Abstract

The indexing algorithms for the high-dimensional nearest neighbor search (NNS) with the best worst-case guarantees are based on the randomized Locality Sensitive Hashing (LSH), and its derivatives. In practice, many heuristic approaches exist to "learn" the best indexing method in order to speed-up NNS, crucially adapting to the structure of the given dataset. Oftentimes, these heuristics outperform the LSH-based algorithms on real datasets, but, almost always, come at the cost of losing the guarantees of either correctness or robust performance on adversarial queries, or apply to datasets with an assumed extra structure/model. In this paper, we design an NNS algorithm for the Hamming space that has worst-case guarantees essentially matching that of theoretical algorithms, while optimizing the hashing to the structure of the dataset (think instance-optimal algorithms) for performance on the minimum-performing query. We evaluate the algorithm’s ability to optimize for a given dataset both theoretically and practically. On the theoretical side, we exhibit a natural setting (dataset model) where our algorithm is much better than the standard theoretical one. On the practical side, we run experiments that show that our algorithm has a 1.8x and 2.1x better recall on the worst-performing queries to the MNIST and ImageNet datasets.

1 Introduction

In the nearest neighbor search (NNS) problem, we are to preprocess a dataset of points \( P \) so that later, given a new query point \( q \), we can efficiently report the closest point \( p^* \in P \) to \( q \). The problem is fundamental to many high-dimensional geometric tasks, and consequently to modern data analysis, with applications from computer vision to information retrieval and others (Shakhnarovich et al., 2006). See surveys (Wang et al., 2015; Andoni et al., 2018).

Depending on whether the algorithm has worst-case theoretical guarantees, the indexing solutions for the NNS problem are essentially split into two categories. The first category of algorithms, with theoretical guarantees, are usually based on randomized space partitions, namely Locality-Sensitive Hashing (LSH), and its derivatives—conceptually similar to the random dimension reduction (Johnson & Lindenstrauss, 1984). In order to provide a worst-case guarantee, one focuses on the \( c \)-approximate version, for some approximation \( c > 1 \), where one has to report a point \( p \in P \) at distance at most \( cr \) as long as \( \|q - p^*\| \leq r \). For example, in the case of the \( d \)-dimensional Hamming space \( \mathbb{H}^d = \{0, 1\}^d \), the original LSH paper (Har-Peled et al., 2012) gives an algorithm with \( O(n^d) \) query time and \( O(n^{1+\rho} + nd) \) space where \( \rho = 1/c \), which is optimal for LSH algorithms (O’Donnell et al., 2014). Crucially, the algorithm guarantees that, if there exists a point \( p^* \) at distance at most \( r \), then the data structure returns a point at distance at most \( cr \) with probability at least, say, 90% over the randomness of the algorithm (termed success probability).

Algorithms from the second category are based on the idea of finding (learning) the best possible space partition (hashing) for the given dataset, which, in practice, is usually "nicer" than a worst-case one. For example, PCA trees use partitions based on the Principal Component Analysis of the dataset (Sproull, 1991; McNames, 2001; Verma et al., 2009; Abdullah et al., 2014; Keivani & Sinha, 2018).
although many more methods exist; see survey (Wang et al., 2015) for some of them as well as more recent (Dong et al., 2020). While usually more efficient in practice, such algorithms come at the cost of losing the worst-case guarantees. Most often, the correctness is not guaranteed per query: there are (adversarial) queries for which the data structure fails. Alternatively, the runtime may devolve into a (naïve) linear scan. To address such issues, one approach has been to prove guarantees assuming the dataset has extra structural properties: e.g., that it has low doubling dimension, or that it is generated according to a random model.

Bridging the gap between these two categories of algorithms has been recognized as a big open question in Massive Data Analysis, see e.g. the National Research Council report (NRC13, 2013, Section 5) in the closely-related setting of random dimension reduction. We summarize this challenge as the following “instance optimality” question:

**Challenge 1.1.** Develop NNS algorithms that adapt optimally to the input dataset, while retaining provable guarantees for all, including adversarial, queries.

We address the above challenge in this paper. Before delving into our specific results, we comment on two non-answers. First, a recent line of research led to *data-dependent hashing* algorithms that similarly have worst-case guarantees (Andoni et al., 2014; Andoni & Razenshteyn, 2015; Andoni et al., 2015), improving, for example, the original exponent $\rho$ of (Har-Peled et al., 2012) to $\rho = \frac{1}{c-1} + o(1)$. While this line of work shows that adapting to the dataset can improve the performance for a worst-case dataset, it does not seek to improve the performance further if the dataset is "nice". Second, a straight-forward solution to the challenge could be to run both a practical heuristic and a theoretically-guaranteed algorithm (timing out the latter one if needed). Such a solution however still does not seek to improve the performance for all, especially adversarial, queries.

We also note that it generally seems hard to adapt the heuristic algorithms to have theoretical guarantees for all queries. Most such algorithms learn the best partition, yielding a deterministic index—i.e., building a few indexes does not help failed queries (in contrast to the LSH-based randomized indexes). At the same time, it is known that the deterministic algorithms are unlikely to yield worst-case guarantees (Panigrahy et al., 2010). In particular, it is usually possible (and easy) to construct an adversarial query, by planting it "on the other side" of the part containing its near neighbor. Hence, a solution for the above challenge would likely involve randomized partitions (as LSH does).

1.1 Our results

We address Challenge 1.1 in the case of (approximate) NNS problem under the Hamming space, for which we design an algorithm that adapts to the dataset’s potential structure, while maintaining the performance guarantees for all queries. Our algorithm should be seen from the perspective of *instance optimal* algorithms: an algorithm that is the best possible, within a class of algorithms, for the given dataset.

Our algorithm directly optimizes the performance for all possible queries, for the given fixed dataset. We obtain the following properties (see Theorem 3.1 in Section 3):

1. Correctness: For any query $q$, the algorithm is guaranteed to return the $c$-approximate near neighbor with success probability at least $\Omega(n^{-\rho})$ for some $\rho \leq 1/c$, the exponent obtained by the optimal LSH (Har-Peled et al., 2012; O’Donnell et al., 2014). (Probability is over the randomness of the algorithm only.)

2. Performance: The query time is $O(d^2)$ and the space is $O(n)$, and the preprocessing time is $O(n \cdot \text{poly}(d))$. Note that, as is standard for LSH algorithms, we can boost the success probability to, say, 90% by repeating the algorithm for $O(n^\rho)$ times, obtaining the usual tradeoff of $O(n^{\rho+1} \cdot \text{poly}(d))$ query time and $O(n^{1+\rho} + nd)$ space overall (but for smaller $\rho$).

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1In particular, that would merely split the queries into two classes: those on which the heuristic is successful with improved performance, and those on which it is not and hence the performance is that of a worst-case theoretical algorithm.

2While some use randomization, it is usually used to find the optimal partition (e.g., via SGD), but not to randomize the partition itself.
3. Data-adaptive: The algorithm adapts to the input dataset, and can obtain better success probability for "nicer" datasets. In fact, under certain conditions, the algorithm is "instance optimally" adaptive to the dataset.

We now discuss the last claim of data-adaptivity. The ideal goal would be to obtain an instance-optimal algorithm. Our algorithm becomes instance-optimal (in a precise sense described in the next section), if we are given optimal values for certain parameters $\rho$ during the construction. Alas, we do not know how to compute these parameters efficiently (and thus do not achieve instance optimality).

Instead, we evaluate the last claim by showing that our algorithm achieves theoretical and practical improvements over standard LSH indexes for a range of parameters. On the theoretical side, we formulate a concrete model for the dataset, for which our algorithm improves on the success probability for all queries. We specifically consider the case where the dataset is a mixture model: it is composed of several clusters, where each point is generated iid. We note that our algorithm is not designed specifically for this model; instead it is a natural theoretical model for "nicer" datasets to evaluate improvement of an algorithm. See Section 4 and Section D in supplemental material.

On the practical side, we run experiments that show that our algorithm has a 1.8x better recall on the worst-performing queries to the MNIST dataset, and a 2.1x better recall on the bottom tenth of queries to the ImageNet dataset. See Section 5.

1.2 Technical description of our algorithm

We now give an overview of our main algorithm and the tools involved. Our algorithm is based on the LSH Forest method (Bawa et al., 2005) for Hamming space, in which the dataset is iteratively partitioned according to the value in a coordinate, thereby progressing down the constructed tree. In particular, beginning with the entire dataset in the root of an LSH tree, in each node, we pick a random hash function and use it to partition the dataset. The partitioning stops once the dataset becomes of size $\leq C$ for some constant $C$, termed stopping condition. Otherwise, we recurse on each new part (child of the current node in the tree).

The key new component of our algorithm is that, in each node, we optimize for the best possible distribution over hash functions, for the given dataset. In particular, in each node, we solve an optimization to produce a distribution $\pi$ over coordinates $[d]$, that maximizes the probability of success over all (worst) possible queries. Following this optimization, we draw a coordinate from the optimized distribution $\pi$, hash the dataset on the resulting coordinate (to produce two children corresponding to bits 0 and 1 at that coordinate). We then recurse on each of the hashed datasets (children) until the current dataset is less than a fixed constant (stopping condition). The formal algorithm, BUILDTREE, is described in Alg. 1.

The main technical challenge is to compute the optimal distribution $\pi$, for which we use a two-player game to solve a min-max problem. Note that this is a question of efficiency—it is easy to compute the optimal $\pi$ in exponential time (and an instance optimal algorithm in general)—and hence our goal is to do so in polynomial time. Specifically, our method directly optimizes for robustness by computing solutions to a min-max optimization (minimum over queries, maximum over distributions). What are the exact quantities we want to optimize at a given node? Consider a distribution $\pi \in \Delta[d]$ over hash functions, and a query/near neighbor pair $p, q \in \mathbb{H}^d$. The true instance optimal objective function at each node is the following:

$$
\Pr_{\text{Alg}}[\text{success}] = \sum_{i \in [d]} \pi_i \Pr_{\text{Alg}}[\text{success} | \text{hash on coordinate } i, \text{ bit } q_i] \cdot \mathbb{I}\{p_i = q_i\},
$$

which is a function of the success probability on the remainder of the dataset, $\Pr_{\text{Alg}}[\text{success} | \text{hash coord. } i, \text{ bit } q_i]$. However, exactly computing the probability of success on the remainder of the tree appears computationally intractable, as one would need to have considered all possible subsets of hashes (exponential in dimension). Instead, we approximate the recursive probabilities by using a lower bound on the probability of success in the remainder of the tree. In fact, there’s already a natural candidate for such a lower bound: the success probability of the standard LSH, which hashes on uniformly-random coordinate(s). Hence, our optimization becomes as follows, where the maximum is over distributions $\pi \in \Delta[d]$, $n_i, p_i$ is the size of the dataset after hashing on
coordinate \(i\), bit \(p_i\), and for a chosen parameter \(\rho \in (0, 1)\), the function we optimize is:

\[
\max_{\pi \in \Delta[d]} \min_{p \in P} \sum_{q:\|p-q\| \leq r} d n_{\pi,p} \mathbb{I}\{p_i = q_i\}
\]  

(2)

Notably, if we set \(\rho = p_i\) for each \(i \in [d]\), where \(n^{-p_i}_{\pi,p} = \Pr[\text{success} | \text{hash coordinate } i, \text{bit } p_i]\), we obtain exactly the instance optimal objective. We don’t know the values of \(p_i\)’s but can use an upper bound instead: \(\rho_i \leq 1/c\). (In fact, one can compute directly an upper bound using any data-independent distribution \(\pi\)—e.g., even uniform distribution \(\pi\) sometimes yields better estimates than \(1/c\).)

We solve the min-max program from Eqn. 3 by finding a Nash equilibria in an equivalent two-player zero sum game, in which the worst-performing queries are iteratively presented to a "player" who learns hash functions to maximize the success probability on those queries. The main question is under what circumstances can we find such a Nash equilibrium efficiently? In the case of our hash/query game, although there are exactly \(d\) hash functions available to hash player, there are \(n^d\) potentially exponential in \(d\)—many query/NN pairs available to the query player.

Nonetheless, it turns out we can approximately solve this game efficiently, in \(n \cdot \text{poly}(d)\) time! We use a variation on the so-called fictitious play dynamic (Abernethy et al. 2021), in which the hash player performs the multiplicative weights update and the query player chooses the query that minimizes their loss on the hashes played so far (the “Follow-the-Leader” (FTL) approach (Kalai & Vempala 2005)). Indeed, while the complexity of the game is polynomial in the number of hash player strategies, it is essentially independent of the number of possible queries, as we have reduced the query player’s complexity contribution to that of a single minimization (see details in Sec 3.1 and Sec. B Supplemental Material).

1.3 Other related work

This paper focuses on indexing NNS algorithms, which can be contrasted to the sketching algorithms; see (Wang et al. 2015). In the latter, the goal is to produce the smallest possible sketch for each point in order to speed-up a linear scan over the dataset (of sketches). Such solutions have a query time (at least) linear in \(n\), in contrast to the indexing algorithms, which are sublinear, typically \(n^\rho\) for \(\rho < 1\). Furthermore, one can often combine the two: use the indexing NNS algorithm to filter out all but a smaller set of candidate points and then use (preprocessed) sketches for faster distance evaluations on them (Wu et al. 2017, Johnson et al. 2019).

We also note that there exist other practical NNS algorithm, which do not directly fit into the "learning to hash" paradigm alludes to before. For example, the algorithm from (Malkov & Yashunin 2018) builds a graph on the dataset, such that a future query will perform a graph exploration to reach the nearest neighbor. While very competitive in practice, it again provides no guarantees. It remains a formidable challenge to derive theoretical guarantees for such algorithms.

2 Preliminaries

We label the dataset as \(P \subset \{0,1\}^d = \mathbb{R}^d\) where \(|P| = n\). Formally, we solve the \(c\)-approximate near neighbor problem, where, given a threshold \(r > 0\), and approximation \(c > 1\), we need to build a data structure on \(P\) so that, given a query \(q\), we return a point \(p \in P\) with \(||q-p||_1 \leq cr\), as long as there exists a point \(p^*\) with \(||q-p^*||_1 \leq r\). In that case, for the given \(q\), we call such a point \(p^*\) a near neighbor of \(q\), and \(p\) an approximate near neighbor.

**Definition 2.1.** For a given query \(q\) and a near neighbor \(p^*\), we consider an LSH tree to be successful on that pair if when the query algorithm halts on a node \(v\), \(q\) and \(p^*\) are both in the bucket at node \(v\). The probability with which it happens (over the randomness of the algorithm) is referred to as success probability, denoted \(\Pr[\text{success}]\).

Our algorithm builds a tree top-down, from a node to its children partitioning the dataset according to the chosen hash function. For a node \(v\), we use \(P^v \subset P\) to denote the set of dataset points that reached the node \(v\) (have been hashed to \(v\) according to the hash function of the ancestors of \(v\)). We also call \(P^v\) as the "bucket" at \(v\), and let \(n_v = |P^v|\). Each (internal) node \(v\) has an associated hash
function used to partition $P^0$, which is described by the coordinate $i \in [d]$ by which we partition $P^0$. In particular, $P^0_{i,b}$ indicates the subset of datapoints in $P^0$ that have bit $b$ at coordinate $i$. The node $v$ splits $P^0$ into $P^0_{i,0}$ and $P^0_{i,1}$. We let $n_{i,v} := |P^0_{i,v}|$.

**Definition 2.2.** A coordinate $i \in [d]$ is called $\epsilon$-balanced for the dataset $P^0$ and $0 \leq \epsilon \leq 0.5$ if:

$$\max(|P^0_{i,0}|, |P^0_{i,1}|) = (1 - \epsilon)|P^0|.$$  \hfill (3)

For the analysis that follows, we make the trivial assumption that hashing is done without replacement (i.e. once a coordinate $i$ is used to hash, it is never used again in a tree descendant).

**Notation.** For two vectors $x, y \in \mathbb{R}^d$, we denote their element-wise product by $x \odot y \in \mathbb{R}^d$. We denote the transpose of a vector $x$ by $x'$. For a vector $x$, we denote its $i$-th coordinate by $x(i)$ or $x_i$. Let $e_i$ be the $i$-th standard basis vector.

### 3 Main Algorithm

We now present and analyze our LSH forest algorithm with hash functions adapting to the given dataset. We then show that our algorithm (1) is correct, and (2) has worst-case performance guarantees. We show our algorithm has improved performance in experiments in Section 5, and on "nice" datasets in Section D (Supplemental Material).

We present our algorithm in Alg. 1. The algorithm is an LSH forest algorithm, where, beginning with the entire dataset at the root, we construct the tree by performing a min-max optimization at the current node to compute the best distribution over hashes, picking a random hash function from this optimized distribution, and recursing on the hashed datasets until the datasets are of constant size.

The main component of the algorithm is to compute the optimal distribution for the given node, described in Alg. 2. Specifically, for this goal, we setup a min-max optimization, Eqn. (2), which we solve efficiently by iterating an equivalent two-player zero sum game (see Section 3.1).

Our main correctness and worst-case performance guarantee is in the following theorem. We remark that the main algorithm requires an input parameter $\rho$, which we discuss, along with an interpretation of the probability guarantee in Section 3.2.

**Theorem 3.1 (Correctness and Runtime).** Fix stopping condition $C \geq 1$ to be a constant, and query algorithm parameter $m \geq 1$. Suppose there exists a $\rho \in (0, 1)$, such that for any node $v$, there is a distribution $\pi_v$ over hash functions such that for any query/near neighbor pair $q, \rho^* \in \mathbb{R}^d$, both hashing into node $v$, such that fewer than $\frac{1}{m}\rho$ fraction of the bucket $P^v$ are approximate near neighbors of $q$, $\mathbb{E}_{i \sim \pi_v} [\mathbb{I}[\rho^*_i = q_i] \cdot f_{i,\rho^*_i,v}] \geq 1$ where $f_{i,\rho^*_i,v} = |P^v_{i,\rho^*_i,v}|/|P^v|$. Then, using $\rho$ as the input parameter, Algorithm 1 constructs a tree that satisfies:

$$\Pr_{\text{Alg}} [\text{success on } q, \rho^*] \geq n^{-\rho} - 2\epsilon d,$$  \hfill (4)

where $\epsilon > 0$ is the input parameter. Furthermore, $\rho \leq \gamma/c$ for $\gamma = \frac{1}{1-1/m}$.

The pre-processing time to construct a single tree as in Algorithm 1 is $O\left(\frac{1}{\epsilon} nd^4 \ln^2 d\right)$, and the resulting query time is $O\left(md^2\right)$.

### 3.1 Min-Max Optimization Analysis

To solve the min-max optimization, Eqn. (2), efficiently, we iterate a two-player zero-sum game (Def. 3.7). In this game, the "hash" player selects a distribution over coordinates to hash the dataset on, and the "query" player selects a query/nearst neighbor pair adversarially for the least probability of success at the end of the tree. Using such a method, we can find an approximate solution to the min-max program in the following runtime.

**Theorem 3.2 (Solving the Min Max Optimization).** For any desired $\epsilon > 0$, there exists an algorithm (Algorithm 2) that solves the min-max optimization in Eqn. (2) for the node $v$, up to an additive approximation $\epsilon > 0$ in $O\left(\frac{1}{\epsilon^2} nd^3 \ln^2 d\right)$ time.
Algorithm 1 Main Algorithm

1: function BUILDTREE($P^v, \rho, C, \epsilon$)  \small{$\triangleright$ $P^v$ is the dataset at the current node}
2: \hspace{1em} create an empty node $v$
3: \hspace{1em} set $v$.dataset = $P^v$
4: \hspace{1em} if $|P^v| > C$ then
5: \hspace{2em} set $\pi_v = \text{MinMaxOpt}(P^v, \rho, \epsilon)$ \small{$\triangleright$ $\pi_v \in \Delta^d$}
6: \hspace{2em} draw $i \sim \pi_v$
7: \hspace{2em} set $v$.coordinate = $i$
8: \hspace{2em} set $v$.left_child = BuildTree($P^v_i, 0, \rho, C, \epsilon$)
9: \hspace{2em} set $v$.right_child = BuildTree($P^v_{i+1}, \rho, C, \epsilon$)
10: \hspace{1em} end if
11: \hspace{1em} return $v$
12: end function

13: function QUERYTREE($q, v, m, c$)
14: \hspace{1em} $P^v = v$.dataset
15: \hspace{1em} Select $m$ uniform random points from the current bucket.
16: \hspace{1em} If one of these points is an approximate near neighbor, then return it.
17: \hspace{1em} Otherwise,
18: \hspace{2em} if $|P^v| > C$ then
19: \hspace{3em} if $q[v$.coordinate$] = 0$ then
20: \hspace{4em} return QueryTree($q, v$.left_child)
21: \hspace{3em} else
22: \hspace{4em} return QueryTree($q, v$.right_child)
23: \hspace{2em} end if
24: \hspace{2em} else
25: \hspace{3em} if approximate near neighbor is in dataset then
26: \hspace{4em} return approximate near neighbor
27: \hspace{3em} else
28: \hspace{4em} return $\emptyset$
29: \hspace{3em} end if
30: \hspace{2em} end if
31: end function

Algorithm 2 Min-Max Optimization

1: function MINMAXOPT($P^v, \rho, \epsilon$)
2: \hspace{1em} initialize distribution $\pi_1 = \mathbf{1}_d \cdot \frac{1}{d}$
3: \hspace{1em} initialize query strategy arbitrarily to $y_1 = (p_1, q_1)$
4: \hspace{1em} $T = \Omega(\frac{d^2 \ln d}{\epsilon^2})$ \small{$\triangleright$ choose a sufficiently large constant pre-factor}
5: \hspace{1em} $\beta = 1 - \sqrt{\frac{\ln d}{T}}$
6: \hspace{1em} for $t = 2, \ldots, T$ do
7: \hspace{2em} $y_t = \arg\min_y \left( \sum_{s=1}^{t-1} \pi'_s A_{vy}^s \right)$ \small{$\triangleright$ query player minimization}
8: \hspace{2em} $\pi_t = \pi_{t-1} \odot \beta'(\pi_{t-1}, y_{t-1})$ \small{$\triangleright$ hash player update}
9: \hspace{2em} end for
10: \hspace{1em} return $\pi_T$
11: end function

We introduce the following definitions to understand this theorem.

Definition 3.3. A (simultaneous) two-player game is when two actors (players) are each able to play a weighted mixture of actions (as in Definition 3.4), without knowledge of the other players mixture, where each action incurs a reward that is a function of the mixtures of both players. The game is characterized by two reward matrices $R$, $C$ (one for each player) whose entries are indexed by pairs of single actions. The reward for each player is a function of these matrices (as in Definition 3.5). This game is called iterated if the game is repeated in sequential rounds.
**Definition 3.4.** Suppose a player in a two-player game has \( N \) actions available to them. One such action is called a **pure strategy**, and is represented by a standard basis vector \( e_i \) for \( i \in [N] \). Further, a **mixed strategy** \( s \in [0,1]^N \) is a convex combination of these pure strategies.

**Definition 3.5.** Suppose the first player plays a mixed strategy \( x \in [0,1]^N \), and the second player plays a mixed strategy \( y \in [0,1]^M \). The **reward** or **payoff** for the first player (whose reward matrix is \( R \)) is \( x' R y \), and for the second player (whose reward matrix is \( C \)) it is \( x' C y \). We call the first player, whose strategy left-multiplies their reward matrix, the **row player**; while the second player, whose strategy right-multiplies their reward matrix, is the **column player**.

**Definition 3.6.** (Daskalakis n.d.) Consider a two player game where the row player has \( N \) possible pure strategies, and the column player has \( M \) possible pure strategies. Suppose that the row player has reward matrix \( R \in \mathbb{R}^{N \times M} \), and the column player has reward matrix \( C \in \mathbb{R}^{N \times M} \). (A two player game is called **zero-sum** when \( R = -C \).) Then, a pair of mixed strategies \((x_0, y_0)\) for \( x_0 \in \mathbb{R}^N, y_0 \in \mathbb{R}^M \) is considered an \( \epsilon \)-**approximate Nash equilibrium** if and only if the following two conditions hold:

1. \( x_0' R y_0 \geq \max_x x' R y_0 - \epsilon \),
2. \( x_0' C y_0 \geq \max_y x_0' C y - \epsilon \),

where \( x, y \) are taken from the convex hull of available strategies to each player.

**Definition 3.7.** The **hash/query zero sum game** is a two-player zero sum game at a given node \( v \) with exponent \( \rho \). In this game, the hash player has reward matrix \( R = A_v^h \) and the query player has reward matrix \( C = -A_v^q \). In this case, the hash player has \( N = d \) possible pure strategies (coordinates to hash on), while the query player has \( M = n(d) \) many pure strategies, as this is the number of possible query/near-neighbor pairs.

For our problem, the hash and query players iterate the above two-player zero-sum game. By the celebrated min-max theorem of Nash, there exists a pair of mixed strategies for the hash and query players (i.e. distributions over pure strategies) in the aforementioned game for which no player can improve their reward by deviating from them (Nash, 1950) (a Nash equilibrium). To treat the min-max optimization in equation (2) as such a game, we must first show that solving the desired min-max program is equivalent to solving a min-max optimization where distributions over query/NN pairs are permitted.

**Definition 3.8.** Suppose we are performing min-max optimization at node \( v \) in an LSH tree with a given exponent \( \rho \). We define the matrix \( A_v^h \) to be the **payoff matrix** for that node. The entries of this matrix \( A_v^h \) correspond to a query/near-neighbor pair \((q, p^*)\) (indexed \( j \)) and dimension \( i \). These entries in particular are: \( A_v^h \) := \( \left[ P_{v,q_i} \right]^{\rho} \cdot 1_{\{q_i = p_i^*\}} \). Note that this matrix is exponentially large, and so is never written explicitly.

**Theorem 3.9.** Consider a node \( v \) in the LSH tree. For \( M \) total query/near-neighbor pairs, let \( y \in \Delta[M] \) be a distribution over all possible query/NN pairs. Then, a hash distribution that solves \( \max_{\pi} \min_{p \in P} \sum_{q \in q_v, p \leq r} \pi, \gamma \quad p \quad y \quad 1 \{p_i = q_i\} = \max_{\pi} \min_{y} \pi' A_v^h y \)

To prove the main theorem (Theorem 3.2), it will be useful to introduce the following standard concept of regret.

**Definition 3.10.** Suppose a player in a two-player zero-sum game has played a sequence of mixed strategies \( x_1, ..., x_T \) up to time \( T \), each of which has experienced some loss according to the functions \( \ell_s(x) \) for \( s \in 1, ..., T \). Then, that player’s regret is defined as follows.

\[
\text{Regret}(x_1, ..., x_T) := \sum_{s=1}^{T} \ell_s(x_s) - \min_{x} \sum_{s=1}^{T} \ell_s(x)
\]
best strategy in hindsight), then iterating a two-player zero-sum game will efficiently lead to a Nash equilibrium (Freund & Schapire 1999). The hash player can simply use the multiplicative weights update rule to achieve sublinear regret (Definition 3.11). Recall that the FTL dynamic is the choice of strategy selection in which a player in each round of an iterated game selects the mixed strategy that performs the best on the loss vectors incurred in hindsight. Notably, although FTL strategies on their own do not imply no-regret, as the hash player uses a no-regret dynamic, the query player can still achieve no-regret with FTL (as in Definition 3.12).

Definition 3.11. Suppose a player in some game has available to them \( N \) pure strategies. Fix some parameter \( \beta \in (0, 1) \). The multiplicative weights update (MWU) method is a method for choosing a mixed strategy over these \( N \) possible actions so as to minimize one’s loss on a sequence of loss vectors. In particular, suppose a player experience a sequence of losses \( \ell_s(x) \) for \( s = 1, \ldots, T \). Let \( \pi_s \) be their distribution over strategies at round \( s \). For the MWU update rule, the player initializes their distribution to \( \pi_{1,i} = \frac{1}{N} \) for all \( i \in [N] \). In subsequent rounds, the player updates their distribution according to \( \pi_{s+1,i} = \pi_{s,i} \cdot \beta^{\ell_s(i)} \).

Definition 3.12. Let the payoff matrix be \( A^p \) the set of possible query/near-neighbor pairs \( y \), and \( \ell_s^p(y) \) a sequence of loss functions for \( s = 1, \ldots, t \). The following equation is defined as the query player minimization (which is an instance of Follow-the-Leader):

\[
\arg\min_y \left( \sum_{s=1}^{t} \ell_s^p(y) \right) = \arg\min_y \left( \sum_{s=1}^{t} \pi_s^t A^p v \right)
\]  

(7)

Key to the polynomial efficiency of our algorithm, despite the fact that there are superpolynomially many potential query/NN pairs, is that the query player minimization returns single queries (pure strategies). This way we can avoid ever explicitly considering all possible queries. We express this fact in the following lemma.

Lemma 3.13. Optimal query strategies produced by the query player minimization are pure (standard basis vectors) in game 3.7.

It is a well known result that multiplicative weights update achieves sublinear regret in online learning, as stated in lemma 3.14. Further, we show in Theorem 3.15 that the regret of the query player is also sublinear, exactly because the distributions in consecutive rounds of MWU change relatively slowly.

Lemma 3.14 (MWU is No-Regret (Freund & Schapire 1999)). The multiplicative weights update rule yields \( O(\sqrt{T} \ln N) \) regret for a player with losses bounded between \([0, 1]\), and \( N \) available pure strategies.

Theorem 3.15. Consider any sequence of losses \( \{ -x_i^C \}_{t \in [T]} \) for the query (column) player in game 3.7. Then, the regret of the query player on this sequence is bounded by \( O \left( d \sqrt{T \ln d} \right) \).

Using these claims to adapt the result of Freund and Schapire, we can conclude the following theorem.

Definition 3.16. For node \( v \) in the LSH tree, \( \rho \in (0, 1) \), distribution \( \pi \in \Delta [d] \), query/NN pair \( y = (q, p^*) \) indexed by \( j \), and \( i \in [d] \), the loss vector for the hash player in a round of game 3.7 \( \ell(\pi, y) \in [0, 1]^d \), has entries:

\[
\ell(\pi, y)_i = 1 - A^p_{ij, v}
\]  

(8)

Theorem 3.17 (Adapted from Freund & Schapire [1999]). Consider the the hash/query zero sum game 3.7. Suppose the hash player uses MWU to select strategies with losses as in Definition 3.16. Suppose the query player uses FTL as in the query player minimization to select strategies (Definition 3.12). Let \( M = n^{d/2} \) be the total number of possible query/NN pairs to the given dataset (recall this is super-polynomial in dimension). Suppose \( T \) rounds of this iterated game have been executed, and let \( x_1, \ldots, x_T \in [0, 1]^d \) and \( y_1, \ldots, y_T \in \{ e_i \}_{i=1}^M \) be the mixed row (hash) and pure column (query) player strategies from these rounds, respectively. Then, for a universal constant \( K > 0 \), the pair of strategies \( \left( \frac{1}{T} \sum_{t=1}^{T} x_t, \frac{1}{T} \sum_{t=1}^{T} y_t \right) \) for the hash and query players, respectively, is a \( 2Kd^{d/2} \sqrt{T} \) approximate solution to max_{\pi} min_y \( \pi^t A^p v \) (and Nash equilibrium in game 3.7).

Theorem 3.12 follows from this theorem, Theorem 3.9 and that the query player minimization can be solved in time \( O(n_d d \ln d) \) (Alg. 5 Supplemental Material).
3.2 Success Probability Guarantee

For any query/near neighbor pair \( q, p^* \in \mathbb{H}^d \), Theorem 3.1 requires a parameter \( \rho \) that satisfies: 
\[
\mathbb{E}_{i \sim \pi} [ \mathbb{I} \{ p_i^* = q_i \} \cdot f_{q^*,q} \geq 1 \text{ for all nodes } v \text{ in the tree that contain } q, p^* (\text{with fewer than } \frac{1}{m} \text{ approximate near neighbors of } q) \}, \]
where each node \( v \). The second inequality in the theorem states that this \( \rho \) can always upper bounded by \( \gamma/c \approx 1/c \) (the upper bound for theoretical LSH). A practitioner may interpret this exponent in the following way: provided that your parameter choice \( \rho \) is an upper bound for the least possible \( \rho \) such that this condition (3.2) holds, then you are guaranteed \( n^{-\rho} \) performance. Further, as the practitioner also may choose \( c \) (as in the \((c,r)\)-ANN problem), they may tune this \( \rho \) aggressively to achieve maximal improvement, and then set \( c = \frac{1}{\rho} \) to obtain worst-case guarantees.

4 Improvement on Datasets Generated from a Mixture Model

We now describe a data model (and a variant) in which our algorithm can provably perform strictly better than the standard, optimal Hamming LSH (Har-Peled et al. 2012; O’Donnell et al. 2014). In particular, recall that the LSH from Har-Peled et al. (2012) simply samples coordinates at random (which would correspond to the LSH Forest with a uniform distribution \( \pi \) in each node).

We consider the case of a dataset \( P \) where each point \( x \in P \) is generated randomly such that each coordinate \( i \in [d] \) is drawn independently according to \( x_i \sim \text{Bernoulli}(\epsilon_i) \), for some fixed \( \epsilon_i \in (0,1) \). This model has been studied before, e.g., in Dubiner (2012) (but, for random queries, not worst-case like we do here). There are settings of the \( \epsilon_i \)'s where the uniform distribution is still optimal for the independent Bernoulli above (e.g. \( \epsilon_i = 1/2 \) for all \( i \in [d] \)). To achieve strict improvement over uniform, we instead consider datasets with balances that are heterogeneous across coordinates.

Specifically, we consider the case where the coordinates \([d]\) can be partitioned into two sets \( S_1, S_2 \subset [d] \) that are \( \epsilon_i \)-balanced, for \( 0 < \epsilon_1 < \epsilon_2 \leq \frac{1}{2} \) respectively. In particular, \( p_j \sim \text{Bernoulli}(\epsilon_i) \), if \( j \in S_i \), for each \( p \in P \). Further, we assume the cardinalities of these sets satisfy \( |S_1| = \alpha_i \) with \( \alpha_i \gg k \), where \( k \) is the number of hashes chosen by the algorithm (tree depth). The sizes of these sets change as hashing is performed, so we denote these sets relative to a node \( v \) in the LSH tree by \( S_i^v \).

Interestingly, this setting is not sufficient to obtain improvement over uniform, as uniform hashing is essentially optimal for one cluster of independent coordinates (Theorem E.1). We incorporate the notion of mixture models into this setting to obtain improvement for the minimum query over uniform hashing. This is informally stated in Theorem 4.1 and formally treated for standard LSH (Indyk & Motwani 1998) in Theorem D.1 and for LSH Forests (Bawa et al. 2005) in Theorem D.2.

To simplify the analysis, suppose we plant a point \( p_o = 0^d \) and \( \sqrt{d} \) points next to the point \( p_o \) to form cluster. Suppose further that these points are generated i.i.d. at distance \( r + 1 \) from \( p_o \), where the coordinates on which they each differ from \( p_o \) are all in \( S_1 \). In the high-dimensional limit, these additional points will not affect the balances of the coordinates for subsets larger than \( d \) (as these planted points compose at most \( 1/\sqrt{d} \rightarrow 0 \) fraction of the bucket). However, as we will see, the worst-case query in this model is the query with bits flipped on only the coordinates that differentiate \( p_o \) from its approximate near neighbors.

Further, we suppose the data are in the high-dimensional limit — specifically where \( d \gg \ln(n) \), with \( n \gg d \) (e.g. \( n = \text{poly}(d) \)), and \( d \rightarrow \infty \).

Theorem 4.1 (Informal). In the above mixture model, with exponent parameter \( \rho \in (0.1,1) \), algorithm \( T \) obtains a factor of \( \Omega \left( \exp(\Omega(\sqrt{\ln d})) \right) \) improvement on the minimum query over LSH forests (Bawa et al. 2005) and standard LSH (Indyk & Motwani 1998).

5 Experiments

We performed experiments on the first 750 images of MNIST’s training dataset (Chris Burges 2021), and on the first 624 images of ImageNet’s 3x8x8 validation subset (Deng et al. 2009).

For MNIST, the dataset was binarized using a threshold. In particular, all pixel values below a threshold pixel value of 1 were set to 0, and the complement is set to 1. The distribution of
digits (labels) is roughly uniform over the MNIST subset. The implementation details can be found in Section C, Supplemental Material. We tested Algorithm 1 for several fixed settings: $\rho \in \{1, \frac{5}{6}, \frac{1}{4}, 1, \frac{1}{10}\}$. In these experiments, we do not sample uniform pivots as in Algorithm 1. Instead, the algorithm halts only when the size of the dataset is less than $C = 5$ (i.e. when the stopping condition is reached). This is well justified for nice datasets where there are very few or exactly one (approximate) near neighbors, as the success probability guarantee still holds without sampling random points in this case (see the $(c, r)$-Gap-ANN problem in [Andoni et al., 2017]). Two additional parameters are listed for the experiments - the number of rounds $T$ the game was executed for, and the base $\beta \in (0, 1)$ used for MWU.

For ImageNet, we flattened the image to 1x192, and binarized the dataset with a threshold (pixel value 16). We then ran our algorithm with stopping condition $C = 10$, radius $r = 5$, exponent parameter $\rho = 1$, and the other specified parameters in Tables 1 and 2. Again, no pivots were selected at random. The success probabilities are presented in Table 1 and Figure 3. On querying, we measured the time until the near neighbor was returned for a given query/NN pair using the “time” library for Python. We recorded the maximum and average query times in Tables 1 and 3 for ImageNet and MNIST. The bottom tenth percentile of success probabilities refers to the average success probability over the bottom tenth of success probabilities for random queries to the given dataset. This is a proxy for the minimum success probability, as for some trees the success probability was too small to be measured. This occurs because we are not using pivots in our experiments.

We compare trees generated using these exponent settings to trees generated by uniformly sampling hash functions. To assess the performance of our algorithm in these settings, for MNIST, we sample 100 points uniformly at distance $r = 10$ from each point in the dataset. We sample 110 trees for each of these strategies, and estimate the probability of success for each query/NN pair by computing the fraction of trees which co-locate the pair in their final bucket. For ImageNet, we sampled 2 points at distance $r = 5$ from each point, and compute success probability similarly.

The experiments reveal that our algorithm with certain parameters produces trees with a 1.8 $\times$ improvement over uniform hash trees in the success probability for the minimum query for MNIST (Table 4), and 2.1 $\times$ improvement for the bottom tenth percentile of queries to ImageNet (Table 2). These success probability improvements are accompanied by large query time improvements for both datasets (Tables 1 and 3).

Further, we constructed Recall/Query-rate tradeoff curves for both datasets. Recall was measured as the fraction of near neighbors that were recovered for a given query with a fixed number of trees. Queries-per-second was calculated by taking the inverse of query time. These data are an average over 1500 and 3120 random queries for MNIST and ImageNet, respectively. Because the recall was too high to resolve differences among tree types for our settings, we increased the query radius $r$ to 10 at query time for the ImageNet dataset, and $r$ to 25 for the MNIST dataset. These curves demonstrate the empirical improvement of our algorithm over uniform hashing.

![Figure 1: Normalized and centered distributions for MNIST (Learned Distributions)](image)

**Figure 1:** Normalized and centered distributions for MNIST (Learned Distributions)

| Parameters | Maximum Query Time (s) | Average Query Time ($s \times 10^{-6}$) |
|------------|------------------------|----------------------------------------|
| Uniform   | 0.0013                 | 13.2                                   |
| $\rho = 1$, $T = 3000$, $\beta = 0.68$ | 0.00046                | 7.37                                   |

Table 1: Query Times on Random Queries to ImageNet Subset.
Table 2: Success Probability on Random Queries to ImageNet Subset.

| Parameters       | Bottom 10th Percentile Succ. Prob. | Average Success Prob. |
|------------------|-----------------------------------|-----------------------|
| Uniform          | 0.275                             | 0.621                 |
| $\rho = 1, T = 3000, \beta = 0.68$ | 0.576                             | 0.772                 |

Table 3: Query Time for Random Queries to MNIST Subset.

| Parameters       | Maximum Query Time (s) | Average Query Time ($s \times 10^{-5}$) |
|------------------|------------------------|----------------------------------------|
| Uniform          | 0.0012                 | 4.03                                   |
| $\rho = 1, T = 3000, \beta = 0.68$ | 0.00048               | 1.10                                   |
| $\rho = 0.83, T = 3000, \beta = 0.68$ | 0.0011               | 1.29                                   |
| $\rho = 0.67, T = 1600, \beta = 0.88$ | 0.037               | 2.30                                   |
| $\rho = 0.25, T = 1600, \beta = 0.88$ | 0.0033               | 2.15                                   |
| $\rho = 0.1, T = 1600, \beta = 0.88$ | 0.0027               | 3.06                                   |

Table 4: Success Probability on Random Queries to MNIST Subset.

| Parameters       | Minimum Success Probability | Average Success Probability |
|------------------|-----------------------------|-----------------------------|
| Uniform          | 0.35                        | 0.737                       |
| $\rho = 1, T = 3000, \beta = 0.68$ | 0.6                       | 0.877                       |
| $\rho = 0.83, T = 3000, \beta = 0.68$ | 0.63                      | 0.878                       |
| $\rho = 0.67, T = 1600, \beta = 0.88$ | 0.56                      | 0.838                       |
| $\rho = 0.25, T = 1600, \beta = 0.88$ | 0.42                      | 0.834                       |
| $\rho = 0.1, T = 1600, \beta = 0.88$ | 0.36                      | 0.785                       |

Figure 2: Distribution of Success Probabilities for Random Queries to MNIST Subset.

(a) $\rho = 1, T = 3000, \beta = 0.68$  (b) $\rho = \frac{3}{4}, T = 3000, \beta = 0.68$  (c) $\rho = \frac{1}{4}, T = 1600, \beta = 0.88$

Figure 3: Distribution of Success Probabilities for Random Queries to ImageNet Subset.

(a) $\rho = 1, T = 3000, \beta = 0.68$
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Supplement to "Learning to Hash Robustly, with Guarantees"

Preface

We briefly outline the structure of the supplement. We highlight the Discussion in Section F which includes, among other discussion points, an important note regarding the dimensions dependence of the algorithm. Crucially, although in the worst-case we require $d^2 \ln d$ rounds to solve the main min-max game, we can halt the optimization with a data-dependent approximation guarantee (potentially achieving much shorter runtimes). Otherwise, in Section A we include proofs for theorems that appear in section 3 of the main document (particularly for min-max game theory). In Section B we describe an algorithm for efficiently implementing the query player minimization. In Section C we derive the main correctness and performance theorem. In Section D we describe a data model and prove for that model that our algorithm can perform much better than uniform hash functions on the worst-case queries. In Section E we demonstrate that for a reasonable LSH variant, the uniform distribution is optimal for a single cluster with independent coordinates. In Section G we include hardware details for our experiments and the link to the code used to generate our empirical results. We include table of contents below for ease of reference.

Contents

1 Introduction .................................................... 1
   1.1 Our results .................................................... 2
   1.2 Technical description of our algorithm ....................... 3
   1.3 Other related work ............................................ 4

2 Preliminaries .................................................. 4

3 Main Algorithm ............................................... 5
   3.1 Min-Max Optimization Analysis ............................... 5
   3.2 Success Probability Guarantee ............................... 9

4 Improvement on Datasets Generated from a Mixture Model ........ 9

5 Experiments .................................................... 9

A Proofs for Section 3.1 ......................................... 17
   A.1 Proof of Theorem 3.9 .......................................... 17
   A.2 Proof of Theorem 3.15 ........................................ 17
   A.3 Proof of Theorem 3.17 ........................................ 19

B Implementing Query Player Minimization ........................ 20

C Proof of Theorem 3.1 (Success Probability) .................... 21

D Formal Treatment of Mixture Model ............................ 22

E Uniform Distribution is Optimal for Independent Coordinates .... 25

F Discussion ..................................................... 27
A Proofs for Section 3.1

A.1 Proof of Theorem 3.9

Proof. Recall that $A_c^*$ has entires equal to $n_i^p q_i \{ p_i = q_i \}$, for fixed $i \in [d]$ and query/NN pair $p^*, q$. Consider a solution $\pi^*, y^*$ to the RHS of (5). Suppose for contradiction that the theorem is false, i.e. for all query/NN pairs $q, p^*$, $\sum_{i=1}^d \pi^*_i n_i^p \{ p_i = q_i \} > (\pi^*)' A_c^* y^*$. This means there is a coordinate $j \in [M]$ such that $\sum_{i=1}^d \pi^*_i n_i^p \{ p_i = q_i \} > (\pi^*)' A_c^* y^* \geq ((\pi^*)' A_c^*)_j$. We can re-write this as $\sum_{i=1}^d \pi^*_i n_i^p \{ p_i = q_i \} > (\pi^*)' A_c^* e_j$, which contradicts the supposition, as these quantities are exactly equal for query/NN pair $j$.

□

A.2 Proof of Theorem 3.15

We first introduce a somewhat boiler-plate lemma for proving sublinear regret bounds in online learning.

Lemma A.1. [Haghtalab, 2020] Let $y_\ell$ be the resulting strategy from the query player minimization performed at round $t'$ in game 3.7. Explicitly, $y_\ell \leftarrow \arg \min_{y} \sum_{s=1}^{t'} \ell_s^y(y)$. Then,

$$\text{Regret}(y_1, ..., y_t) \leq \sum_{s=1}^{t} \left[ \ell_{\pi_s}(y_s) - \ell_{\pi_s}(y_{s+1}) \right]$$

In order to ensure that the query player minimization gives sublinear regret, we introduce lemma A.2 which shows that the distributions played by the hash player change slowly between rounds of the game.

Lemma A.2. Suppose we perform multiplicative weights update on a vector $w_{t+1} \leftarrow w_t \odot \beta^t$ with base $\beta = 1 - \epsilon_T$ and loss vector $\ell_t \in [0, 1]^N$. Then, for $i \in [N]$, $w_t(i) - w_{t+1}(i) \leq w_t(i) \cdot \epsilon_t$. This implies that for mixed strategies in consecutive rounds $x_{t+1}, x_t$ over $[N]$, $\|x_{t+1} - x_t\|_{\infty} \leq 2\epsilon_T$.

Proof of Lemma 3.15. For any action $i \in [N]$ at time $t$, using the update MWU rule with $\beta = 1 - \epsilon_T$, we get:

$$w_t(i) - w_{t+1}(i) = w_t(i) (1 - \beta^t(i))$$

$$\leq w_t(i) (1 - \beta)$$

$$= w_t(i) \epsilon_T$$

For the second part of the lemma,

$$x_{t+1}(i) - x_t(i) = \frac{w_t(i)}{\sum_j w_t(j)} - \frac{w_{t+1}(i)}{\sum_j w_{t+1}(j)}$$

$$\leq \frac{1}{1 - \epsilon_T} \frac{w_t(i)}{\sum_j w_t(j)}$$

$$= \frac{(1 + \epsilon_T + \epsilon_T^2 + \cdots) w_{t+1}(i) - w_t(i)}{\sum_j w_t(j)}$$

$$= \frac{w_{t+1}(i) - w_t(i) + \epsilon_T \cdot (1 + \epsilon_T + \epsilon_T^2 + \cdots) w_{t+1}(i)}{\sum_j w_t(j)}$$

$$\leq \frac{\epsilon_T w_t(i)}{\sum_j w_t(j)}$$

$$\leq 2\epsilon_T$$

Further,
Before proving the main theorem of this section, we complete the proof that the query player minimization returns pure strategies.

**Proof of Lemma 3.13**  Recall that query strategies are produced by the Follow-the-Leader dynamic (Definition 3.12). In this case, we seek the non-negative vector $y$ with $\|y\|_1 = 1$ such that $\sum_{i=1}^n \pi_i A^i y$ is minimized. We can re-write this as minimizing (for $u = \sum_{i=1}^n \pi_i A^i$): min $u \cdot y$, which is minimized by setting $y = e_i$ for $\arg \min_i u(i)$.

Now, we are equipped to prove sublinear regret for the query player.

**Proof of Theorem 3.15**  We adapt the proof method from (Grnarova et al., 2017). By Lemma A.1

$$\text{Regret}_{FTL}(y_1, ..., y_T) \leq \sum_{t=1}^T \ell_t(y_t) - \ell_t(y_{t+1})$$

(22)

$$= - \sum_{t=1}^T x_t' C(y_t - y_{t+1})$$

(23)

$$= - \sum_{t=1}^{T-1} \left( x_t' C(y_t - y_{t+1}) + x_{t+1}' C(y_{t+1} - y_{t+1}) \right) - \left( x_T' C(y_T - y_{T+1}) \right)$$

(24)

$$= - \sum_{t=1}^{T-1} (x_{t+1} - x_t)' C y_{t+1} - \sum_{t=1}^{T-1} \left( x_t' C y_t - x_{t+1}' C y_{t+1} \right) - \left( x_T' C y_T - x_T' C y_{T+1} \right)$$

(25)

$$= \sum_{t=1}^{T-1} (x_{t+1} - x_t)' C y_{t+1} - \left( x_1' C y_1 - x_T' C y_{T+1} \right)$$

(26)

$$\leq \sum_{t=1}^{T-1} \|x_{t+1} - x_t\|_\infty \|C y_{t+1}\|_1 - \left( x_1' C y_1 - x_T' C y_{T+1} \right)$$

(27)

$$\leq O\left( \sum_{t=1}^{T-1} \frac{d \sqrt{\ln(d)}}{\sqrt{T}} \right) + 1$$

(28)

$$\leq O(d \sqrt{T \ln d})$$

(29)

The sixth line is from applying Holder’s. The seventh line is from Lemma A.2 Lemma 3.13 and noting that the linear form $x' C y$ is within $[0, 1]$. 

\[\square\]
A.3 Proof of Theorem 3.17

Now, we adapt the result of Freund and Schapire to our game, proving that sublinear regret from both players leads to a Nash equilibrium through an iterated two player zero sum game, and this equilibrium pair is a solution to the desired min-max program. (The proof for Theorem 3.17 is inspired by these [Daskalakis, n.d.] lecture notes on algorithmic game theory).

Proof of Theorem 3.17. Consider the row player’s moves up to round $T$. Let $\mathbb{1}$ be the matrix of all ones. Then, Theorem 3.15 implies the following by the definition of regret for some universal constant $c$ (note this constant is not defined in the theorem statement, but appears in it by typo):

$$\text{Regret}(x_1, \ldots, x_T) := \sum_{t=1}^{T} \ell_t(x_t) - \min_{x} \sum_{t=1}^{T} \ell_t(x) \leq cd\sqrt{T \ln d}$$

$$\Longleftrightarrow \sum_{t=1}^{T} x'_t (\mathbb{1} - R) y_t - \min_{x} \sum_{t=1}^{T} x'(\mathbb{1} - R) y_t \leq cd\sqrt{T \ln d}$$

$$\Longleftrightarrow \sum_{t=1}^{T} (1 - x'_t R y_t) - \min_{x} \sum_{t=1}^{T} (1 - x' R y_t) \leq cd\sqrt{T \ln d} \quad (32)$$

$$\Longleftrightarrow \max_{x} \sum_{t=1}^{T} x' R y_t - \sum_{t=1}^{T} x'_t R y_t \leq cd\sqrt{T \ln d} \quad (33)$$

$$\Longleftrightarrow \frac{1}{T} \sum_{t=1}^{T} x'_t R y_t \geq \max_{x} x'R \left( \frac{1}{T} \sum_{t=1}^{T} y_t \right) - c\frac{d\sqrt{\ln d}}{\sqrt{T}} \quad (34)$$

The second line is by substituting the losses for the hash player. The third line is by (1) noting the hash strategies are distributions, and so $x' \mathbb{1}$ is the vector of all ones, and (2) query strategies are standard basis vectors (Lemma 3.13), so $x' \mathbb{1} = 1$. The fourth line follows from: $-\min -x = \max x$. The final line is by re-arranging and dividing by $T$.

Using a symmetric for the column case, except with a different regret dependence on dimension and the loss matrix $-C$, we can derive:

$$\frac{1}{T} \sum_{t=1}^{T} x'_t C y_t \geq \max_{y} \left( \frac{1}{T} \sum_{t=1}^{T} x_t \right)' C y - c\frac{\sqrt{\ln d}}{\sqrt{T}} \quad (35)$$

Summing equations 34 and 35 and noting that $R = -C = A^e_v$, we derive:

$$\min_{y} \left( \frac{1}{T} \sum_{t=1}^{T} x'_t \right)' A^e_v y \geq \max_{x} x'A^e_v \left( \frac{1}{T} \sum_{t=1}^{T} y_t \right) - c\frac{d\sqrt{\ln d}}{\sqrt{T}} - c\frac{\sqrt{\ln d}}{\sqrt{T}} \quad (36)$$

(37)

Observing that,

$$\left( \frac{1}{T} \sum_{t=1}^{T} x_t \right)' A^e_v \left( \frac{1}{T} \sum_{t=1}^{T} y_t \right) \geq \min_{y} \left( \frac{1}{T} \sum_{t=1}^{T} x_t \right)' A^e_v y$$

We can combine the prior two inequalities to derive:

$$\left( \frac{1}{T} \sum_{t=1}^{T} x_t \right)' A^e_v \left( \frac{1}{T} \sum_{t=1}^{T} y_t \right) \geq \max_{x} x'A^e_v \left( \frac{1}{T} \sum_{t=1}^{T} y_t \right) - 2c\frac{d\sqrt{\ln d}}{\sqrt{T}} \quad (38)$$

Using a symmetric argument for the query player, we can show:
This pair is thus an approximate Nash equilibrium. By the definition of the maximum:

\[
\left( \frac{1}{T} \sum_{t=1}^{T} x_t \right)^{'} A^c_v \left( \frac{1}{T} \sum_{t=1}^{T} y_t \right) \leq \min_y \left( \frac{1}{T} \sum_{t=1}^{T} x_t \right)^{'} A^c_v y + 2c \frac{d\sqrt{\ln d}}{\sqrt{T}}
\]

(39)

And,

\[
\left( \frac{1}{T} \sum_{t=1}^{T} x_t \right)^{'} A^c_v \left( \frac{1}{T} \sum_{t=1}^{T} y_t \right) \geq \max_x x^{'} A^c_v \left( \frac{1}{T} \sum_{t=1}^{T} y_t \right) - \min_y \max_x x^{'} A^c_v y - 2c \frac{d\sqrt{\ln d}}{\sqrt{T}}
\]

(40)

The final claim of this theorem follows by Von Neumann’s minimax theorem \cite{Neumann1928}. \qed

## B Implementing Query Player Minimization

The implementation of the MWU strategy selection is fairly self-explanatory, but how should we efficiently perform the query player minimization? We now show that the query player minimization is efficiently implementable and prove the runtime of the entire pre-processing procedure.

**Algorithm 3** Query Player Minimization

1: function QPM($\pi_v$, $v$, $\rho$)  
\(\triangleright \pi_v\) is the distribution over bits, current node $v$
2: 3: compute objective values $n_{i,b}^{\rho}$ for $i \in [d]$ and $b \in \{0,1\}$
4: 5: min probability = $\infty$
6: 7: for $j = 1, \ldots, n_v$, do.
8: set $u_j \in \mathbb{R}^d$ to the objective values for the given datapoint.
9: compute $s_j = u_j \odot \pi_v$
10: sort $s_j$, while tracking the positions of the original coordinates
11: Set the top $r$ values in the sorted list to 0 and sum the remaining values (call this sum $z_j$)
12: if $z_j < \text{(min probability)}$ then
13: set (min probability) = $z_j$
14: set (min query) to the current datapoint $j$ with the top $r$ coordinates flipped.
15: end if
16: end for
17: 18: return min query
19: end function

**Proof of Theorem 3.1 (Pre-processing Time).** The query player minimization (step 7 of Algorithm 2) can be implemented exactly using Algorithm 3.

Suppose the current node is $v$, and the current bucket is of size $n_v$. By theorem 3.2, a single min-max optimization can be solved in time $O(\frac{T}{\epsilon^2} n_v d^3 \ln^2 d)$. In a given layer of the tree, each node contains a bucket that is disjoint from all other buckets in that layer. Therefore, the total runtime for the
algorithm on a single layer of the tree is $O(\frac{1}{\rho} nd^3 \ln^2 d)$. Further, there are at most $d$ layers in the tree, as we hash without replacement when we progress to the next layer. This gives the pre-processing time in the theorem.

\section{Proof of Theorem 3.1 (Success Probability)}

We now prove the success probability guarantee as in Theorem 3.1. Let $\delta = \frac{1}{m}$ for chosen tradeoff parameter $m > 0$. (We do not define $\delta$ in the theorem by omission). The query time is $O(md^2)$, in particular, suppose we are given a dataset with a datapoint $p^*$ and a query $q$ with $\|p^* - q\|_1 \leq \rho$. Recall that we want to guarantee that when the querying procedure terminates (Algorithm 1), the probability that the pair of points collide on the final bucket is at least $n^{-\rho} \geq n^{-\frac{d}{2}}$, for $\rho$ satisfying $\mathbb{E}_{i \sim \pi,} [\mathbb{I}\{p^*_i = q_i\} \cdot f_{i,p^*,v}] \geq 1$ on all nodes $v$ in the LSH tree (where $f_{i,p^*,v} = |P^*_i|/|P^v|$).

**Proof.** The proof is by induction over the size of the dataset. Fix any query/NN pair $q, p^* \in \mathbb{H}^d$. For the base case assume the size of the dataset is $|P| = 1$. Then, by assumption that there is a near neighbor in the dataset, and as the stopping condition is reached ($1 \leq C$ for all choices of $C$), the probability of success is exactly 1.

We now prove the induction step of the claim. Consider the tree of possible hashes from the given dataset, with each child corresponding to a hash event. Note this is a $d$-ary tree. Consider a dataset of size $n_v$ at some node $v$ in the tree, with some children that have additional optimizations performed and perhaps some children that don’t. Suppose all children have size $n_{i,v} < n_v$. If not, we re-direct this argument to the child with $n_{i,v} = n_v$. If this child also has children of size $n_v$, then we again focus on the grandchild node, repeating this recursion until we reach a descendant node with children all of size strictly less than $n_v$. We can then "unpeel" the argument to prove the inductive hypothesis for the original node using the same calculation as below.

Assume for induction that the optimizations in the children (one child for each $i \in [d]$) produce a distribution that has minimum probability of success greater than $n_{i,v}^{-\rho}$ for all queries with $n_{i,v} < n_v$. The current node optimizes assuming the children have probability of success $\{n_{i,v}^{-\rho}\}_i$. We follow a similar approach to (Andoni et al., 2017) to prove lower bounds with uniform hashing.

For the first inequality, recall by the theorem assumption, there exists a distribution over hashes $\pi_v$ such that $\mathbb{E}_{i \sim \pi,} [\mathbb{I}\{p^*_i = q_i\} \cdot f_{i,p^*,v}] \geq 1$. Then, we have the following by the induction hypothesis:

\begin{equation}
\Pr[success] = \sum_i \mathbb{I}_{\pi_v, \mathbb{I}\{p^*_i = q_i\}} \cdot \Pr[success \mid P^v_i] \geq \sum_i \mathbb{I}_{\pi_v, \mathbb{I}\{p^*_i = q_i\}} \cdot n_{i,v}^{-\rho}
\end{equation}

\begin{equation}
= n_v^{-\rho} \cdot \mathbb{E}_{i \sim \pi,} [\mathbb{I}\{p^*_i = q_i\} \cdot f_{i,p^*,v}] \geq n_v^{-\rho}
\end{equation}

This completes the proof for the first guarantee of the success probability.

To ensure the second inequality in the theorem holds (namely $\rho \leq \frac{d}{2}$), we follow the strategy suggested in (Andoni et al., 2017) to handle datasets with many approximate near neighbors. In particular, we select points uniformly at random at each node and compare these to our query, halting the query procedure if an approximate near neighbor is found. Suppose then for the node $v$ in the LSH tree, the current bucket $P^v$ has $\delta n_v$ points at distance less than $\epsilon r$ from the query. Then, with constant probability, selecting $m = \Theta(\frac{1}{\rho})$ (as the algorithm parameter) random points in the dataset will include one such near point. Note that this is why the query time in Theorem 3.1 is $md^2$, as a single query comparison takes $d$ time and there are at most $O(md)$ comparisons at query time. Now suppose to the contrary that fewer than $(1 - \delta)n_v$ points are at distance less than $\epsilon r$ from all queries.
For the second inequality in the theorem \((\rho \leq \frac{\ln n}{d})\), we note for randomized hash function \(h\) with distribution \(\pi \in \Delta[d]\), where we let \(\rho_0 = \frac{1}{2}\):

\[
\Pr[\text{success}] = \Pr_{i \sim \pi} [\text{success on } P_{i,q_i}^c] \geq \Pr_{i \sim \pi} [\text{success on } P_{i,q_i}^c, \text{ and } p_i^* = q_i] = \Pr_{i \sim \pi} [\text{success on } P_{i,q_i}^c, p_i^* = q_i] \cdot \Pr_{i \sim \pi} [p_i^* = q_i] \geq \mathbb{E}[n_i^{-\rho_0}] \cdot \Pr_{i \sim \pi} [p_i^* = q_i],
\]

where the fourth step follows by the induction assumption. If we choose \(h\) to be distributed uniformly, then applying Jensen’s inequality we get:

\[
\Pr[\text{success}] \geq \left(1 - \frac{r}{d}\right) \cdot \mathbb{E}[n_i^{-\rho_0}] \geq \left(1 - \frac{r}{d}\right) \left(\sum_{p \in \rho^v} \Pr[p_i^* = p_i]\right)^{-\rho_0} \geq \left(1 - \frac{r}{d}\right) \left(\frac{\delta n_v}{n_v} + (1 - \delta)n_v (1 - \frac{cr}{d})\right)^{-\rho_0} \cdot n_i^{-\rho_0} \cdot n_v^{-\rho_0}.
\]

The third line is because we assume at most \(\delta\) fraction of points are at distance at most \(cr\), and at least \(1 - \delta\) fraction are at distance at least \(cr\). To complete the proof, we now show the last formula is lower bounded by \(n_v^{-\rho_0}\).

\[
\left(1 - \frac{r}{d}\right) \left(\frac{\delta n_v}{n_v} + (1 - \delta)n_v (1 - \frac{cr}{d})\right)^{-\rho_0} \geq 1 \iff \rho_0 \geq \ln\left(\frac{1}{(1 - \delta)^d}\right) \ln^{-1}\left(\frac{1}{\delta + (1 - \delta)(1 - \frac{cr}{d})}\right) \iff \rho_0 \geq \ln\left(\frac{1}{1 - \frac{cr}{d}}\right) \ln^{-1}\left(\frac{1}{\delta + (1 - \delta)(1 - \frac{cr}{d})}\right).
\]

Note that \(\frac{1}{1 - \frac{cr}{d}} \geq \ln\left(\frac{1}{1 - \frac{cr}{d}}\right) \ln^{-1}\left(\frac{1}{1 - (1 - \delta)^2}\right)\), and so we can set \(\rho_0 \geq \frac{1}{(1 - \delta)^2}\). As the true probabilities of success are greater than the "lower bound" objective by the induction assumption in both inequalities, the true probability of success is greater still than \(n_v^{-\rho}\) (or \(n_v^{-\rho_0}\) in the second inequality), proving the theorem.

\(\square\)

## D Formal Treatment of Mixture Model

We first define the uniform LSH algorithm [Indyk & Motwani [1998]] for the general ANN problem. In this algorithm, for a chosen approximation factor \(c\), a fixed number of hash functions are chosen such that the probability of success for the algorithm, for any query at distance \(r\) from its near neighbor, is exactly \(n^{-\rho}\) where \(\rho = \frac{\ln(1 - \frac{1}{r})}{\ln(1 - \frac{1}{d})}\).

**Theorem D.1.** Suppose we have a dataset drawn according to the above data model, with \(r = d/\sqrt{\ln d}\), \(n = d^6\), \(\epsilon_1 = 0.3\), \(\epsilon_2 = 0.5\), \(\alpha_1 = \alpha_2 = \frac{d}{2}\). Then with probability 0.99 over the data distribution, Algorithm 2 with algorithm parameters \(m, \rho \in (0.1, 1)\) until the bucket size is \(d\), and after that \(\rho = 0\) until stopping condition \(C = 1\), for
we conclude

\[ \pi \]

Then, as,

\[ \text{The probability of success for the uniform distribution on the worst-case query on reaching this} \]

\[ \text{first class is lower bounded by} \]

\[ n \]

\[ \text{Proof of Theorem D.1.} \]

\[ \text{We must first understand what it means for a query to be "worst-case" for the} \]

\[ \text{standard uniform LSH. In particular, this algorithm in its original formulation uses a fixed number of} \]

\[ \text{uniform hash functions, and so the probability of success is the same for all queries at a fixed distance} \]

\[ \text{from their near neighbor. To define the probability of success for uniform LSH as applied to our data} \]

\[ \text{model, we divide the potential queries to this dataset into two classes. In the first class, we consider} \]

\[ \text{queries to any arbitrary point (not equal to } p_a \text{ and its cluster), which all require an equal number of} \]

\[ \text{hashes to reach expected bucket size 1. In the second, we consider queries to } p_a \text{ with bits flipped} \]

\[ \text{on the coordinates that differentiate } p_a \text{ from its planted approximate near neighbors. For the second} \]

\[ \text{class to be "worst-case" we need that the probability of success for queries in this class are less than} \]

\[ \text{the first.} \]

The probability of success for the second class is exactly \( \sqrt{d^{-r_a}} \) where \( r_a = \frac{\ln(1-\frac{2}{d})}{\ln(1-\frac{2}{d}+\epsilon)} \). We can

lower bound this success probability by \( \sqrt{d^{-r_a + O(\frac{1}{r})}} \geq \frac{1}{d^{1/2+\alpha(\frac{1}{r})}} \).

The probability of success for the first class is lower bounded by \( n^{-0.5/c_0} \) where \( c_0 r \) is the average
distance between two points (chosen iid from the model). We can compute this distance as \( c_0 r = \frac{d}{2} \cdot 2(1-\epsilon_1)\epsilon_1 + \frac{d}{2} \cdot 2(1-\epsilon_2)\epsilon_2 = d(1-\epsilon_1)\epsilon_1 + d(1-\epsilon_2)\epsilon_2. \) As we have set \( n = d^n \), we have that
the probability of success for this first class is,

\[
\text{Pr[success | for phase 1] } \geq -6 \cdot \frac{0.5}{0.464} \ln d \tag{59}
\]

\[
> -7 \cdot \ln d \tag{60}
\]

\[
= -7 \sqrt{\ln d} \tag{61}
\]

\[
\iff \text{Pr[success | for phase 1] } \geq \exp(-7\sqrt{\ln d}) \tag{62}
\]

\[
\gg \exp(-0.5 \ln d) \tag{63}
\]

\[
= \frac{1}{\sqrt{d}} \tag{64}
\]

\[
\approx \text{Pr[success | for phase 2]} \tag{65}
\]

proving that the second class queries are indeed worst-case in the high-dimensional limit.

Because the distribution for the optimized hash functions are maximal for their objective (by definition), we can choose any distribution we’d like and derive a lower bound for the performance of a single optimized hash distribution. We consider distributions that are marginally uniform on each group \( S_i \), as the planted point has a 0 on each coordinate (and so the coordinates are symmetric across groups). Suppose the optimized distribution is \( \pi = (0, 1) \). This is the distribution that would be returned by our algorithm for almost all \( \rho \), but certainly including e.g. \( \rho \in (0.1, 1) \). To see this, we first note that the objective function (the lower bound for the probability of success for \( \pi = (\pi_1, \pi_2) \)) is:

\[
\text{Objective } = \frac{d}{2} \pi_1 (1-\epsilon_1)^{-\rho} + \frac{d}{2} \pi_2 (1-\epsilon_2)^{-\rho} \tag{66}
\]

Then, as,

\[
(1-\frac{2r}{d}) (1-\epsilon_2)^{-\rho} > \frac{1}{2} (1-\epsilon_1)^{-\rho} + \frac{1}{2} (1-\frac{2r}{d}) (1-\epsilon_2)^{-\rho} \tag{67}
\]

we conclude \( \pi = (0, 1) \) is the distribution returned by our algorithm.

Suppose we choose \( k_u \) hash functions to reach \( d/n \) fraction of points remaining in the original dataset.

The probability of success for the uniform distribution on the worst-case query on reaching this fraction is \( (1-\frac{2}{d})^{k_u} \).
As a uniform hash function reduces the dataset to at least $\epsilon_1$ fraction of the original dataset size, $k_u \geq \ln(\frac{2}{\epsilon}) \ln^{-1}(1/\epsilon_1)$.

Meanwhile, for the worst-case query, as we have assumed all of the coordinates that differentiate the cluster center $p_u$ from its approximate near neighbors are in $S_1$, and therefore all the flipped coordinates of the worst-case query are in $S_1$, the probability of success for this query in hashing to size $d$ from the root is exactly 1. In the remaining hashing from the size $d$ subset, the optimized algorithm has probability at least $d^{-\rho_0}$, where $\rho_0 = \frac{\ln(1-\frac{\epsilon_1}{2})}{\ln(1-\frac{\epsilon_1}{2d})}$, from equation (58) in the proof of theorem 3.1.

Once the dataset is of size $d$, according to the uniform (theoretical) LSH algorithm (Indyk & Motwani 1998), the probability of success is exactly equal to $d^{-\rho_u}$, where $\rho_u = \frac{\ln(1-\frac{\epsilon}{2d})}{\ln(1-\frac{\epsilon}{2d})}$. The total probability of success for this worst-case query in uniform LSH is then,

$$\Pr[\text{success} \mid \text{uniform}] \leq d^{-\rho_u} (1 - \frac{r}{d}) \ln(\frac{2}{\epsilon}) \ln^{-1}(1/\epsilon_1)$$  \hspace{1cm} (68)

The final advantage of our algorithm over uniform LSH follows from these formulae.

One fact that remains to show is that in the high-dimensional limit, the balances of the coordinates remain concentrated at $\epsilon$.

Consider a node $v$ in the tree that was generated by hashing on $k_u$ coordinates. Consider an unhashed dimension $i \in [d]$. Let $f_{i,v}$ be the balance of coordinate $i$ at this node. As the dataset has independently drawn coordinates, the distribution of balances for $i$ is independent of the previous hashes, and so $f_{i,v} = \frac{1}{n_u} \cdot \text{Binomial}(n_v, \epsilon_i)$. Then, we can apply the standard Chernoff bound:

$$Pr[|f_{i,v} - \epsilon_i| > \delta] \leq 2 \exp \left( -\frac{1}{3} \epsilon_i n_v \delta^2 \right)$$  \hspace{1cm} (69)

$$\leq 2 \exp \left( -\frac{1}{3} \epsilon_2 \delta^2 \right)$$  \hspace{1cm} (70)

$$= \frac{1}{100d^{k+1}}$$  \hspace{1cm} (71)

Note there are a total of at most $d^k$ nodes and $d$ coordinates we must consider for $\leq k$ possible hashes. Thus, we set the failure probability to $10^{-k+1} d^{k+1}$ so that the probability of success on all nodes is at least $(1 - \frac{1}{100d^{k+1}}) d^{k+1} \approx e^{-0.01} = 0.99$. Solving the previous equation for $d$ gives the requirement that

$$d \geq \frac{3(k+1) \ln(d) + 3 \ln 200}{\delta^2 \epsilon_2 k_u}.$$  \hspace{1cm} For fixed, $\delta$, $\epsilon_2$, and $k \leq \frac{\ln(\frac{1}{\epsilon})}{\ln(1-\epsilon_1)}$, the left-hand-side grows faster with dimension than the right. Therefore, in the high-dimensional limit we can drive $\delta \to 0$ while maintaining a 0.99 probability of success.

We also show improvement over the LSH forest algorithm. Recall that in this algorithm, for a given query, a coordinate is chosen uniformly at random, one at a time, until the current bucket has size less than or equal to 1.

**Theorem D.2.** Suppose we have a dataset drawn according to the aforementioned data model, with $d = 100r$, $n = d^3$, $\epsilon_1 = 0.3$, $\epsilon_2 = 0.5$, $\alpha_1 = \alpha_2 = \frac{d}{r}$, but only one planted approximate near neighbor to $p_u$. Then with probability 0.99 over the data distribution, Algorithm 7 with parameters $m = 0$, $p \in (0.2, 0.8)$ until the bucket is of size $d$, and then $p = 0$ for the remainder of the tree until stopping condition $C = 1$, where $k_u = \ln(\frac{\epsilon}{d^3}) \ln^{-1}(1/\epsilon_1)$, has $(1 - \frac{\epsilon}{d})^{-k_u}$ times greater success probability than uniform LSH trees for all queries (over the randomness of the algorithm and data model).

**Proof.** We first prove that the minimum-performing query to this dataset (for uniform LSH trees) is one with all coordinates flipped in $S_1$ (on the bits differentiating an approximate near neighbor...
from \( p_a \). As there are \( r + 1 \) coordinates for which \( p_a \) differs from all other near neighbors, we must hash until the single coordinate that is not flipped in the worst-query, is flipped. The probability of this is \( \frac{1}{2}^{r+1} \approx \frac{1}{2}^r \), where \( k \ll d \) is the number of hashes chosen to get the dataset to size \( d \), and increases to \( \frac{1}{2}^{r+1} \) for \( s \) additional hashes. Then, we will need at least \( \frac{k}{2} \) additional hashes to get \( O(1) \) probability of getting to a single point, using uniform hashing. (This is because \( (1 - \frac{1}{2}) \cdots (1 - \frac{3}{2}) \approx (1 - \frac{3}{2})^4 = O(1) \)).

The probability of success for this query doing this is \( (1 - \frac{r}{d})^2 \approx e^{-r/2} \), which is clearly vanishing with \( r \), and is greater than for all queries which are not designed to have \( r \) of the \( r + 1 \) differing coordinates flipped. Suppose we only flip \( r - \ell + 1 \) of these \( r + 1 \) bits, for \( \ell \geq 2 \), then the probability of eventually hashing on one of the unflipped bits is \( (1 - \frac{r}{d})^{2\ell} \approx e^{-r/2\ell} \). Suppose pessimistically the probability of success for other queries is \( \frac{1}{d} \) (as good as randomly sampling points) times the probability of selecting one of the differing coordinates \( e^{-r/2\ell} \). Suppose optimistically it is \( e^{-r} \) for designed queries with \( r \) of the \( r + 1 \) bits flipped. Then we just require \( \frac{1}{d} e^{-r/2\ell} (1 - \frac{r}{d})^k e^{-r/2} \geq e^{-r/2} \) for the designed query to be the true minimum, where \( k_o \) is the number of hash functions needed to get to bucket size \( d \) for optimized hashing. This inequality is true for large \( r \) and \( d = 100r \), proving the worst-case query is as claimed.

Consider the first phase, where we hash the dataset until it is of size \( d \). The probability of success for the optimized distribution on the worst-case query is exactly 1, while for the uniform hash tree it is at most \( (1 - \frac{r}{d})^k \), where \( k_o = \ln(\frac{d}{2}) \ln^{-1}(\epsilon_1) \) (as we proved in the previous theorem). With very high probability, we will not have chosen the necessary differentiating bit to separate the approximate near neighbor from \( p_a \). Therefore, the probability for the remainder of the tree for uniform is (with high probability) equal to that of our algorithm (as the datasets of size \( d \) should be the same in expectation for both algorithms, given the independent coordinates assumption, the probability of success over the randomness in both the algorithm and the data model is equal for both algorithms).

\section{E Uniform Distribution is Optimal for Independent Coordinates}

Suppose the data are drawn from the data model in section \( \ref{sec:uniform} \) without an additional planted cluster. Suppose further that instead of two groups, there are \( M \) groups \( S_i \) with \( M \ll d \), balances \( \epsilon_i \in (0, \frac{1}{2}] \), and cardinalities \( d/M \). We also consider the limit where \( r \ll d \). For simplicity of analysis, suppose we plant the point \( 0^d \) in the dataset.

We consider a variant of the LSH tree where a fixed number of hash functions are selected from a chosen distribution \( \pi \) until the dataset of size \( n_0 \), where \( d < n_0 \). In a standard LSH tree, where \( w_i \) is the fraction of points remaining in the dataset after hashing for the \( i \)-th time, we select hashes \( k_o \) in total such that:

\begin{equation}
\prod_{i=1}^{k_o} w_i = \frac{n_0}{n} \tag{72}
\end{equation}

\begin{equation}
\iff \sum_{i=1}^{k_o} \ln w_i = \ln \frac{n_0}{n} \tag{73}
\end{equation}

As \( k_o \) is a random variable, we instead consider the number of hash functions \( k_o \) needed in expectation to reach the stopping size. In other words, we compute \( k_o^* \) such that:

\begin{equation}
\mathbb{E} \left[ \sum_{i=1}^{k_o^*} \ln w_i \right] = \ln \frac{n_0}{n} \tag{74}
\end{equation}

In the LSH variant we propose here, we use this fixed \( k_o^* \) number of hashes.

\textbf{Theorem E.1}. \textit{When the data are sampled according to the above data model, the uniform distribution is optimal for the worst-case query to the above LSH variant.}
Proof. We derive the exact value of the number of hash functions $k_o^*$. By assuming the coordinates are drawn independently, we use the linearity of expectation to derive:

$$
\mathbb{E} \left[ \sum_{i=1}^{k_o^*} \ln w_i \right] = \ln \frac{n_0}{n} \quad (75)
$$

$$
\iff k_o^* = \ln \frac{n_0}{n} \mathbb{E}^{-1} [\ln w_i] \quad (76)
$$

$$
= \ln \frac{n_0}{n} \left( \sum_{i=1}^{M} \pi_i \ln (1 - \epsilon_i) \right)^{-1} \quad (77)
$$

The last step follows from two facts. First, we only need to consider distributions over coordinates that are marginally uniform across coordinates in a single group. This is because the worst queries to the dataset will be to the planted point $0^d$, whose balances are uniform across coordinates of a single group. Second, because we are in the high-dimensional limit (as in the previous section), when we hash on a single coordinate $i$, the fraction of points in the dataset that remains in the bucket is exactly $1 - \epsilon_i$, as this is the fraction of points that have a 1 at coordinate $i$.

Consider a query at distance $r$ from $0^d$ with its $r$ coordinates flipped in an arbitrary group $j \in [M]$. To begin with, suppose $M = 2$. The probability of success over the entire tree for this query is, using $k_o^*$ total hashes:

$$
\Pr[success] = \left( 1 - \pi_j \frac{2r}{d} \right)^{k_o^*} \quad (78)
$$

$$
\iff \ln \Pr[success] = \ln \left( \frac{n_0}{n} \right) \ln \left( 1 - \pi_2 \frac{2r}{d} \right) \mathbb{E}^{-1} [\ln w_i] \quad (79)
$$

$$
\approx \ln \left( \frac{n_0}{n} \right) \frac{2\pi_2 r}{d} \mathbb{E}^{-1} [\ln w_i] \quad (80)
$$

$$
\propto \frac{\pi_2}{\pi_1 \ln w_1 + \pi_2 \ln w_2} \quad (81)
$$

$$
= \frac{\pi_1}{(1 - \pi_2) \ln w_1 + \pi_2 \ln w_2} \quad (82)
$$

As the logarithm is increasing, we can compute the derivative of the RHS to understand the optimal setting of $\pi_2 = 1 - \pi_1$. Doing so, we find that the derivative is $\frac{d}{d\pi_2} (\text{RHS}) = \frac{\ln w_1}{(1 - \pi_2) \ln w_1 + \pi_2 \ln w_2} < 0$. Therefore, the probability of success increases by decreasing $\pi_2$. Further, if the query has its bits flipped on group $S_1$ instead, the probability of success is also decreasing in $\pi_1$. Therefore, the optimal distribution decreases $\pi_2$ until the probability of success for both types of queries are equal. Setting these two query probabilities to be equal:

$$
\frac{\pi_2}{(1 - \pi_2) \ln w_1 + \pi_2 \ln w_2} = \frac{\pi_1}{(1 - \pi_2) \ln w_1 + \pi_2 \ln w_2} \quad (83)
$$

we derive that $\pi_1 = \pi_2$, i.e. the uniform distribution is optimal.

Generalizing to many groups (for increasing, non-negative functions $F_j(\pi_j)$):

$$
\ln \Pr[success] \approx \ln \left( \frac{n}{n_0} \right) \frac{\pi_j M r}{d} \mathbb{E}^{-1} [\ln w_i] \quad (84)
$$

$$
\propto \frac{\pi_j}{\sum_{i=1}^{M} \pi_i \ln w_i} \quad (85)
$$

$$
= F_j(\pi_j) + \frac{\pi_j}{\sum_{i=1}^{M} \pi_i \ln w_i} \quad (86)
$$

As the logarithm is increasing, we can compute the derivative of the RHS to understand the optimal setting of $\pi_j$. Doing so, we find that the derivative is $\frac{d}{d\pi_j} (\text{RHS}) = \frac{F_j(\pi_j) - \pi_j F_j'(\pi_j)}{(\pi_j \ln w_2 - F_j(\pi_j)) \pi} < 0$. Again,
the probability of success is decreasing in $\pi_j$. Further, the denominator is the same regardless of where the query’s bits are flipped (i.e., which group is chosen to flip). So, for a fixed distribution, the log of the probability of success is proportional to the probability of choosing the group with bits flipped for that query. In this independent case, there are essentially $M$ possible types of queries - one with bits flipped entirely in each one of the groups. Suppose that for a chosen distribution, the probability of success is higher for queries in one group versus another. Then, by the derivative argument above, we can increase the success probability for the worse query by moving weight from that group to the other. Therefore, any distribution that has this inequity is not optimal. Therefore, the optimal distribution is such that for all $j, k \in [M]$:}

$$\frac{\pi_k}{\sum_{i=1}^{M} \pi_i \ln w_i} = \frac{\pi_j}{\sum_{i=1}^{M} \pi_i \ln w_i}$$  \hfill (87)

Hence, the uniform distribution is again optimal. \hfill \Box

### F Discussion

**Challenges for designing instance optimal NNS algorithms.** An ideal goal for data-aware NNS would be an instance-optimal algorithm: one that achieves the best possible performance (success probability/query time) amongst all possible algorithms. To avoid hard computational complexity issues, it is only reasonable to ask for all possible algorithms from a restricted class of algorithms $\mathcal{C}$, for as large class $\mathcal{C}$ as possible.

We considered the class $\mathcal{C}$ of, essentially, (random) decisions trees, where each node is a coordinate cut (in the Hamming space). Our algorithms is instance optimal as long as the algorithm knows the correct parameters $\rho$ at each node.

It would be natural to try to extend the class $\mathcal{C}$ to include other possible hashes (node decision functions), most notably hyperplane cuts for the Euclidean space, and ball cuts (for both Hamming and Euclidean spaces). Such hashes are popular for practical and theoretical LSH algorithms.

There are some challenges in extending our algorithm to the above settings. Specifically, while one can efficiently extend the algorithm in this paper to other hash functions and metrics, the runtime must depend polynomially either on the number of possible hash functions or the number of possible queries. Indeed, one can solve the two-player game by implementing MWU strategy selection for the player with polynomially many strategies (in the dataset size), and FTL for the other player. Alas, both for hyperplane and ball cuts the number of hash functions and queries are essentially exponential in $d$. It may be possible to reduce the number of hash functions/queries by making an assumption: e.g., consider ball cuts with centers at dataset points, or assume queries come from a distribution.

Yet it is still conceivable to design an efficient algorithm for instance optimal hashing even when there are exponentially many queries and hash functions. Intuitively, say, from the perspective of the hash function distribution, we do not actually need the optimal distribution—merely a sample from it. In fact, if Karlin’s weak conjecture holds (Karlin, 1962), namely that both players can use FTL to achieve sublinear regret, then neither player must explicitly consider all of their exponentially many strategies! There is some hope that this conjecture is true (see (Abernethy et al., 2021)).

**Effect of the parameter $\rho$ to the algorithm.** Depending on the exponent $\rho$ chosen for the optimizations in the experiments, the distributions returned by the min-max optimization in Algorithm 2 could be qualitatively quite different. In the experiment with exponent $\rho = \frac{1}{10}$ (Figure 1), the distribution at the root placed a large amount of weight on the most balanced bits. However, when the exponent was decreased to $\rho = \frac{1}{100}$, the optimal distribution (roughly) uniformly weighted many balanced and unbalanced bits.

We illustrate why the optimal distributions might be very different depending on input $\rho$ with the following examples. Suppose there are two groups of bits with balances $0.1, 0.5$, respectively, and with sizes $5r, r$ for queries at radius $r$. Then, the optimal distribution will have less weight on the more balanced group, as the worst-case query with have all $r$ of the more balanced bits flipped. Suppose instead that the two groups have balances $0, 0.5$, with sizes $r, 100r$, respectively. Then, the optimal distribution will place no weight on the first, unbalanced group, as these bits make no progress on hashing the dataset, while the second group is sufficiently large that you can increase the weight on that group without increasing the probability of failure substantially.
Theorems D.1 and D.2 show large improvement over uniform hashing by exploiting the nice structure of the dataset to isolate the cluster later down the tree. There we make an assumption that the coordinates differentiating the cluster all appear in the less-balanced group. We expect that, in practice, with sufficiently "diverse" data, a given dataset might consist of many clusters whose differentiating coordinates are spread across balances. (Note we still see theoretical improvement in this case.) The function of these clusters is really to introduce adversarial quality to the dataset so that the current balances at the root (or a nearby descendant) do not indicate the true difficulty of hashing on a particular coordinate. In this case, the worst-case queries are not those with the most balanced coordinates flipped, but rather those embedded in these adversarial clusters. In effect, the worst-case analysis of the LSH tree is reduced to average-case analysis (as the differentiating coordinates are likely spread across a large spectrum of balances).

Recall that with the "correct" objective values our algorithm is exactly instance-optimal. Given the discussion above, this suggests that there might be a different choice of objective values in our min-max game that more closely approximates instance-optimality. In particular, rather than setting a single exponent $\rho$ for the entire algorithm, this parameter should vary for each possible bucket, and should be tuned reflect the difficulty of hashing uniformly on that bucket. In other words, while our algorithm optimizes for the snapshot of a dataset at a given node, an instance optimal algorithm must be able to look ahead and use information about what the buckets will look like in future nodes.

As we showed in section E if the coordinate balances remain constant throughout the hash tree (in which case the bucket looks identical to the optimizer at every node), it may not be possible to improve over uniform at all! Therefore, to guarantee improvement over uniform sampling, we need that the balance profiles of the coordinates change throughout the hash tree. This is likely what occurred in our experiments - namely, which coordinates were balanced early in the tree were distinct from (or independent of) which coordinates were balanced later down the tree. To exploit this feature of a dataset in practice, one may try to obtain a better lower bound on the probability of success than merely $n^{-\rho}$, for $\rho$ from the uniform LSH—e.g., by setting up a convex program and relaxing it. This is an interesting route for future work.

**Pre-processing.** Recall that the runtime for pre-processing of our algorithm is $n \cdot \text{poly}(d) \cdot \frac{1}{\epsilon^2}$, where $\epsilon$ is the approximation factor in the min-max game. To closely approximate the optimum success probability, we need to set $\epsilon$ to be on the order of (ideally less than) the optimum. Therefore, an equivalent runtime is $n \cdot \text{poly}(d) \cdot (\Pr[\text{success}])^{-2} = n^{1+O(\rho)} \cdot \text{poly}(d)$.

**Convergence of the min-max game.** The number of steps to convergence depends as $1/\epsilon^2$ on the error $\epsilon$ to success probability. As noted above, $\epsilon$ must be of the order $\Pr[\text{success}]$ hence quite small, and it is normal to wonder whether this step can be sped-up. As we discuss below, the game can be stopped much earlier, in a data-aware way, while retaining the theoretical guarantees.

Indeed, in our experiments, we used far fewer iterations than are required by Theorem 3.2. We used 3000 iterations, while the theoretical bound requires $\frac{784^2 \ln(784)}{4 \cdot 10^6} > 4 \cdot 10^6$. How can we show that the distributions are converged? In general, how might a practitioner improve our algorithm’s polynomial dependence on the dimension? In the proof of Theorem 3.17 the proximity to a Nash equilibrium is bounded by the sum of the average regret of the two players. Therefore, a practitioner can simply halt the game when the sum of the average regrets of the two players is less than their desired approximation threshold.

We consider the distribution at the root for an experiment with $\rho = 0.5$, $T = 3000$, and $\beta = 0.08$ (Figure 1). For the query player, the average loss achievable by the best query (least probability of success) is 0.00051286, while the loss incurred by the query player is 0.0005134, meaning that the average regret of the query player is $5.78 \cdot 10^{-7}$. For the hash player, we compute the best distribution in hindsight by solving the following linear program:

\[
\min_{\pi} \frac{1}{T} \sum_{t=1}^{T} (1 - \Pr[\text{success on } (p^t, q^t)]) = \min_{\pi} \left( 1 - \sum_{t=1}^{T} \sum_{i=1}^{d} \pi_i \mathbb{1}\{p^t_i = q\} \cdot n_{i,t}^{-\rho} \pi_i \right) 
= 1 - \min_{\pi} \sum_{i} \pi_i \left( \sum_{t} \mathbb{1}\{p^t_i = q\} \cdot n_{i,t}^{-\rho} \right)
\]
Where $\pi$ is constrained to $\Delta[d]$.

Solving this program gives that the loss of the best distribution is $0.99739$, while the loss incurred by the hash player is $0.99949$, and so the regret of the hash player is at most $0.0021$. Therefore, the query/hash strategies are within $0.0022$ of the game’s value, which in this case is on the order of the optimum.

G Implementation Details

A link to the experiment code repository can be found at (https://github.com/dmbeaglehole/Instance-Adaptive-LSH-Forests/blob/main/README.md). The experiments were implemented in C++, and compiled with g++-5 using the -march=native and -O3 flags for improved runtime. In addition, our implementation was highly parallelized using OpenMP pre-processor directives. Efficient matrix/vector computation was done with the Eigen library for C++ (Guennebaud et al., 2010). The experiments were performed on an Intel(R) Xeon(R) W-2155 CPU @ 3.30GHz with 65 GB of RAM (all 20 physical cores were used for the experiment). The runtime to generate 110 trees with 3000 game rounds varied, but took on average 40 hours to complete with these hardware specs.