) is a straightforward task \[2\]. However, the inference step, e.g., finding the class \( x \) that maximize \( p(y \mid x) \) is non-trivial when we have billions of data points/classes. Some special cases of this problem have been addressed in the literature. For example, assume \( x \) and \( y \) are vectors of the same size in \( \mathbb{R}^S \) (\( S \) is the dimension of the data), and \( P(y \mid x) \) has a Gaussian probability distribution centered at \( x \), i.e.,

\[
P(y \mid x) = \frac{1}{\sqrt{2\pi\sigma}} e^{-\frac{|y - x|^2}{2\sigma^2}}
\]

It is easy to derive that given this conditional probability distribution, ML classification is equivalent to finding \( x \in X \) that has minimum Euclidean distance to the data-point \( y \), i.e.,

\[
\arg \max_{x \in X} P(y \mid x) = \arg \min_{x \in X} ||y - x||^2
\]

where \( ||.|| \) is the Euclidean distance function. This problem is called the nearest neighbor search problem, and has been extensively studied in the past \[3, 4\]. It can also be shown that the nearest neighbor search in binary case \[3\], and the problem of finding similar sets \[5\] are also special cases of the ML classification problem.

As there is no efficient method for solving the exact form of the nearest neighbor search problem in the case of high-dimensional data, many of the researchers consider the approximate nearest neighbor search problem \[6, 7\]. Given \( c > 1 \), the approximate nearest neighbor search problem can be formulated as follows. For each \( y \), find \( x \in X \) which satisfies

\[
||y - x|| < c||y - x_{\min}||
\]

where \( x_{\min} = \arg \min_{x \in X} ||y - x|| \). One of the most popular methods for approximate nearest neighbor search is locality sensitive hashing (LSH) \[8, 3\]. For any metric space \( \mathcal{M} = (M, d) \), a family of functions \( h: \mathcal{M} \to S \) is \( \mathcal{F}(R, cR, p_1, p_2) \)-sensitive if for any two points \( x, y \in \mathcal{M} \):

\[
\begin{align*}
\text{If } d(x, y) &\leq R, \text{ then } h_X(x) = h_Y(y) \text{ with probability at least } p_1. \\
\text{If } d(x, y) &\geq cR, \text{ then } h_X(x) = h_Y(y) \text{ with probability at most } p_2.
\end{align*}
\]

Currently, there is no sub-linear solution for the exact ML Classification problem. Therefore, we focus on the Approximate ML Classification Problem as follows. Given \( c < 1 \) and for each \( y \), find \( x \in X \) which satisfies

\[
\log (P(y \mid x)) > c \log (P(y \mid x_{\text{max}}))
\]

where \( x_{\text{max}} = \arg \max_{x \in X} P(y \mid x) \). Define \( P_X(x) \) and \( P_Y(y) \) as the marginal probability distributions of \( P(x, y) \) and \( Q(x, y) = P_X(x)P_Y(y) \). Similar to the theory of locality sensitive hashing \[8, 3\], we solve
the approximate ML classification problem by designing hashes \( h_X : X^S \to \mathbb{N}, h_Y : Y^S \to \mathbb{N} \) such that for some arbitrary \( 0 \leq \beta \leq \alpha \leq 1 \)

\[
\begin{align*}
\text{Prob}(h_X(x) = h_Y(y) | x, y \sim P) &< e^T, (x, y) \sim \rho P + (1 - \rho) Q = \alpha \quad (9) \\
\text{Prob}(h_X(x) = h_Y(y) | x, y \sim P) &> e^T, (x, y) \sim \rho P + (1 - \rho) Q = \beta \quad (10)
\end{align*}
\]

where \( \alpha \) and \( \beta \) stand for the probabilities that the data points \( x \) and \( y \) are hashed to the same bucket under the constraints \( \frac{P(x,y)}{P_X(x)P_Y(y)} < e^T \) and \( \frac{P(x,y)}{P_X(x)P_Y(y)} > e^T \) for some log-likelihood threshold \( T \). Moreover, \( \rho \) denotes the prior probability of \( (x, y) \) being generated from \( P \) while \( 1 - \rho \) stands for the prior probability \( (x, y) \) being generated from \( Q \).

In order to design such hashes, we show that when \( P \) is factorizable into independent and identically distributed (i.i.d) factors, i.e.,

\[
P(x,y) = \prod_{s=1}^{S} p(x_s, y_s) \quad (11)
\]

and \( S \) is large enough, finding hashes \( h_X \) and \( h_Y \) that satisfy (9) and (10) is equivalent to finding hashes \( h_X \) and \( h_Y \) that satisfy:

\[
\begin{align*}
\text{Prob}(h_X(x) = h_Y(y) | (x,y) \sim P) &= \alpha \quad (12) \\
\text{Prob}(h_X(x) = h_Y(y) | (x,y) \sim Q) &= \beta \quad (13)
\end{align*}
\]

See Appendix A for the proof of equivalence.

This article is structured as follows. In Section 2, we define ”distribution sensitive hashes”. In Section 3, we assume that an oracle has given us a family of distribution sensitive hashes, and use them to design an algorithm for ML classification in known probabilistic settings (discrete joint probability distributions). We further demonstrate that if hashes satisfying (9) and (10) exist, the approximate ML problem can be solved in \( O(\log(N)^{1 - \log(\alpha) / \log(\beta)}, N \log(\alpha) / \log(\beta)) \) query time. In Section 4, in the special case where \( P \) is factorizable to i.i.d components we present a method to construct a family of distribution sensitive hashes using a decision tree structure (TreeDSH). While the number of nodes in these decision trees could grow exponentially with the dimension, in Section 5 we propose a method to hash the data and classes through the decision trees without the need to construct the complete tree. In Sections 6 and 7, we compare TreeDSH to existing nearest neighbor search algorithms LSH-hamming and Minhash across various probability distributions, both theoretically and experimentally. Finally, we apply TreeDSH to the problem of peptide identification from mass spectrometry data.

1.1 Related work

In the past, multiclass classification methods have been introduced to efficiently solve the maximum likelihood problem for large number of classes \([9][10][11]\). These methods speed up the prediction by rejecting a significant portion of classes for each query. However, all these methods suffer from

\[
^2\text{The notation } (x, y) \sim P \text{ stands for } (x, y) \text{ are sampled from the probability distribution } P.
\]

\[
^3\text{The data point } x \text{ hashes to the bucket } h_\ast(x) \text{ under the hashing function } h_\ast.
\]

\[
^4\text{Note that, in contrast to inequalities in (6) and (7), we have equalities in (9) and (10).}
\]
the curse of dimensionality, i.e., when the dimension of the data increases, the complexity of these methods increases linearly with the number of classes. In [8], the $\epsilon$-approximate nearest neighbor search is studied where the goal is to find a point $p \in P$ that for all the other points $p' \in P$ and $q$ we have $d(p, q) \leq (1 + \epsilon)d(p', q)$. $P$ is the set of all feasible points. Later on, in [12], a similarity search that returns $m$ results is studied. The authors in [12] design a self tuning index structure which returns $m$ neighbors, such that the distance between the query $q$ and the $i$-th neighbor is at most $1 + \epsilon$ times the distance between the query $q$ and the actual $i$-th neighbor. While the approximate nearest neighbor search methods can scale to high dimensional data, these methods are limited to specific metrics, and can not generalize to arbitrary joint probability distributions for which the triangle inequality does not hold [6, 7, 8, 13, 14, 15].

The problem of finding high dimensional approximate nearest neighbors in a known probabilistic setting using a bucketing tree algorithm has been studied previously in [16, 17]. Dubiner uses a strategy to hash the data points from an arbitrary joint probability distribution into the leafs of the tree in a way that the paired data collide with a probability higher than the random pairs. However, the algorithm introduced in Dubiner requires solving computationally intractable optimizations, making it impossible to implement (e.g. see equation (126) from [16]).

In this paper, we rely on tree-hashes similar to [12, 16] to design a universal hashing scheme for arbitrary joint probability distributions. We provide an efficient algorithm for setting the parameters and a correctness analysis. Our result shows that TreeDSH outperforms LSH-hamming and Minhash for all joint probability distributions and our simulations confirm the theory. We use the idea of constructing a decision-tree-based hash incrementally such that at each node a choice is made in such a way that the odds of reaching the next node under the true joint probability distribution $P(x, y)$ is higher than under an independent probability distribution $Q(x, y) = \prod_{s=1}^{S} p(x_s, y_s)$. The tree is built in a way that the ratio of these two probabilities, i.e., $\frac{P(x, y)}{Q(x, y)}$ at each leaf exceeds some minimum threshold. In Section 4, among many trees that can be constructed in this way, we determined the tree that optimizes the complexity.

Notation: The cardinality of a set $A$ is denoted as $|A|$. The sets $\mathbb{N}$ and $\mathbb{R}$ stand for the sets of natural and real numbers, respectively. We use $P(\cdot)$ and $Q(\cdot)$ to denote the probability function $\text{Prob}(\cdot)$. We use the notation $[n]$ for the set $\{1, 2, \cdots, n\}$.

2 Definitions

Definition 1 (Alphabets) Define two alphabets $A$ and $B$ as

\[
A = \{a_1, a_2, \cdots, a_k\}
\]

\[
B = \{b_1, b_2, \cdots, b_l\}
\]

for some natural numbers $k$ and $l$. Moreover, assume the product probability distribution:

\[
P : A^S \times B^S \rightarrow [0, 1], \quad P(x, y) = \prod_{s=1}^{S} p(x_s, y_s)
\]

for $x = (x_1, x_2, \cdots, x_S) \in A^S$ and $y = (y_1, y_2, \cdots, y_S) \in B^S$. Note that, we assume the same probability distribution $P(x, y)$ for each dimension $s \in S$. Moreover, define: $p(x_s = i, y_s = j) = p_{i,j}$

\footnote{The curse of dimensionality holds for non-deterministic probability distributions. When $p(y \mid x)$ is deterministic, there is no curse of dimensionality. In this paper, we are interested in the case of non-deterministic probability distributions.}
satisfying:

\[
\sum_{i \in [k], j \in [l]} p_{i,j} = 1 \tag{17}
\]

The marginal probability distributions \( P_X(x) \), \( P_Y(y) \) and \( Q(x,y) \) are also defined as,

\[
P_X(x) : A^S \rightarrow [0,1] \quad P_X(x) = \prod_{s=1}^{S} p_X(x_s) \tag{18}
\]

\[
P_Y(y) : B^S \rightarrow [0,1] \quad P_Y(y) = \prod_{s=1}^{S} p_Y(y_s) \tag{19}
\]

\[
Q : A^S \times B^S \rightarrow [0,1] \quad Q(x, y) = \prod_{s=1}^{S} q(x_s, y_s) \tag{20}
\]

where

\[
p_X(x_s) = \sum_{j=1}^{l} p(x_s, b_j) \tag{21}
\]

\[
p_Y(y_s) = \sum_{i=1}^{k} p(a_i, y_s) \tag{22}
\]

\[
q(x_s, y_s) = p_X(x_s) \times p_Y(y_s) \tag{23}
\]

**Definition 2** For sets \( I \subset A \) and \( J \subset B \), we define

\[
p_X(I) = \sum_{a \in I} p_X(a) \tag{24}
\]

\[
p_Y(J) = \sum_{b \in J} p_Y(b) \tag{25}
\]

\[
p(I \times J) = \sum_{a \in I, b \in J} p(a, b) \tag{26}
\]

**Definition 3 (Family of Distribution sensitive hashes)** Given \( P, Q, \alpha, \beta \), a family of hashes \( h_i^X : A^S \rightarrow \mathbb{N} \) and \( h_i^Y : B^S \rightarrow \mathbb{N} \) for \( i \in \mathbb{N} \) is called \( (P, Q, \alpha, \beta) \)-distribution sensitive, if \([12]\) and \([13]\) hold.

### 3 Approximate ML classification by distribution sensitive hashing

In this section, we assume an oracle has given us a set of \( (P, Q, \alpha, \beta) \)-distribution sensitive hashes \( h_i^X(x) \) and \( h_i^Y(y) \) for \( i \in \mathbb{N} \) that satisfies \([12]\) and \([13]\). Using these hashes, we propose an algorithm for approximate maximum likelihood classification problem and show that its complexity is bounded by \( O(N \log^{\alpha} \log^{\beta}) \). In section 4, we introduce a family of hashes that satisfy \([12]\) and \([13]\) using decision trees and provide guarantees on their run time.
3.1 Distribution Sensitive Hashing Algorithm

Our algorithm start with \( b \times r \) randomly selected hashes from the DSH family, where \( r \) is the number of rows and \( b \) is the number of bands. We recall a pair \((x, y)\), if \( x \) and \( y \) are hashed to the same value in all \( r \) rows in at least one of the \( b \) bands. It is straightforward to show that

\[
TP = 1 - (1 - \alpha)^b \quad (27)
\]

\[
FP = 1 - (1 - \beta)^b \quad (28)
\]

where \( TP \) is the probability of recalling matched pairs generated from \( P \) and \( FP \) is the probability of recalling random pairs generated from \( Q \).

Algorithm 1 Approximate Maximum Likelihood by distribution sensitive hashing.

**Inputs:** Numbers of rows \( r \), number of bands \( b \), \( h_{ij}^X(x) \), \( h_{ij}^Y(y) \) for all \( 1 \leq i \leq r, 1 \leq j \leq b \) that satisfy (12) and (13), classes \( X = \{x_1, \cdots, x_N\} \) and query \( y \).

**Outputs:** Matched pairs \((x, y)\).

**For** \( 1 \leq j \leq b \)

Step 1: Hash each data point \( x \) according to \( h_{1,j}^X(x), \cdots, h_{r,j}^X(x) \) and sort the results.

Step 2: Hash \( y \) according to \( h_{1,j}^Y(y), \cdots, h_{r,j}^Y(y) \) and search the signature in the corresponding sorted list of signatures from the previous step. For classes \( x \) with hashes matching \( y \) in all \( r \) rows, recall \( x \).

Here, we demonstrate that the complexity for Algorithm 1 is \( O(\log(N)\frac{\log(\alpha)}{\log(\beta)} \cdot N\frac{\log(\alpha)}{\log(\beta)}) \) where \( N \) is the number of classes. Note that the true positive and false positive rates are computed as (27) and (28). Using the inequality \((1 - x)^{\frac{1}{x}} < e^{-c}\), we have

\[
b < \frac{\log \frac{1}{1-TP}}{\alpha^r} \quad (29)
\]

and using the inequality \((1 - x)^y > 1 - xy\) when \( x, y > 0 \), we have

\[
FP < b\beta^r \quad (30)
\]

Therefore, the expected complexity of Algorithm 1 is equal to the complexity of \( rb \) hashes and checking \( N \times FP \) recalls. Therefore, expected value of the complexity is equal to

\[
E(\text{complexity}) = c_{FP}N \times FP + c_H \times r \times b \quad (31)
\]

where \( c_{FP} \) is the complexity of checking each false positive, and \( c_H \) is the complexity of hashing a data point for each hash. From (29) and (30), we have

\[
c_{FP}N \times FP + c_H \times r \times b < \frac{\log \frac{1}{1-TP}}{\alpha^r} (c_{FP}N\beta^r + c_H r) \quad (32)
\]

The value of \( r \) minimizing the right hand side of (32) is

\[
r \approx \log \left( \frac{-c_H\log(\alpha)\log N}{c_{FP}N\log(\beta)} \right) \quad (35)
\]

is minimized by differentiating with respect to \( r \):

\[
g(r) = c_{FP}N \log \left( \frac{\beta}{\alpha} \right) \left( \frac{\beta}{\alpha} \right)^r + c_H \times r \log \left( \frac{1}{\alpha} \right) \left( \frac{1}{\alpha} \right)^r + c_H \left( \frac{1}{\alpha} \right)^r = 0 \quad (33)
\]
This results in the complexity,

\[ O((\log N)^{1 - \frac{\log(\alpha)}{\log(\beta)}} \cdot N ^ {\frac{\log(\alpha)}{\log(\beta)}}) \]  

(36)

**Remark 1** If \( \frac{\log(\alpha)}{\log(\beta)} \to 0 \), the complexity tends to \( O(\log N) \) which is the complexity of binary search.

If \( \frac{\log(\alpha)}{\log(\beta)} \to 1 \), the complexity tends to \( O(N) \) which is the complexity of brute force search.

### 4 Tree-wise hashing

![Hash tree](image)

**Figure 1**: Hash tree.

In the previous section, we proposed an efficient algorithm for solving the approximate ML classification problem based on a family of distribution sensitive hashes that satisfy (12) and (13). In this section, we design a universal family of hashes based on the decision trees that have Minhash and LSH-hamming as special cases (see Figure [13] in Appendix [B]).

We focus on probability distributions that can be factorized as the product of i.i.d components. Consider a decision tree \( G = (V, E, f) \) where \( V \) is the set of nodes, \( E \) is the set of edges, \( V_l \subset V \) is the set of leaf nodes in the tree, \( f_X : A \times V/V_l \to V \) and \( f_Y : B \times V/V_l \to V \) are the set of decisions. Here, we assume that at each edge of depth \( s \) in the tree, the decision is made based on single elements \( x_s \) and \( y_s \) where \( x = (x_1, \cdots, x_s, \cdots, x_S) \) and \( y = (y_1, \cdots, y_s, \cdots, y_S) \). Given the data point \( x = (x_1, \cdots, x_S) \), hash of \( x \) can be computed through the following iterations:

\[
\begin{align*}
v_0 & \leftarrow \text{root} \\
v_{s+1} & \leftarrow f_X(x_s, v_s), \quad 0 \leq s
\end{align*}
\]

(37)

(38)

\( g(r) \) is an increasing continuous function respect to \( r \) in \((0, \infty)\). Moreover, we have \( g(0) = c_H - c_{FP} N \log \left( \frac{\alpha}{\beta} \right) < 0 \) for large enough \( N \) and \( g(\infty) = \infty \). Therefore, (33) has a unique solution. Therefore, (32) has only one local minimum which is the solution of (33). From (33), we have \( r = \frac{\log \left( -c_H (r \log \frac{\alpha}{\beta} + 1) \right)}{c_{FP} N \log \frac{\alpha}{\beta}} \). Bounding the term \( r \log \frac{1}{N} + 1 \) with \( \frac{\log \alpha}{\log \beta} \log N \), we conclude (35). In order to see if bounding the term \( r \log \frac{1}{N} \) with \( \frac{\log \alpha}{\log \beta} \log N \) is reasonable, note that

\[
\log \frac{\alpha}{\log \beta} \log N > \frac{\log \left( -c_H \log \frac{\alpha}{\log \beta} \log N \right)}{c_{FP} N \log \frac{\alpha}{\beta}} \log \frac{1}{\alpha} \log \frac{\alpha}{\log \beta}
\]

(34)

which is true as for large enough \( N \), we have \( \log \left( \frac{N}{\log N} \right) \leq \log N \).
We stop whenever we reach a leaf node in the decision tree. Every iteration increment depth by one. Therefore, we eventually reach a leaf node, and we set \( h_X(x) \) as the index of that leaf node. We do a similar procedure for \( h_Y(y) \). We call this family of hashes the TreeDSH family. Algorithm 2 describes our method for computing the hashes used in Step 2 and 3 of Algorithm 1.

**Algorithm 2** Computing TreeDSH

**Inputs:** A decision tree \( G = (V, E, f_X, f_Y) \) with leaf nodes \( V_l \), decisions \( f_X : \mathcal{A} \times V/V_l \rightarrow V \) and a data point \( x = (x_1, \ldots, x_S) \).

**Outputs:** Hash \( h_X(x), 1 \leq h_X(x) \leq |V_l| \).

Initialize \( v = \text{root}(G) \) and \( s = 0 \).

While \( v \notin V_l \):

\[
\begin{align*}
  v & \leftarrow f_X(x_s, v) \\
  s & \leftarrow s + 1.
\end{align*}
\]

Return the index of the leaf node \( v \).

**Remark 2** In general, Algorithm 2 requires storing \( f_X : \mathcal{A} \times V \rightarrow V \) decision, where \( |V| \), the number of nodes in the tree, grows exponentially with the data dimension \( S \). This is also the case with the \( k-d \) tree approach [9]. In order to avoid exponential growth in the space complexity in Algorithm 4, in Section 5 we will provide a method to calculate the hashes without storing the decision tree. In this way, the complexity of hashing a data point through the tree will grow with the depth of the tree rather than the size of the tree.

In order to calculate the complexity of hashing using decision trees, we use the following lemma which provides a way to compute the collision probability of matched/random pairs in arbitrary decision trees.

**Definition 4** We define \( \alpha(G) \) and \( \beta(G) \) as

\[
\begin{align*}
  \alpha(G) & = \text{Prob}(h_X(x) = h_Y(y) \mid (x, y) \sim \mathcal{P}) \\
  \beta(G) & = \text{Prob}(h_X(x) = h_Y(y) \mid (x, y) \sim \mathcal{Q})
\end{align*}
\]

**Lemma 1** Let \( G = (V, E, f) \) Assume \( h_X(x) \) and \( h_Y(y) \) are the hashes constructed from the decision tree \( G \) using Algorithm 2. Then:

\[
\begin{align*}
  \alpha(G) & = \sum_{v \in V_l} A(v) \\
  \beta(G) & = \sum_{v \in V_l} B(v)
\end{align*}
\]

where \( V_l \) is the set of leaf nodes in the tree, \( A : V \rightarrow \mathbb{R} \) and \( B : V \rightarrow \mathbb{R} \) are defined iteratively as \( A(\text{root}) = 1, B(\text{root}) = 1 \), for \( w = f_X(x, v), x \in \mathcal{A}, v \in V \):

\[
\begin{align*}
  I & : V/\text{root} \rightarrow 2^\mathcal{A}, I(v) = \{x \in \mathcal{A} \mid f_X(x, v) = w\} \\
  J & : V/\text{root} \rightarrow 2^\mathcal{B}, J(v) = \{x \in \mathcal{B} \mid f_Y(y, v) = w\} \\
  A(w) & = A(v), \mathcal{P}(I(v) \times J(v)), \forall v \in V/\text{root} \\
  B(w) & = B(v), \mathcal{P}_X(I(v))\mathcal{P}_Y(J(v)), \forall v \in V/\text{root}
\end{align*}
\]
Note that, $A(v)$ and $B(v)$ can be implied as the probability ratios which we assign to each node in the decision tree satisfying the quality that the probability assigned to $v$ is $\mathbb{P}(I(v) \times J(v))$ times and $\mathbb{P}_{X}(I(v))\mathbb{P}_{Y}(J(v))$ times smaller than those assigned to its parent.

Proof of Lemma 1. Using induction we can show that for any $c \in V_t$,

$$A(v) = \text{Prob}(h_{X}(x) = \text{index}(v), h_{Y}(y) = \text{index}(v) \mid (x, y) \sim \mathbb{P})$$

Therefore,

$$\text{Prob}(h_{X}(x) = h_{Y}(y) \mid (x, y) \sim \mathbb{P}) = \sum_{v \in V_t} \text{Prob}(h_{X}(x) = \text{index}(v), h_{Y}(y) = \text{index}(v) \mid (x, y) \sim \mathbb{P})$$

$$= \sum_{v \in V_t} A(v)$$

$$= \alpha(G)$$

and (42) can be shown similarly.

In order to avoid exponential growth in space complexity, the algorithms 4 and 5 proposed in Section 5 provides an efficient way to find the decision trees that optimizes the complexity $\log \alpha / \log \beta$ where $\alpha$ and $\beta$ are given by (39) and (40).

We further show that the optimal tree is a homogeneous tree if the decisions at each node are independent of the node. In other words, the tree is homogeneous if there exist partitionings $I(1), I(2), \cdots, I(z) \subset 2^A$ and $J(1), J(2), \cdots, J(z) \subset 2^B$ such that:

$$\forall u, 1 \leq u \leq z, x \in I(u), v \in V, I(f_{X}(x, v)) = I(u)$$

$$\forall u, 1 \leq u \leq z, y \in I(u), v \in V, I(f_{Y}(y, v)) = I(u)$$

where each node $v$ has exactly $z$ children $\{w_1, \cdots, w_z\}$ with exception of the leaf nodes. Moreover, the decisions are fixed at each node of the tree:

$$\begin{cases} I(w_u) = I(u) \\ J(w_u) = J(u) \end{cases}, 1 \leq u \leq z$$

5  Constructing optimal decision trees for DSH

Consider the partitions

$$\mathcal{I} = \{I(1), \cdots, I(z) \mid I(u) \subset \mathcal{A}, 1 \leq u \leq z\}$$

$$\mathcal{J} = \{J(1), \cdots, J(z) \mid J(u) \subset \mathcal{B}, 1 \leq u \leq z\}$$

of alphabets $\mathcal{A}$ and $\mathcal{B}$ where

$$I(u) \cap I(u') = \emptyset, \text{ if } u \neq u'$$

$$J(u) \cap J(u') = \emptyset, \text{ if } u \neq u'$$

and define

$$\lambda = \min_{\mathcal{I}, \mathcal{J}} \frac{\mu - 1}{\mu}, \text{ s.t. } \sum_{1 \leq u \leq z} p_u^\mu q_u^{1-\mu} = 1,$$
where
\[ p_u = \mathbb{P}(I(u) \times J(u)) \]  \hspace{1cm} (59)
\[ q_u = \mathbb{Q}(I(u) \times J(u)) = \mathbb{P}_X(I(u))\mathbb{P}_Y(J(u)) \]  \hspace{1cm} (60)

Then\footnote{Note that \( p_u \) and \( q_u \) do not depend on the value of \( s \) as \( \mathbb{P} \) is factorizable to i.i.d. components.}

1. Lemma\footnote{Note that \( r_u \) does not depend on the value of \( s \).} 2 below shows that it is possible to design a homogeneous decision tree with complexity \( \lambda \). Therefore, this lemma provides an upper bound for the complexity.

2. Lemma 3 below shows that there is no homogeneous or heterogeneous decision tree with complexity below \( \lambda \). Thus, this lemma results in a lower bound for the complexity.

**Definition 5** Define
\[ r_u = \frac{p_u}{q_u} \]  \hspace{1cm} (61)
for \( 1 \leq u \leq z \). Without loss of generality, assume \( p_u \geq q_u \) for \( 1 \leq u \leq z \).

**Definition 6** Given a threshold \( T \), we define the decision tree \( G(T) \) as the output of Algorithm 3. In this algorithm, we start from the root and construct the tree and a function \( R : V \to \mathbb{R} \) recursively, stopping whenever we reach a node \( v \) where \( R(v) > e^T \).

**Algorithm 3** Constructing the decision tree \( G(T) \)

**Inputs:** Partitionings \( \{I(1), I(2), \cdots, I(z)\} \) of \( A \) and \( \{J(1), J(2), \cdots, J(z)\} \) of \( B \), ratios \( r_1, \cdots, r_z \) and the threshold \( T \).

**Outputs:** Decision tree \( G = (V, E, f_X, f_Y) \).

**Initialization:**
Create a new node \( \text{root} \).
\( R(\text{root}) \leftarrow 1 \).
\( \text{ConstructTree(\text{root}).} \)

**Procedure** \( \text{ConstructTree}(v) \).

For \( u = 1 \) to \( z \) # Create \( z \) children for each node \( v \).
Create a new node \( w \).
\( R(w) \leftarrow R(v)r_u \)
If \( R(w) \leq e^T \)
For \( x \in I(u) \)
\[ f_X(x, v) \leftarrow w \]
For \( y \in J(u) \)
\[ f_Y(y, v) \leftarrow w \]
\( V.\text{insert}(w) \).  # Add \( v \) to the nodes of \( G \).
\( E.\text{insert}(v, w) \).  # Add \( (v, w) \) to the edges of \( G \).
\( \text{ConstructTree}(w) \).
Else
Prune \( w \).

Return \( G(T) \).
Lemma 2 Define

\[ r_{\text{max}} = \max_{1 \leq u \leq z} r_u \]  

Then, for any decision tree \( G(T) \) defined above, we have

\[ e^{-(\mu - 1)T} \leq \alpha(G(T)) \leq r_{\text{max}}^{\mu - 1} e^{-(\mu - 1)T} \]  
\[ e^{-\mu T} \leq \beta(G(T)) \leq r_{\text{max}} \mu e^{-\mu T} \]  

Therefore:

\[ \lim_{T \to \infty} \frac{\log(\alpha(G(T)))}{\log(\beta(G(T)))} = \frac{\mu - 1}{\mu} \]  

Lemma 3 There is no hash-tree with complexity below \( \lambda \).

5.1 Proof of Lemma 2

First of all, note that from (58) and using \( r_u = \frac{p_u}{q_u} \) we have

\[ \sum_{1 \leq u \leq z} p_u r_u^{\mu - 1} = 1 \]  

and for each leaf nodes \( v \) of \( G(T) \) with parent \( w \), we have

\[ \frac{R(v)}{r_{\text{max}}} \leq R(w) < R(v) \]  

Therefore, we have

\[ e^T < R(v) < r_{\text{max}} e^T \]  

Moreover, for leaf nodes \( V_l^G \) of \( G(T) \) we have

\[ \sum_{v \in V_l(G)} A(v) R(v)^{\mu - 1} = 1 \]  

(See Appendix C for the proof) From (68) and (69) we conclude that

\[ e^{-(\mu - 1)T} \leq \sum_{v \in V_l(G)} A(v) \leq e^{-(\mu - 1)T} r_{\text{max}}^{\mu - 1} \]  

Similarly, we have

\[ e^{-\mu T} \leq \sum_{v \in V_l(G)} B(v) \leq e^{-\mu T} r_{\text{max}}^{\mu} \]  

From Lemma 1, we have \( \alpha(G(T)) = \sum_{v \in V_l(G)} A(v) \) and \( \beta(G(T)) = \sum_{v \in V_l(G)} B(v) \). Therefore, Lemma 2 holds.
5.2 Proof of Lemma 3

Before proving Lemma 3 for the decision tree $G = (V, E, f_X, f_Y)$ we define

$$D : V \rightarrow \mathbb{R}$$

$$D(v) = A(v)^\mu B(v)^{1-\mu}, \forall v \in V$$

where $\mu$ is defined in (58). Then,

$$\alpha(G) \mu \beta(G)^{1-\mu} \leq \sum_{v \in V_l(G)} D(v) \leq 1$$

where $V_l(G)$ is the set of leaf nodes in $G$. First of all, we show that

$$\sum_{v \in V_l(G)} D(v) \leq 1$$

by induction on the number of nodes in the tree. If the tree has only one node, i.e., root, then (75) holds as $A(root) = 1$ and $B(root) = 1$ from the definition of $A(v)$ and $B(v)$ in (45) and (46). Assume that (75) holds for any decision tree with $|V| < Z$. Our goal is to prove that (75) holds for a decision tree with $|V| = Z$. Assume $w_1$ is the node with maximum length in $G$ and consider a tree $G'$ constructed by removing $w_1$ and all its siblings $w_2, \ldots, w_z$ belonging to the same parent $w$. Then:

$$\sum_{v \in V_l(G)} D(v)$$

$$= \sum_{v \in V_l(G')} D(v) - A(w)^\mu B(w)^{1-\mu} + \sum_{u=1}^z A(w_u)^\mu B(w_u)^{1-\mu}$$

$$= \sum_{v \in V_l(G')} D(v) - A(w)^\mu B(w)^{1-\mu} + \sum_{u=1}^z A(w)^\mu B(w)^{1-\mu} p_{w_u} \mu q_{w_u}^{1-\mu}$$

$$= \sum_{v \in V_l(G')} D(v) - A(w)^\mu B(w)^{1-\mu} \left( 1 - \sum_{u=1}^z p_{w_u} \mu q_{w_u}^{1-\mu} \right)$$

$$\leq \sum_{v \in V_l(G')} D(v)$$

where (76) holds from the definition of tree $G'$, (77) follows from the recursive definition of $A(v)$ and $B(v)$ in (45) and (46). To see why (79) holds, note that from the definition of $\mu$ in (58) we have

$$\sum_{1 \leq u \leq z} p_u \mu q_u^{1-\mu} \leq 1$$

In order to see why (80) is true, assume that for some partitioning $I$ and $J$, $\sum_{1 \leq u \leq z} p_u \mu q_u^{1-\mu} > 1$. Therefore, as $\sum_{1 \leq u \leq z} p_u \mu q_u^{1-\mu}$ is an increasing function respect to $\mu$, there is a $\mu'$ where $\mu' < \mu$ and $\sum_{1 \leq u \leq z} p_u \mu' q_u^{1-\mu'} = 1$. However, $\mu'$ is smaller than $\mu$, and this contradicts with the definition of $\mu$ in (58). Note that $\frac{p_u}{q_u} \geq 1$, therefore, $\sum_{1 \leq u \leq z} p_u \mu q_u^{1-\mu}$ is an increasing function with respect to $\mu$. 

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Therefore, we conclude that

$$\sum_{v \in V_l(G)} D(v) \leq 1 \quad (81)$$

On the other hand,

$$\frac{\sum_{v \in V_l(G)} D(v)}{|V_l|} = \frac{\sum_{v \in V_l(G)} A(v)^\mu B(v)^{1-\mu}}{|V_l|} \geq \left( \sum_{v \in V_l(G)} A(v) \right)^\mu \left( \sum_{v \in V_l(G)} B(v)^{1-\mu} \right) \quad (82)$$

$$= \frac{\alpha(G)^\mu \beta(G)^{1-\mu}}{|V_l|} \quad (84)$$

In order to show (83), note that the function $f(r, s) = r^\mu s^{1-\mu}$ is a convex function when $\mu > 1, p, q \geq 0$. In fact, the Hessian matrix of second partial derivatives of $f(r, s)$ is equal to

$$H(f) = \left| \begin{array}{cc} \frac{\partial^2 r^\mu s^{1-\mu}}{\partial r \partial s} & \frac{\partial^2 r^\mu s^{1-\mu}}{\partial s^2} \\ \frac{\partial^2 r^\mu s^{1-\mu}}{\partial r^2} & \frac{\partial^2 r^\mu s^{1-\mu}}{\partial s^2} \end{array} \right|$$

$$= \begin{vmatrix} \mu(\mu - 1)r^{\mu-2}s^{1-\mu} & \mu(1 - \mu)r^{\mu-1}s^{-\mu} \\ \mu(1 - \mu)r^{\mu-1}s^{-\mu} & \mu(\mu - 1)r^\mu s^{-1-\mu} \end{vmatrix}$$

Determinant of $H(f)$ is equal to zero and its trace is a non-negative real number for $\mu > 1, p, q \geq 0$. Therefore, we conclude that $f(r, s) = r^\mu s^{1-\mu}$ is a convex function and

$$\alpha(G)^\mu \beta(G)^{1-\mu} \leq 1 \quad (85)$$

$$\Rightarrow \frac{\log \alpha(G)}{\log \beta(G)} \geq \frac{\mu - 1}{\mu} = \lambda \quad (86)$$

5.3 Algorithms

Lemma 2 and 3 show that the optimal decision trees are homogeneous. In fact in Lemma 2 we design a homogeneous tree with complexity $\lambda$ and in Lemma 3 we prove that there is no decision tree with the complexity below $\lambda$. Algorithm 4 proposes an efficient method for hashing data points in case of the homogeneous trees without any need for the construction and storage of the complete decision tree, and the complexity of the algorithm is equal to the depth of the tree. Using this method, the complexity of hashing will grow linearly with the number of the data points and the depth of the tree rather than the size of the tree. In fact, in order to compute the hash for each data point $x$, we need to explore a single trajectory from the root to the leaf node with complexity equal to the depth of tree, therefore the complexity per data point is equal to the depth of the tree.

The following algorithm assumes that the number of hashes $b$, threshold $T$ and factors $r_1, \cdots, r_z$ are known. Later in Algorithm 5 we will provide a method for finding the optimal value of these parameters.
Algorithm 4 Computing hashes in the homogeneous trees

**Inputs:** Partitions \( \{I(1), \cdots, I(z)\} \subset A, \{J(1), \cdots, J(z)\} \subset B, \{r_1, \cdots, r_z\} \), threshold \( T > 0 \) and the data point \( x = (x_1, \cdots, x_S) \).

**Outputs:** \( h_X(x) \).

Initialize \( R = 1, s = 0 \) and \( h_X = \emptyset \).

While \( R \leq e^T \)

- Find \( 1 \leq u \leq z \) for which \( x_s \in I(u) \)
- \( R \leftarrow R.r_u \)
- \( s \leftarrow s + 1 \)
- \( h_X(x).append(u) \)

\( \emptyset \) stand for an empty vector and \( h_X(x).append(u) \) is a command for adding an entry \( u \) to the vector \( h_X(x) \).

Remark 3 Note that in the locality sensitive hashing literature, parameter \( r \), i.e., the number of rows, and \( b \), i.e., the number of bands, are used to control the collision probability for matched and random pairs. In the case of TreeDSH, we use the parameters \( T \) and \( b \) to accomplish this.

The following algorithm is used to set parameters in Algorithm 4. Here, we assume that a penalty \( C_{FP} \) for each false positive and \( C_D \) for each decision-making in the decision tree are given, and using these two penalties, we attempt to design a decision-tree with minimum total penalty with a specific true positive rate.

Algorithm 5 Parameters Setting

**Inputs:** \( \{p_1, \cdots, p_z\}, \{q_1, \cdots, q_z\} \), number of classes \( N \), minimum acceptable true positive rate \( TP \), false positive penalty \( C_{FP} \) and decision-making hashing penalty \( C_D \).

**Outputs:** Parameters \( b, T \) and \( \{r_1, \cdots, r_z\} \).

**Step 1:** Compute \( \alpha(G(T)), \beta(G(T)) \) and \( \text{len}_Y(G(T)) \) using (41), (42) and (93).

**Step 2:** Set

\[
b(T) = \frac{\log(1 - TP)}{\log(1 - \alpha(G(T)))} \tag{87}
\]

**Step 3:** Find \( T_{\text{min}} \) as follows.

\[
T_{\text{min}} = \arg \min_{T \geq 0} (C_{FP}.N.FP + C_D.\text{len}_Y(G(T)).b(T)) \tag{88}
\]

where \( FP \) is computed as

\[
FP = 1 - (1 - \beta(G(T)))^{b(T)} \tag{89}
\]

**Step 4:** Report \( r_u = \frac{p_u}{q_u}, 1 \leq u \leq z, T_{\text{min}} \) and \( b(T_{\text{min}}) \).
6 Complexity of TreeDSH

In this section, we derive the complexity for LSH-hamming, Minhash and TreeDSH for perfect recovery of correct pairs. Here, we focus on the case \( \mathcal{A} = \{0,1\}, \mathcal{B} = \{0,1\} \). Assume \( \mathbb{P} = \begin{bmatrix} p_{00} & p_{01} \\ p_{10} & p_{11} \end{bmatrix} \)

and \( \mathcal{Q} = \begin{bmatrix} q_{00} & q_{01} \\ q_{10} & q_{11} \end{bmatrix} \). In case of LSH-hamming, the query complexity is

\[
O((\log N)^{\frac{1}{\mu}}.N^{\frac{\mu-1}{\mu}})
\]

(94)

and the storage required for the algorithm is \( O((\log N)^{1+\min\left(\frac{\log(p_{00}+p_{11})}{\log(q_{00}+q_{11})},\frac{\log(p_{01}+p_{10})}{\log(q_{01}+q_{11})}\right)} \) where \( N \) is the number of data points. Furthermore, for Minhash the query complexity is

\[
N^{\min(mh_1,mh_2,mh_3,mh_4)}
\]

(91)

where \( mh_1 = \frac{\log p_{00}}{\log \frac{p_{00}}{1-q_{11}}} \), \( mh_2 = \frac{\log p_{10}}{\log \frac{p_{10}}{1-q_{01}}} \), \( mh_3 = \frac{\log p_{01}}{\log \frac{p_{01}}{1-q_{10}}} \) and \( mh_4 = \frac{\log p_{11}}{\log \frac{p_{11}}{1-q_{00}}} \). In case of TreeDSH, the complexity is

\[
c_{FP}.N.FP + C_D.len_Y(G(T)).b(T)
\]

(92)

where \( c_{FP} \) is the penalty for false positive, \( C_D \) is the complexity per each decision-making in the decision tree, and \( len_Y(G(T)) \) is defined as

\[
len_Y(G(T)) = \sum_{v \in V_T} \mathbb{P}_Y(v).\text{depth}(v)
\]

(93)

In fact, \( len_Y(G(T)) \) represents the average number of decision-makings required for hashing a data point \( y \) through the tree \( G(T) \). Assuming \( I(0) = J(0) = \{0\} \) and \( I(1) = J(1) = \{1\} \), similar to (29)-(36), the minimum of (92) is

\[
O((\log N)^{\frac{1}{\mu}}.N^{\mu-1})
\]

(94)

where \( \mu \) is the positive solution of the following equality\(^{11}\)

\[
(p_{00})^\mu(q_{00})^{1-\mu} + (p_{11})^\mu(q_{11})^{1-\mu} = 1
\]

(95)

Moreover, the storage complexity for TreeDSH is \( O((\log N)^{\frac{1}{\mu}}.N^{1+\mu-1}) \). Algorithm 5 provides the parameters to reach this minimum for general distributions.

\textbf{Remark 4} For \( z = 2 \) and the \( 2 \times 2 \) probability matrix \( \mathbb{P} = \begin{bmatrix} p_{00} & p_{01} \\ p_{10} & p_{11} \end{bmatrix} \), we need to consider the two partitionings, \( I(0) = J(0) = \{0\}, I(1) = J(1) = \{1\} \) and \( I(0) = J(1) = \{0\}, I(1) = J(0) = \{1\} \). For

\(^{10}\)In this section, we represent the probability distribution \( \mathbb{P} \) with the \( k \times l \) matrix \( \begin{bmatrix} p_{00} & \cdots & p_{0l} \\ \vdots & \ddots & \vdots \\ p_{k0} & \cdots & p_{kl} \end{bmatrix} \) with \( p_{ij} = p(x_i = i, y_j = j) \) in its \( i \)-th row and \( j \)-th column.

\(^{11}\)\( \mu \) has a positive solution as the left side of (92) is less than 1 for \( \mu = 1 \), and greater than one when \( \mu \) tends to \( \infty \).
the first partitioning, \( r_0 = p_{00}/q_{00} \) and \( r_1 = p_{11}/q_{11} \). By computing \( r_0 \) and \( r_1 \), it is observed that if \( p_{00}p_{11} > p_{01}p_{10} \), then \( r_0, r_1 > 1 \). On the other hand, for the other partitioning \( r'_0 = p_{01}/q_{01}, r'_1 = p_{10}/q_{10} \) we have \( r'_0, r'_1 > 1 \) if \( p_{00}p_{11} < p_{01}p_{10} \). Therefore, for \( z=2 \), there always exists a partitioning where the ratios are larger than one.

**Example 1** Assume \( A = \{0, 1\} \) and \( B = \{0, 1\} \) and consider the probability distribution \( P_1 = \begin{bmatrix} 0.215 & 0.0025 \\ 0.255 & 0.5275 \end{bmatrix} \). Minhash has the complexity \( \log \frac{p_{00}}{q_{00}} - \log \frac{p_{11}}{q_{11}} = 0.4512 \) to achieve perfect true positive rate and LSH-hamming algorithm has the complexity \( \log \frac{p_{00} + p_{11}}{q_{00} + q_{11}} = 0.4512 \) for this distribution. For TreeDSH, assuming \( I(0) = J(0) = \{0\} \) and \( I(1) = J(1) = \{1\} \), \( (95) \) has a unique positive solution \( \mu = 1.733 \) resulting in the complexity \( \frac{1}{\mu} = 0.4229 \). In order to design a decision tree that realizes this complexity, we set \( r_0 = \frac{p_{00}}{q_{00}} = 2.103, r_1 = \frac{p_{11}}{q_{11}} = 1.272 \) and trim the tree at threshold \( T = \ln(1.5) \) (Fig. 2). Figure 3 shows another hash-tree for the same probability distribution with \( T = \ln(2.5) \) and \( T = \ln(3) \).

![Hash tree for \( P_1 \) defined in Example 1 and \( T = \ln(1.5) \).](image)

Then, Algorithm \( 4 \) introduces the following hashes in the tree:

\[
\begin{align*}
  h_X(x) &= \begin{cases} 
    1 & \text{if, } x_1 = x_2 = 1 \\
    2 & \text{if, } x_1 = 1, x_2 = 0 \\
    3 & \text{if, } x_1 = 0 
  \end{cases} \\
  h_Y(y) &= \begin{cases} 
    1 & \text{if, } y_1 = y_2 = 1 \\
    2 & \text{if, } y_1 = 1, y_2 = 0 \\
    3 & \text{if, } y_1 = 0
  \end{cases}
\end{align*}
\]  

(96)  

(97)

\(^{12}\)Note that, when \( p_{00}p_{11} = p_{01}p_{10} \), \( r_0 = r_1 = 1 \) no matter what partitioning we choose, resulting in tree with infinite depth and complexity \( O(N) \). In fact \( p_{00}p_{11} = p_{01}p_{10} \) holds only when \( P = Q \) and in this case matching pairs are independent.
From \([41]\), \(\alpha\) is derived as,

\[
\alpha = \text{Prob}(h_X(x) = h_Y(y) \mid (x, y) \sim \mathbb{P}) = \text{Prob}(h_X(x) = h_Y(y) = 1 \mid (x, y) \sim \mathbb{P}) + \text{Prob}(h_X(x) = h_Y(y) = 2 \mid (x, y) \sim \mathbb{P}) + \text{Prob}(h_X(x) = h_Y(y) = 3 \mid (x, y) \sim \mathbb{P})
\]

\[
= p_{11}^2 + p_{00}p_{11} + p_{00} = 0.606
\]

Similarly,

\[
\beta = q_{11}^2 + q_{00}q_{11} + q_{00} = 0.3166
\]

Now the question is how we can use these decision trees to design an algorithm for efficient classification. Assume two data points \((x_1, \cdots, x_S)\) and \((y_1, \cdots, y_S)\). Similar to Algorithm \([1]\), we randomly select \(2b\) numbers \(1 \leq s_{1,j} < s_{2,j} < s\) for \(1 \leq j \leq b\). For each \(1 \leq j \leq b\), we define \(h^j_X(x)\) and \(h^j_Y(y)\) as follows:

\[
h^j_X(x) = \begin{cases} 
1 & \text{if, } x_{s_{1,j}} = 1 \\
2 & \text{if, } x_{s_{1,j}} = 0, x_{s_{2,j}} = 1 \\
3 & \text{if, } x_{s_{1,j}} = x_{s_{2,j}} = 0
\end{cases}
\]

\[
h^j_Y(y) = \begin{cases} 
1 & \text{if, } y_{s_{1,j}} = 1 \\
2 & \text{if, } y_{s_{1,j}} = 0, y_{s_{2,j}} = 1 \\
3 & \text{if, } y_{s_{1,j}} = y_{s_{2,j}} = 0
\end{cases}
\]

Now, for any \(1 \leq j \leq b\) we have

\[
\text{Prob}(h^j_X(x) = h^j_Y(y) \mid (x, y) \sim \mathbb{P}) = \alpha
\]

\[
\text{Prob}(h^j_X(x) = h^j_Y(y) \mid (x, y) \sim \mathbb{Q}) = \beta
\]

Therefore, the probability of collision in at least one of the bands can be computed as:

\[
\text{Prob}(h^1_X(x) = h^1_Y(y) \text{ or } \cdots \text{ or } h^b_X(x) = h^b_Y(y) \mid (x, y) \sim \mathbb{P}) = 1 - (1 - \alpha)^b
\]

\[
\text{Prob}(h^1_X(x) = h^1_Y(y) \text{ or } \cdots \text{ or } h^b_X(x) = h^b_Y(y) \mid (x, y) \sim \mathbb{Q}) = 1 - (1 - \beta)^b
\]

From the values of \(\alpha\) and \(\beta\) in \((100)\) and \((101)\), if we use only one band \((b = 1)\), the chance of matched pairs having collision is \(\alpha = 0.606\), while the chance of random pairs having collision is \(\beta = 0.316\). If we have 3 bands \((b = 3)\), the chance of collision in at least one band for the matched pairs is \(1 - (1 - \alpha)^3 = 0.938\), while the chance for the random pairs is \(1 - (1 - \beta)^3 = 0.679\).

In Section 4 we showed that given \(\alpha\) and \(\beta\), it is possible to design hashes with complexity \(O(N \log \log N)\) to discover almost all of the matched pairs. Now, the question is how we can design the tree that finds optimal \(\alpha\) and \(\beta\). In Lemma 2 and 3, we showed that the optimal tree is homogeneous, and it can be reconstructed based on two parameters \(r_0 = \frac{p_{00}}{q_{00}}\) and \(r_1 = \frac{p_{11}}{q_{11}}\).

**Example 2** Fig. 8, 9, 10 and 11 show \(\alpha(T)\), \(\beta(T)\), \(\frac{\log \alpha(T)}{\log \beta(T)}\) and \(\text{len}(T)\) as a function of \(T\) for the matrix \(\mathbb{P}_1\). From the previous example, Figures 9 and 10 confirm that \(\alpha(T)\) and \(\beta(T)\) are bounded from below and above by the exponential functions as demonstrated in (63) and (64). Fig. 8 shows that for large values of \(T\), \(\frac{\log \alpha(T)}{\log \beta(T)}\) converges to \(\frac{\mu - 1}{\mu}\) as shown in Lemma 2. Figure 11 shows that \(\text{len}_Y(T)\) grows linearly with \(T\).
Figure 3: Equivalent hash trees are depicted for Example 1. T is the factor determining the growth in the tree. For instance, consider the leaf node on the bottom left. For this node, the probability ratio is equal to $r^5_1 = 3.30$ which is greater than the $T = \ln(3)$, while for its parent node the probability ratio is equal to $r^4_1 = 2.617$ which is less than $T = \ln(3)$. Note that, $\alpha(T = \ln(2.5)) = \sum_{v \in V_1} A(v) = 0.4419$ and $\alpha(T = \ln(3)) = \sum_{v \in V_1} A(v) = 0.3635$ are calculated by summing the probability of all six and nine leaves in the corresponding hash trees respectively, e.g., $\alpha(T = \ln(2.5)) = \sum_{v \in V_1} A(v) = p_{00} * p_{00} + p_{00} * p_{11} + p_{00} * p_{00} + p_{11} * p_{11} * p_{11} * p_{11}$, etc. Here, we show an example of the tree construction for the matrix $P_1$ and thresholds $T = \ln(2.5)$ and $T = \ln(3)$. Moreover, $\alpha(T = \ln(2.5))$ and $\alpha(T = \ln(3))$ are computed as $\alpha(T = \ln(2.5)) = \sum_{v \in V_1} A(v) = 0.4419$, $\alpha(T = \ln(3)) = \sum_{v \in V_1} A(v) = 0.3635$. Similarly, we conclude that $\beta(T = \ln(2.5)) = \sum_{v \in V_1} B(v) = 0.1497$, $\beta(T = \ln(3)) = \sum_{v \in V_1} q(v) = 0.09444$. Therefore, the complexity is equal to $\frac{\log \alpha(T = \ln(2.5))}{\log \beta(T = \ln(2.5))} = 0.4301$ and $\frac{\log \alpha(T = \ln(3))}{\log \beta(T = \ln(3))} = 0.4288$ for thresholds $T = \ln(2.5)$ and $T = \ln(3)$, respectively.

7 Experiments

In this section, we will benchmark TreeDSH against LSH-hamming and MinHash, both theoretically and through simulations. Our results show that TreeDSH is a universal hashing scheme that performs well for various probabilistic settings (e.g. sparse and dense). We tried to benchmark TreeDSH complexity with the algorithm presented by Dubiner [16]. However, equation (126) from [16] is computationally intractable which makes it impossible to compute the complexity for the algorithm presented there. In Experiment 3, we further applied TreeDSH to the problem of peptide identification from the mass spectrometry data.

**Experiment 1** Figure 4 shows the false positive rate with respect to $b$ for the three algorithms Minhash, LSH-hamming and TreeDSH, and the probability distribution $P_1$ considered in Example 7.
Figure 4: False positive is plotted with respect to $b$ for TreeDSH, Minhash and LSH-hamming at 99% true positive rate.

In case of TreeDSH, we changed the threshold $T$, from 0 to 7, and for each value of $T$, computed the number of bands $b$ required for achieving the true positive rate 99% \((87)\). We further used $b(T)$ to compute the false positive rate \((89)\). In case of LSH-hamming (Minhash), we changed $r$ from 1 to 16 (1 to 6 for Minhash), and for each value of $r$, we used \((27)\) to find the number of bands $b(T)$ required to achieve the true positive rate 99%. Finally, using \((28)\), we derived the false positive rate. Our results show that at fixed $TP$ and number of bands, TreeDSH achieves smaller false positive rates (Fig. 4).

**Experiment 2** In this experiment, we compared the complexity for the three algorithms LSH-hamming, Minhash and TreeDSH for a range of probability distributions. We benchmark the three methods using matrices $P(t) = P_2(1 - t) + P_3t$ where $0 \leq t \leq 1$ where $P_2 = \begin{bmatrix} 0.345 & 0 \\ 0.31 & 0.345 \end{bmatrix}$ and $P_3 = \begin{bmatrix} 0.019625 & 0 \\ 0.036875 & 0.9435 \end{bmatrix}$. Fig. 5 shows the theoretical complexity of TreeDSH, Minhash and LSH-hamming using equations \((90)\), \((91)\) and \((94)\) for each matrix. In Fig. 6, we simulated $N$

Figure 5: Complexity of LSH-hamming, Minhash and TreeDSH, i.e., $\frac{\log \alpha}{\log \beta}$ is plotted for all the probability distribution matrices $P(t) = P_2(1 - t) + P_3t$ where $0 \leq t \leq 1$. $t$ is between 0 and 1 not $P(t)$.

*S-dimensional classes $\{x_1, \cdots, x_N\}$ and $N$ $S$-dimensional data points $\{y_1, \cdots, y_N\}$ where each
$(x_i, y_i)$ is generated from $\mathbb{P}_1$, and $x_i$ is independent of $y_j$ for $i \neq j$ ($N = 2000, S = 10000$). Then,

**Figure 6:** Total simulation time for the three algorithms is plotted for all the probability distribution matrices $\mathbb{P}(t) = \mathbb{P}_2(1 - t) + \mathbb{P}_3 t$ where $0 \leq t \leq 1$. The results are consistent with the theoretical guarantees in Fig. 5.

we used TreeDSH, LSH-hamming and Minhash to find the matched pairs. In each case, we tuned $T$, $r$ and $b$ to achieve 99% true positive rate, while minimizing the total time spent on hashing and verifying the false positives.

In both the theoretical results in Fig. 5 and simulations in Fig. 6 for sparse matrices ($t \approx 1$), Minhash and TreeDSH outperform LSH-hamming. Moreover, In denser cases ($t \approx 0$) LSH-hamming and TreeDSH outperform Minhash. This experiment shows TreeDSH is a universal hashing scheme that improves on both LSH-hamming and Minhash for various probability distributions.

In Fig. 7 we plot total simulation time for the three algorithms with probability distribution $\mathbb{P}_1$ from Example 1 with respect to number of data points $N$ and $S = 10000$. Here, the optimal parameters for each method is selected to achieve $TP = 99\%$.

**Figure 7:** Total simulation time for TreeDSH, Minhash, LSH-hamming with probability distribution $\mathbb{P}_1$ and $S = 10000$ is plotted for various values of $N$. Here, the optimal parameters for each method is selected to achieve $TP = 99\%$.  

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Figure 8: The complexity $\frac{\log \alpha(T)}{\log \beta(T)}$ is plotted with respect to the threshold $T$.

Figure 9: $\alpha(T)$, the lower bound on $\alpha(T)$ and the upper bound on $\alpha(T)$ are plotted with respect to the threshold $T$. The lower bound and upper bound on $\alpha(T)$ are derived from (63).

Figure 10: $\beta(T)$, the lower bound on $\beta(T)$ and the upper bound on $\beta(T)$ are plotted with respect to the threshold $T$. The lower bound and upper bound on $\beta(T)$ are derived from (64).
Figure 11: \( \text{len}_X(T) \) and \( \text{len}_Y(T) \) grow linearly with respect to threshold \( T \). Note that, \( \text{len}_X(T) \) and \( \text{len}_Y(T) \) determine the complexity of hashing a single data point \( x \) and \( y \), respectively.

**Example 3** Consider the following probability distribution \( P = \begin{bmatrix} p_{00} & p_{01} \\ p_{10} & p_{11} \end{bmatrix} \) with \( p_{00} = p_{11} = \frac{p}{2}, p_{10} = p_{01} = \frac{1-p}{2} \). For the LSH-hamming, we get the complexity \( \log \frac{1}{p} \) while for the TreeDSH from (58) we have

\[
\left( \frac{p}{2} \right)^\mu \left( \frac{1}{4} \right)^{1-\mu} = \frac{1}{2}
\]

\[
\rightarrow \mu \log \frac{p}{2} + (1-\mu) \log \left( \frac{1}{4} \right) = -1
\]

Therefore, the complexity is \( \frac{\mu-1}{p} = \log \frac{1}{p} \) which is the same as the complexity we get for the LSH-hamming. In fact, for this joint probability distribution, the optimal tree hash is the same as LSH-hamming.

**Experiment 3** [Application of TreeDSH to peptide identification in mass spectrometry] In this experiment, we applied TreeDSH to the problem of peptide identification from mass spectrometry data. In this problem, we have a large number of \( S \)-dimensional binary vectors \( x \) (peptides) and \( y \) (spectra) where \( S = 4710 \). The problem of peptide identification from mass spectrometry is to assign each spectra \( y \) to a peptide \( x \) that is most likely to generate it. The state of the art approach to peptide identification is based on learning the conditional probability distribution \( P(y \mid x) = \prod_{s=1}^{S} p(x_s \mid y_s) \) based on a training dataset of matching peptide and spectra. Here, we use \( P(y \mid x) \) introduced in [2]. The next step is to use this model to find peptide \( x \) for each spectra \( y \) that maximize \( P(y \mid x) \).

Currently, the state of the art approach use brute-force to compute \( P(y \mid x) \) for all the candidate peptides[2]. This can be a very time consuming task when we search against all the peptides from the human proteome (billions of peptides). We compared the performance of TreeDSH against the state of art brute-force search. Training on the known peptide and spectra matches, the joint probability distribution is \( P = \begin{bmatrix} 0.975159 & 0.005308 \\ 0.015924 & 0.003609 \end{bmatrix} \). In this case \( \mu = 1.6073 \) and the complexity is \( \frac{\mu-1}{\mu} = 0.3778 \). Algorithm delivers \( T_{\text{min}} = 6.5 \) and \( b(T_{\text{min}}) = 228 \) as the optimal parameters for TreeDSH to achieve 99% true positive rate (Fig. 12). When searching each spectra against 10231 peptides using the TreeDSH method with these parameters, we encounter an average 525 false

\[13\] Note that, the probability distribution \( p_{00} = p_{11} = \frac{p}{2}, p_{10} = p_{01} = \frac{1-p}{2} \), has the marginal probability distribution \( q_{00} = q_{01} = q_{10} = q_{11} = \frac{1}{4} \).
positives. It takes 132 microseconds per spectra to compute the hashes and 2 milliseconds per spectra to resolve all the false positives. The brute-force algorithm takes 493 milliseconds/spectra, and TreeDSH approach is two orders of magnitude faster than the brute-force approach. The complexity of search against $N$ peptides using TreeDSH is $O(N^{0.3778})$ compared to $O(N)$ for the brute-force algorithm.

![Figure 12: Complexity $N.FP + b$ as a function of the threshold $T$ for peptide identification by mass spectrometry problem.](image)

8 Conclusion

In this paper, we proposed a new algorithm for efficient maximum likelihood classification of high dimensional data point $y$ into classes $\{x_1, x_2, \cdots, x_N\}$ when the probability setting $p(y \mid x)$ is known. Multiclass classification methods provide a way to classify among $N$ classes with logarithmic complexity [9, 10, 11]. However, these methods are not applicable to high dimensional data. In order to solve the approximate maximum likelihood classification problem, we introduced the distribution sensitive hashing paradigm, which is adapted from the locality sensitive hashing paradigm to classify probability distributions. We further demonstrated guarantees on the complexity of our algorithms, and provided a method for the construction of these hashes using decision trees. Our method provides a universal technique for finding the optimal decision tree to minimize the complexity for the joint probability distributions that are factorizable to i.i.d factors.

While the size of the decision tree can grow exponentially with the dimension of data, we provided a method to hash each data point without the need to construct/store the whole decision tree (data-dependent hashing). Therefore, the complexity of the algorithm provided in this paper grows with $O(N^{\lambda}(\log N)^{1-\lambda})$ for some $\lambda < 1$. For the deterministic distributions, $\lambda \to 0$ and the complexity is $O(\log N)$, while for the independent distributions $\lambda \to 1$ and the complexity is $O(N)$.

Although our algorithm involves multiple parameters, we provide a method for setting all the parameters and prove its correctness. In the future work, we will further extend our method to do the classification when $p(y \mid x)$ is unknown.

References

[1] R. Aebersold and M. Matthias, “Mass spectrometry-based proteomics,” Nature, vol. 422, no. 6928, p. 198, 2003.

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[2] S. Kim and P. Pevzner, “MS-GF+ makes progress towards a universal database search tool for proteomics,” *Nature communications*, vol. 5, p. 5277, Oct 2014.

[3] A. Gionis, P. Indyk, and R. Motwani, “Similarity search in high dimensions via hashing,” *In Vldb*, vol. 99, no. 6, pp. 518–529, 1999.

[4] M. Datar, N. Immorlica, P. Indyk, and V. Mirrokni, “Locality-sensitive hashing scheme based on p-stable distributions,” *In Proceedings of the twentieth annual symposium on Computational geometry, ACM*, pp. 253–262, June 2004.

[5] E. Cohen, M. Datar, S. Fujiwara, A. Gionis, P. Indyk, R. Motwani, and C. Yang, “Finding interesting associations without support pruning,” *IEEE Transactions on Knowledge and Data Engineering*, vol. 13, no. 1, pp. 64–78, Jan 2001.

[6] A. Andoni and I. Razenshteyn, “Optimal data-dependent hashing for approximate near neighbors,” *Proceedings of the forty-seventh annual ACM symposium on Theory of computing. ACM*, pp. 793–801, June 2015.

[7] A. Andoni, P. Indyk, T. Laarhoven, I. Razenshteyn, and L. Schmidt, “Practical and optimal LSH for angular distance,” *In Advances in Neural Information Processing Systems*, pp. 1225–1233, 2015.

[8] P. Indyk and R. Motwani, “Approximate nearest neighbor: Towards removing the curse of dimensionality,” *In Proceedings of the thirtieth annual ACM symposium on Theory of computing, vol. 8, no. 1*, pp. 604–613, May 1998.

[9] J. Bentley, “Multidimensional binary search trees used for associative searching,” *Communications of the ACM 18*, vol. 18, no. 9, pp. 509–517, 1975.

[10] Y. Prabhu and M. Varma, “Fastxml: A fast, accurate and stable tree-classifier for extreme multi-label learning,” *In Proceedings of the 20th ACM SIGKDD international conference on Knowledge discovery and data mining. ACM*, pp. 263–272, 2014.

[11] J. Friedman, J. Bentley, and R. Finkel, “An algorithm for finding best matches in logarithmic time,” *ACM Trans. Math. Software, 3(SLAC-PUB-1549-REV. 2)*, pp. 209–226, 1976.

[12] M. Bawa, C. Tyson, and G. Prasanna, “LSH forest: self-tuning indexes for similarity search,” *In Proceedings of the 14th international conference on World Wide Web. ACM*, pp. 651–660, May 2005.

[13] A. Chakrabarti and O. Regev, “An optimal randomised cell probe lower bounds for approximate nearest neighbor searching,” *In Proceedings of the Symposium on Foundations of Computer Science*, 2004.

[14] P. Miltersen, “Cell probe complexity-a survey,” *In Proceedings of the 19th Conference on the Foundations of Software Technology and Theoretical Computer Science, Advances in Data Structures Workshop*, p. 2, Dec 1999.

[15] A. Andoni, A. Naor, A. Nikolov, I. Razenshteyn, and E. Waingarten, “Data-dependent hashing via nonlinear spectral gaps,” *In Proceedings of the 50th Annual ACM SIGACT Symposium on Theory of Computing*, pp. 787–800, June 2018.
A Equivalence of the two problems

Here, we prove that in the case of high dimensions, finding hashes to solve the approximate maximum likelihood classification problem is equivalent to finding hashes that satisfy (12) and (13).

**Theorem 1** If $P$ is factorizable to i.i.d distributions, i.e., $P(x,y) = \prod_{s=1}^{S} p(x_s, y_s)$, then we have

\[
\lim_{S \to \infty} \text{Prob}(h_X(x) = h_Y(y) \mid \frac{P(x,y)}{P_X(x)P_Y(y)} > R, (x,y) \sim \rho P + (1-\rho) Q) = 1 \quad (110)
\]

and

\[
\lim_{S \to \infty} \text{Prob}(h_X(x) = h_Y(y) \mid \frac{P(x,y)}{P_X(x)P_Y(y)} < R, (x,y) \sim \rho P + (1-\rho) Q) = 1 \quad (111)
\]

Note that the right-hand sides of $(110)$ and $(111)$ are independent of $R$ and $\rho$.

A.1 Proof of Theorem 1

We first prove the following lemma.

**Lemma 4** If $P$ is factorizable to $S$ i.i.d distributions, then when $S \to \infty$ we have

\[
\lim_{S \to \infty} \text{Prob}(\frac{P(x,y)}{P_X(x)P_Y(y)} > R \mid (x,y) \sim P) = 1 \quad (112)
\]

\[
\lim_{S \to \infty} \text{Prob}(\frac{P(x,y)}{P_X(x)P_Y(y)} < R \mid (x,y) \sim Q) = 1 \quad (113)
\]

**Proof of Lemma 4** We know

\[
\log \left( \frac{P(x,y)}{P_X(x)P_Y(y)} \right) = \sum_{s=1}^{S} (\log p(x_s, y_s) - \log p_X(x_s) - \log p_Y(y_s)) \quad (114)
\]
As \( p(x, y) - p(x, y) - p(y) \) are i.i.d random variables, using the central limit theorem\(^\text{14}\) we conclude that its sum has a Gaussian distribution

\[
\lim_{S \to \infty} \Pr(X, Y) = \left( \frac{p(x, y)}{p(x) p(y)} > R \right) \sim N(0, \sigma^2)
\]

where \( \eta \) and \( \sigma^2 \) are the mean and variance of \( p(x, y) - p(x, y) - p(y) \) under \( (x, y) \sim \mathbb{P} \). Note that \( \eta \) is a positive number as

\[
\eta = E_{p(x,y)} \left[ \log p(x, y) - \log p(x) - \log p(y) \right] = D_{KL}(P|Q) \quad (118)
\]

Therefore, from (116), (112) holds. Similarly, we have

\[
\lim_{S \to \infty} \Pr(X, Y) = \left( \frac{p(x, y)}{p(x) p(y)} < R \right) \sim N(0, \sigma^2)
\]

where \( \eta' \) and \( \sigma'^2 \) are the mean and variance of \( p(x, y) - p(x, y) - p(y) \) under \( (x, y) \sim \mathbb{Q} \). Note that \( \eta' \) is negative number as

\[
\eta' = E_{p(x,y)} \left[ \log p(x, y) - \log p(x) - \log p(y) \right] = -D_{KL}(Q|P) \quad (120)
\]

Therefore, from (119), (113) holds.

**Proof of Theorem 1.** Using (112) and (113), we have

\[
\lim_{S \to \infty} \Pr(X, Y) = \left( \frac{p(x, y)}{p(x) p(y)} > R \right) \sim \rho \mathbb{P} + (1 - \rho) \mathbb{Q}
\]

\[
\lim_{S \to \infty} \Pr(X, Y) = \left( \frac{p(x, y)}{p(x) p(y)} < R \right) \sim \rho \mathbb{P} + (1 - \rho) \mathbb{Q}
\]

\(\text{\textsuperscript{14}}\)Suppose \( \{X_1, X_2, \cdots, X_n\} \) is a sequence of i.i.d. random variables with \( \text{E}[X_i] = \eta \), \( \text{Var}[X_i] = \sigma^2 < \infty \) and \( S_n = \sum_{i=1}^n X_i \). Then as \( n \) approaches infinity, the random variables \( \sqrt{n}(S_n - \eta) \) convergence in distribution to a normal distribution \( N(0, \sigma^2) \):

\[
\sqrt{n}(S_n - \eta) \rightarrow N(0, \sigma^2)
\]

\(\text{\textsuperscript{15}}\) stands for converging in distribution.

\(\text{\textsuperscript{15}}\) \( \Phi(x) \) denotes the cumulative distribution function (CDF) of the standard normal distribution, i.e.,

\[
\Phi(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{x} e^{-t^2/2} \, dt
\]

\(\text{\textsuperscript{16}}\) The Kullback-Leibler divergence between discrete probability distributions \( P \) and \( Q \) is defined as \( D_{KL}(P||Q) = -\sum_{x \in X} P(x) \log \left( \frac{Q(x)}{P(x)} \right) \).
Note that

$$
\lim_{S \to \infty} \text{Prob}(\frac{P(x, y)}{P_X(x)P_Y(y)} > R \mid (x, y) \sim \rho P + (1 - \rho) Q)
$$

$$= \rho \lim_{S \to \infty} \text{Prob}(\frac{P(x, y)}{P_X(x)P_Y(y)} > R \mid (x, y) \sim P)
+(1 - \rho) \lim_{S \to \infty} \text{Prob}(\frac{P(x, y)}{P_X(x)P_Y(y)} > R \mid (x, y) \sim Q)
$$

$$= \rho$$

(123) holds as $\text{Prob}(\frac{P(x, y)}{P_X(x)P_Y(y)} > R \mid (x, y) \sim P) = 1$ and $\text{Prob}(\frac{P(x, y)}{P_X(x)P_Y(y)} > R \mid (x, y) \sim Q) = 0$ when $S$ tends to infinity. Moreover,

$$
\lim_{S \to \infty} \text{Prob}(h_X(x) = h_Y(y), \frac{P(x, y)}{P_X(x)P_Y(y)} > R \mid (x, y) \sim \rho P + (1 - \rho) Q)
$$

$$= \rho \lim_{S \to \infty} \text{Prob}(h_X(x) = h_Y(y), \frac{P(x, y)}{P_X(x)P_Y(y)} > R \mid (x, y) \sim P)
+(1 - \rho) \lim_{S \to \infty} \text{Prob}(h_X(x) = h_Y(y), \frac{P(x, y)}{P_X(x)P_Y(y)} > R \mid (x, y) \sim Q)
$$

$$= \rho \lim_{S \to \infty} \text{Prob}(h_X(x) = h_Y(y) \mid (x, y) \sim P)
$$

(125) holds as $\text{Prob}(\frac{P(x, y)}{P_X(x)P_Y(y)} > R \mid (x, y) \sim Q) = 0$ when $S$ tends to infinity. (126) is concluded as follows.

$$0 \leq \lim_{S \to \infty} \text{Prob}(h_X(x) = h_Y(y) \mid (x, y) \sim P)
$$

$$= \lim_{S \to \infty} \text{Prob}(h_X(x) = h_Y(y), \frac{P(x, y)}{P_X(x)P_Y(y)} > R \mid (x, y) \sim P)
$$

$$\leq \lim_{S \to \infty} \text{Prob}(\frac{P(x, y)}{P_X(x)P_Y(y)} \leq R \mid (x, y) \sim P)
$$

$$= 1 - \lim_{S \to \infty} \text{Prob}(\frac{P(x, y)}{P_X(x)P_Y(y)} > R \mid (x, y) \sim P)
$$

$$= 1 - 1 = 0$$

(127) holds as the left hand side of (127) is a non-negative real number, (126) is concluded. From (121), (123) and (126), (110) holds. Similarly, (111) holds.
B Decision Tree for Minhash Algorithm

![Decision Tree Diagram](image)

Figure 13: Equivalent decision tree for the Minhash algorithm.

C Proof of (69)

The proof is done by induction on the number of vertices in the tree. For a tree with only one node, the statement is trivial as

\[ A(\text{root})R(\text{root}) = 1 \]  \hspace{1cm} (132)

Assume (69) holds for all the trees with the number of vertices below \( Z \). Consider a tree \( G \) with \( Z \) nodes and assume \( w_q \) is the node in \( G \) with maximum depth. Define a tree \( G' \) as the tree obtained after removing \( w_1 \) and all of its siblings \( w_2, \ldots, w_z \) in \( G \). Therefore, \( G' \) has \( Z - z \) nodes. Assume that \( w \) is the parent of \( w_1, w_2, \ldots, w_z \). Then, we have

\[
\sum_{v \in V(G)} A(v)R(v)^{\mu-1} = \sum_{v \in V(G')} A(v)R(v)^{\mu-1} - A(w)R(w)^{\mu-1} + \sum_{u=1}^{z} (A(w)p_u)(R(w)r_u)^{\mu-1} 
\]  \hspace{1cm} (133)

\[
= \sum_{v \in V(G')} A(v)R(v)^{\mu-1} - A(w)R(w)^{\mu-1} \left( 1 - \sum_{u=1}^{z} p_u(r_u)^{\mu-1} \right) 
\]  \hspace{1cm} (134)

\[
\leq \sum_{v \in V(G')} A(v)R(v)^{\mu-1} \hspace{1cm} (135)
\]

\[ \text{(135) is true as } \sum_{u=1}^{z} p_u(r_u)^{\mu-1} \leq 1 \text{ and (136) is concluded as from the induction hypothesis we have } \sum_{v \in V(G')} A(v)R(v)^{\mu-1} = 1. \]
D Further Examples and Experiments

Example 4 Consider the following probability distribution $P_2 = \begin{bmatrix} p_{00} & p_{01} \\ p_{10} & p_{11} \end{bmatrix} = \begin{bmatrix} 0.345 & 0 \\ 0.31 & 0.345 \end{bmatrix}$.

For the Minhash and LSH we get the complexities $\log \frac{p_{00} + p_{11}}{q_{00} + q_{11}} = 0.5207$, $\log \frac{p_{00} + p_{11}}{q_{00} + q_{11}} = 0.4672$. For the TreeDSH, we should derive the solution of (58) for the probability distribution $p_{00} = p_{11} = 0.345, p_{01} = 0, p_{10} = 0.31$. (58) has a unique positive solution $\mu = 1.8770$ resulting in the complexity $\frac{\mu - 1}{\mu} = 0.4672$. Similarly, for the probability distribution $P_3 = \begin{bmatrix} p_{00} & p_{01} \\ p_{10} & p_{11} \end{bmatrix} = \begin{bmatrix} 0.019625 & 0 \\ 0.036875 & 0.9435 \end{bmatrix}$, we get the complexities $\log \frac{p_{00} + p_{11}}{q_{00} + q_{11}} = 0.2509$, $\log \frac{p_{00} + p_{11}}{q_{00} + q_{11}} = 0.4893$ and $\frac{\mu - 1}{\mu} = 0.2469$ for Minhash, LSH-hamming and TreeDSH, respectively.

Experiment 4 Similar to Experiment 2, the complexity is plotted for all the probability distribution matrices $P(t) = P_2(1 - t) + P_1t$ in Fig. 14 and $P(t) = P_1(1 - t) + P_3t$ in Fig. 15 where $0 \leq t \leq 1$.

![Figure 14](image1.png)

Figure 14: Complexity is plotted for all the probability distribution matrices $P(t) = P_2(1 - t) + P_1t$ where $0 \leq t \leq 1$.

![Figure 15](image2.png)

Figure 15: Complexity is plotted for all the probability distribution matrices $P(t) = P_1(1 - t) + P_3t$ where $0 \leq t \leq 1$. 
E  Codes

For the codes, see https://github.com/mohimanilab/TreeDSH.