GRAPH-BASED NEAREST NEIGHBOR SEARCH IN HYPERBOLIC SPACES

Anonymous authors
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ABSTRACT

The nearest neighbor search (NNS) problem is widely studied in Euclidean space, and graph-based algorithms are known to outperform other approaches for this task. However, hyperbolic geometry is found to be very useful for data representation in various domains, including natural language processing, computer vision, and information retrieval. In this paper, we show that graph-based approaches are also well suited for hyperbolic geometry. From a theoretical perspective, we rigorously analyze the time and space complexity of graph-based NNS, assuming that an n-element dataset is uniformly distributed within a d-dimensional ball of radius R in the hyperbolic space of curvature -1. Assuming the dense setting ($d \ll \log n$), we derive the time and space complexity of graph-based NNS and compare the obtained results with known guarantees for the Euclidean case. Interestingly, under some assumptions on dimension d and radius R, graph-based NNS has *lower* time complexity in the hyperbolic space. From a practical perspective, we illustrate this result on word embedding data: we compare graph-based NNS for GloVe and Poincaré GloVe word embeddings. It turns out that for the same corpus, graph-based NNS is more efficient in the hyperbolic space. We also demonstrate that graph-based methods outperform other existing baselines on Poincaré GloVe word embeddings. Overall, our theoretical and empirical analysis suggests that graph-based NNS can be considered a default approach for similarity search in hyperbolic spaces.

1 INTRODUCTION

Given a dataset $\mathcal{D}$ of n elements and an arbitrary query $\mathbf{q}$, the goal of the nearest neighbor search (NNS) is to quickly retrieve one or several elements from $\mathcal{D}$ closest to $\mathbf{q}$. NNS is extensively used in a wide range of machine learning systems: for non-parametric classification and regression, language modeling, information retrieval, recommendations, and many others (Bishop, 2006; Chen et al., 2018; May & Ozerov, 2015; Shakhnarovich et al., 2006). In large-scale applications, searching for the nearest neighbors can be a bottleneck, so this operation's efficiency is of the essence.

Many efficient NNS algorithms exist for Euclidean and, generally, ℓ_p spaces. Among them are methods based on recursive partitions of the space, e.g., k-d trees and random projection trees (Bentley, 1975; Dasgupta & Freund, 2008; Dasgupta & Sinha, 2015; Keivani & Sinha, 2018), well studied Locality Sensitive Hashing (LSH) (Indyk & Motwani, 1998), and methods based on similarity graphs (Fu et al., 2019; Iwasaki & Miyazaki, 2018; Malkov et al., 2014; Malkov & Yashunin, 2018).

However, hyperbolic geometry was recently found to be more suitable for data representation in various domains, including graphs, words, and images (Khrulkov et al., 2020; Nickel & Kiela, 2017; 2018; Tifrea et al., 2018). Hence, a natural question is: how to perform efficient NNS in hyperbolic spaces? This problem has started to gain attention recently. For instance, Wu & Charikar (2020) propose several algorithms for NNS in hyperbolic spaces and analyze them theoretically and empirically. In a nutshell, they show how any given *Euclidean* NNS algorithm can be applied to the *hyperbolic* space. To get convergence guarantees, one has to call the chosen NNS method several times, which leads to the increased hyperbolic NNS complexity compared to the original Euclidean algorithm. In the current paper, we choose an opposite approach and apply a leading NNS technique *directly* to the hyperbolic space. We demonstrate that under some assumptions, the proposed method

does not have increased complexity and may even *reduce* the query time compared to its Euclidean counterpart.

We focus on graph-based NNS methods that are based on a best-first routing over similarity graphs. Namely, at the pre-processing step, a similarity graph is constructed on the elements of the dataset. Then, given a query $\mathbf{q}$, we start from some element of $\mathcal{D}$ and measure distances between its neighbors and $\mathbf{q}$. The neighbors are added to a priority queue. Then, we pick the closest to $\mathbf{q}$ candidate from this queue and continue the process (Fu et al., 2019; Iwasaki & Miyazaki, 2018; Malkov et al., 2014; Malkov & Yashunin, 2018). It was found empirically that graph-based NNS outperforms other approaches in many large-scale applications (Aumüller et al., 2019).

In contrast to other NNS methods, graph-based approaches can be easily applied to non-Euclidean spaces. Indeed, for most algorithms, both graph construction and graph routing can be performed without appealing to the geometry of the underlying space — only the relative ordering of neighbors is used. Thus, one can easily replace Euclidean distance with the hyperbolic one in a favorite graph-based approach. However, it is a priori not known how graph-based approaches would work in such a non-standard scenario.

In this paper, we show that graph-based approaches are well suited for NNS in hyperbolic spaces. From the theoretical perspective, we analyze the time and space complexity of graph-based NNS, assuming that the data elements are distributed uniformly within a ball of radius R in the hyperbolic space of curvature -1. In this regard, we compare the obtained results with Prokhorenkova & Shekhovtsov (2020) who studied graph-based algorithms assuming the uniform distribution over a d-dimensional sphere. In the dense setting (assuming that $d \ll \log n$ and that R does not grow too fast), we derive the time and space complexity using the fact that locally hyperbolic graph-based NNS behaves similarly to the spherical case. However, globally, graph-based search in hyperbolic spaces requires *fewer search steps*. Thus, hyperbolic NNS can be even *more efficient* compared to its Euclidean counterpart.

From a practical perspective, we first illustrate the obtained findings via synthetic experiments on uniform data. Then, we compare Euclidean and hyperbolic geometry in a more realistic setup. Indeed, while our theoretical results give some insights into why and how graph-based NNS works in hyperbolic spaces, our assumptions are too strong to claim that the results would transfer to real datasets with non-uniform distributions. Thus, we consider the word embedding problem and two vector representations: GloVe (Pennington et al., 2014) and Poincaré GloVe (Tifrea et al., 2018). Both representations use the same text corpus, and Poincaré GloVe was shown to outperform the standard representation for tasks of similarity, analogy, and hypernymy detection. Interestingly, we observe that graph-based NNS is *more efficient* for hyperbolic representations: we reach the same accuracy of NNS with fewer distance computations. Finally, we compare graph-based NNS with existing baselines proposed by Wu & Charikar (2020). Using the Poincaré GloVe dataset, we show that graph-based approaches have significantly better performance.

2 PRELIMINARIES

Graph-based nearest neighbor search Graph-based algorithms for NNS are known to outperform other approaches in many large-scale applications (Aumüller et al., 2019). The main idea is to construct a proximity graph at the pre-processing stage and traverse this graph towards the query $\mathbf{q}$ at query time. The best-first search is usually used for traversal: we maintain a priority queue, and at each step, we pick the closest to $\mathbf{q}$ candidate from this queue, measure distances between its neighbors and $\mathbf{q}$, and add the neighbors to the queue. Many algorithms are based on this idea (Baranchuk et al., 2019; Fu et al., 2019; Iwasaki & Miyazaki, 2018; Malkov & Yashunin, 2018).

Unfortunately, despite their success in practice, graph-based approaches do not have solid theoretical guarantees. This problem was first approached by Laarhoven (2018) who provided time–space trade-offs for approximate nearest neighbor (ANN) search in sparse datasets ($d \gg \log n$) uniformly distributed on a d-dimensional Euclidean sphere. This work considered nearest neighbor graphs, where each point is connected to its neighborhood lying within a ball of a fixed radius, and assumed greedy graph traversal. Prokhorenkova & Shekhovtsov (2020) further extended this result: for the uniform distribution the authors consider both sparse ($d \gg \log n$) and dense ($d \ll \log n$) regimes. In addition to the analysis of simple nearest neighbor graphs, they also consider the effect of two

improvements commonly used in practice: replacing greedy search by best-first (or beam) search provably allows for reducing the graph degree and the time complexity; adding long edges with a proper distribution reduces the number of steps which improves time complexity for small d.

In this paper, we aim at understanding graph-based NNS in hyperbolic spaces. For this, we adopt a similar setup to Prokhorenkova & Shekhovtsov (2020), but instead of a uniform distribution over a sphere, we assume a uniform distribution within a ball of a certain radius in the hyperbolic space. The obtained time and space complexity heavily relies on this radius: for small values, the obtained results are similar to the spherical case, while for larger values, the exponential growth of hyperbolic volumes (see the next section) allows us to obtain even faster convergence.

Hyperbolic geometry In this section, we discuss the basics of hyperbolic geometry. Let $\mathbb{R}^{d,1}$ be the $(d+1)$-dimensional *Minkowski space*, i.e., the real vector space $\mathbb{R}^{d+1}$ equipped with the inner product of signature $(d,1)$:

$$\langle \mathbf{x}, \mathbf{y} \rangle_h = -x_0 y_0 + x_1 y_1 + \ldots + x_d y_d. \tag{1}$$

The *vector model* of the *d-dimensional hyperbolic Lobachevsky space* $\mathbb{H}^d$ is the connected component of the standard two-sheeted hyperboloid $H_d = \{\mathbf{x} \in \mathbb{R}^{d,1} \mid \langle \mathbf{x}, \mathbf{x} \rangle_h = -1\}$ contained in the *future light cone*:

$$\mathbb{H}^d = \{\mathbf{x} \in \mathbb{R}^{d,1} \mid \langle \mathbf{x}, \mathbf{x} \rangle_h = -1, x_0 > 0\}.$$

The hyperbolic metric is given by $\cosh \rho(\mathbf{x}, \mathbf{y}) = -\langle \mathbf{x}, \mathbf{y} \rangle_h$. From the definition of the hyperbolic space, we see that $x_0 = \sqrt{1 + x_1^2 + \ldots + x_d^2}$. The volume element in $\mathbb{H}^d$ is (see Ratcliffe (2019))

$$\frac{dx_1 \ldots dx_d}{\sqrt{1 + x_1^2 + \ldots + x_d^2}}.$$

Hyperbolic space is known to be useful for data representation in various domains. It is especially convenient for embedding hierarchical data (Nickel & Kiela, 2017). The reason is that the volume of a ball in the hyperbolic space grows exponentially with its radius, in contrast to the Euclidean space, where the growth is polynomial.

Formally, let $B(\mathbf{x}, r)$ be a closed hyperbolic ball centered at a point $\mathbf{x} \in \mathbb{H}^d$ of radius $r > 0$. Then,

$$\mathrm{Vol}_{\mathbb{H}^d}(B(\mathbf{x}, r)) = \mathrm{Vol}(\mathbb{S}^{d-1}) \int_0^r \sinh^{d-1}(t)\, dt\,, \tag{2}$$

where $\mathbb{S}^{d-1}$ is the unit $(d-1)$-sphere and $\mathrm{Vol}(M)$ denotes the full volume of a Riemannian manifold M. That is, $\mathrm{Vol}(\mathbb{S}^{d-1}) = 2\pi^{d/2}/\Gamma(d/2)$. For $r \gg \log d$, we have

$$\mathrm{Vol}_{\mathbb{H}^d}(B(\mathbf{x}, r)) \sim \mathrm{Vol}(\mathbb{S}^{d-1})\, e^{r(d-1)}\, \Theta(d^{-1} 2^{-d}).$$

The main term here is $e^{r(d-1)}$, so the ball volume $\mathrm{Vol}_{\mathbb{H}^d}(B(\mathbf{x}, r))$ grows exponentially when r is large. However, for small hyperbolic balls (as $r \to 0$), we have $\sinh(r) \sim r$. Hence, the volume of a ball (2) behaves similarly to the Euclidean case. In Section 4.1, we provide a formal general result that shows that not only the above argument is correct, but also the volume of a measurable subset of a hyperbolic ball behaves asymptotically exactly like its Euclidean analog. This is essential for our proof since we need to estimate the volumes of balls intersections.

Nearest neighbor search in hyperbolic space While there are many NNS algorithms for ℓ_p spaces, little is known about efficient hyperbolic analogs. Krauthgamer & Lee (2006) proved the existence of an approximate near neighbor algorithm for general geodesic spaces of hyperbolicity δ. From a theoretical perspective, the bound is given in terms of the doubling dimension. For uniform datasets, we may conclude that the obtained time complexity is $2^{O(d)} \log^2 n$. Thus, for large d, the constant in the exponent of the main term is not given. In contrast, we specify this term as we focus on $d \to \infty$. Another difference is that the algorithm of Krauthgamer & Lee (2006) requires $O(n^2)$ storage that is usually infeasible in practice. In contrast, graph-based algorithms require $n\, M^d$ if $d \ll \log n$. Finally, while the theoretical analysis is given in a very general setup, there is no implementation of the proposed algorithm, and extracting an efficient implementation from the proof is challenging.

In a recent paper, Wu & Charikar (2020) reduce the problem of hyperbolic NNS to Euclidean NNS. Namely, assume that we have an efficient Euclidean algorithm and a dataset represented in the Poincaré ball model. Then, we can apply the algorithm assuming that the coordinates are Euclidean. To guarantee convergence, the algorithm should be applied several times. There are several alternatives proposed. In one of them, one applies the algorithm to the whole dataset, but after each run, appropriately changes the query point to get better hyperbolic neighbors at subsequent iterations. The time complexity of this algorithm is $k+1$ times larger than the Euclidean search if the Euclidean nearest neighbor for the query is the k-th nearest hyperbolic neighbor. In another algorithm, one splits the ball into thin annuli and performs the approximate Euclidean NNS for each of them separately. From a theoretical perspective, it is hard to compare our results since Wu & Charikar (2020) do not consider any particular algorithm. We cannot apply this general result to graph-based algorithms since known guarantees for the Euclidean space assume a uniform distribution. However, if we consider the uniform distribution in the Poincaré model of the hyperbolic space, the corresponding Euclidean distribution is far from uniform, i.e., the guarantees cannot be transferred. From a practical perspective, we compare graph-based algorithms with the method of Wu & Charikar (2020) and show that graph-based NNS is more efficient.

3 SETUP AND NOTATION

The current paper aims at analyzing how hyperbolic geometry of the underlying space affects the time and space complexity of NNS. In this regard, we compare our results with Prokhorenkova & Shekhovtsov (2020), so we use a similar setup and notation for convenience.

To make the analysis feasible, Laarhoven (2018) and Prokhorenkova & Shekhovtsov (2020) assumed that the dataset is uniformly distributed on a sphere. The uniformity assumption is fairly strong. In Prokhorenkova & Shekhovtsov (2020), this setup was partially motivated by techniques allowing to make a dataset more uniform while approximately preserving the distances (Sablayrolles et al., 2018), which are helpful in some practical applications. Let us additionally note that in hyperbolic spaces, the uniform distribution of nodes within a ball leads to structures that are similar to real ones: if we consider a geometric graph on such nodes, we obtain the power-law degree distribution, small diameter, and high clustering coefficient (Krioukov et al., 2010), which further supports the meaningfulness of the uniform distribution in our scenario.

The compactness of the sphere simplifies the analysis in previous work as it allows for avoiding boundary effects. However, we cannot make this assumption in our setup, as a sphere in the hyperbolic space is isometric to a sphere in the Euclidean space. Hence, to use the advantages of hyperbolic geometry, we assume that the dataset is uniformly distributed within a ball of some radius in the hyperbolic space.

Formally, consider a ball $B(R) \subset \mathbb{H}^d$ of radius $R > 0$. Assume that the dataset is a finite collection of points $\mathcal{D} = \{\mathbf{x}_1, \dots, \mathbf{x}_n\} \subset \mathbb{H}^d$, where $\mathbf{x}_i \in \mathcal{D}$ are i.i.d. random vectors uniformly distributed in $B(R)$. For a given query $\mathbf{q} \in B(R)$, let $\overline{\mathbf{x}} \in \mathcal{D}$ be its nearest neighbor. Then, the goal of the exact NNS is to find $\overline{\mathbf{x}}$. For completeness, following Laarhoven (2018); Prokhorenkova & Shekhovtsov (2020), we also consider c, r-approximate near neighbor problem (c, r-ANN). In this scenario, it is assumed that $\mathbf{q}$ is *planted* uniformly within a fixed distance $r > 0$ from its nearest neighbor $\overline{\mathbf{x}}$ and the goal is to return any $\mathbf{x}'$ such that $\rho(\mathbf{q}, \mathbf{x}') \le c\,r$ for a fixed value $c > 1$ (Chen et al., 2018). Formally, in the exact nearest neighbor search, we also assume that $\mathbf{q}$ is planted uniformly within a distance r from some element $\mathbf{x}$. However, we do not restrict the radius r (the only restriction is that $\mathbf{x}$ should be the nearest neighbor for $\mathbf{q}$).

We follow the standard assumption that the dimension $d = d(n)$ is an increasing function of n (Chen et al., 2018). In the present paper, we study the so-called dense regime, where $d \ll \log n$, see more details in the next section.

Graph-based approaches usually imply constructing a nearest neighbor graph (or its approximation), where each element is connected to its k nearest neighbors. As we deal with uniformly distributed datasets, we assume that each node $\mathbf{x}$ is connected to all nodes $\mathbf{y}$ at a distance $\rho(\mathbf{x}, \mathbf{y}) \le \rho^*$ for some ρ^* chosen at the preprocessing stage.[1] Hence, at the preprocessing stage, we construct a similarity

[1]This approach is rigorously substantiated by the fact that the number of nodes within a distance ρ^* is concentrated around its expectation for uniformly distributed datasets. Results for k-NN graphs can be derived from our theorem, see Appendix D.

graph using ρ^*. Next, we receive a query $\mathbf{q}$, sample a random node $\mathbf{x} \in \mathcal{D}$, and at each step of the graph-based greedy descent, we measure the distances between the neighbors of the current node and $\mathbf{q}$ and move to the closest neighbor while we can make such greedy steps.

4 CONVERGENCE AND COMPLEXITY OF GRAPH-BASED NNS

4.1 LOCAL PROPERTIES OF HYPERBOLIC SPACE

Further in this section, we give formal statements regarding the convergence and complexity of greedy graph-based algorithms. Convergence depends on the probability of making a step towards the query from a given element. This probability, in turn, depends on the volumes of some balls' intersections. As follows from our proof, only 'local' properties are important for convergence. Let us show that under some conditions, the local properties in the hyperbolic space are similar to the Euclidean one.

Formally, let $\mathbf{z} = (1, 0, \ldots, 0)$ and let $T_{\mathbf{z}}\mathbb{H}^d = \{\mathbf{x} \in \mathbb{R}^{d,1} \mid x_0 = 1\} \simeq \mathbb{R}^d$ be the tangent space. Let c be the central projection $c : \mathbb{H}^d \to T_{\mathbf{z}}\mathbb{H}^d \simeq \mathbb{R}^d$ from the origin $\mathbf{o} = (0, \ldots, 0)$. The following lemma holds.

Lemma 1. *Suppose that $U \subset \mathbb{H}^d$ is a measurable set such that $U \subset B(0, r)$. If $r \ll \frac{1}{\sqrt{d}}$ and $d \to \infty$, then we have*

$$\mathrm{Vol}_{\mathbb{H}^d}(U) = \mathrm{Vol}_{\mathbb{E}^d}(c(U)) \left(1 - O\left(d\, r^2\right)\right).$$

This result allows us to apply the bounds on volumes of Euclidean balls intersections to such volumes in the hyperbolic case for small radii.

4.2 INTUITION BEHIND THE CHOICE OF PARAMETERS

Our theoretical analysis is asymptotic, meaning that the number of elements n tends to infinity. Hence, we assume that the dimension $d = d(n)$ and the ball radius $R = R(n)$ depend on n. This section discusses our restrictions on $d(n)$ and $R(n)$ and how they affect the analysis. Here, we do not aim at giving mathematically rigorous statements but rather explain underlying intuitions. The formal results can be found in Section 4.3.

Assuming that the dataset is uniformly distributed on a unit sphere, Prokhorenkova & Shekhovtsov (2020) considered two principally different regimes: dense with $d \ll \log n$ and sparse with $d \gg \log n$. In the dense regime, the distance from any element to its nearest neighbor tends to zero as n grows. Hence, locally, graph-based NNS operates in the Euclidean space. In this case, the greedy algorithm reaches the nearest neighbor with probability $1 - o(1)$ if graph degree is M^d for $M > \sqrt{2}$. In the sparse regime, informally speaking, all nodes are at a spherical distance about $\pi/2$ from each other, making the NNS much more challenging. In this case, the graph degree has to grow as n^{φ} for some $\varphi > 0$ in order to solve the approximate near neighbor problem (Prokhorenkova & Shekhovtsov, 2020).

In this paper, we focus on the dense regime with $d \ll \log n$. Let us note that assuming larger values of d is not realistic for uniform distributions. Indeed, while in practice datasets are often embedded into spaces of large dimension, they usually have much smaller *intrinsic* dimension (Beygelzimer et al., 2006; Lin & Zhao, 2019). Moreover, according to Prokhorenkova & Shekhovtsov (2020), in the sparse regime, graph-based NNS is expected to converge in just two steps (for the uniform distribution) which contradicts practical observations. Finally, the optimal degree of a graph rarely exceeds 64. Referring to the analysis of Prokhorenkova & Shekhovtsov (2020), we can speculate that in terms of complexity such datasets have effective dimension not larger than $\log_{\sqrt{2}} 64 = 12$.

We further assume that the dataset is uniformly distributed within a ball $\mathcal{B} = B(R)$ in the hyperbolic space. Note that changing this radius is equivalent to changing the curvature of the space (Petersen, 2016). So, we may either assume that the curvature $c = -1$ is fixed while the radius of the ball $R = R(n)$ may change or assume that the radius is fixed while the curvature $c = c(n)$ changes. We further assume that $c = -1$ is fixed. Thus, we have three parameters: the number of elements n, the dimension $d = d(n)$, and the radius $R = R(n)$.

Denote by $V_d(R)$ the volume of $\mathcal{B}$, i.e., $V_d(R) := \mathrm{Vol}_{\mathbb{H}^d}(B(R))$ and by $v_d(R)$ the normalized volume, i.e., $v_d(R) := V_d(R)/\mathrm{Vol}(\mathbb{S}^{d-1})$.

Let us analyze (approximately) the distance α from an element to its nearest neighbor. Intuitively, we should have

$$\frac{\mathrm{Vol}_{\mathbb{H}^d}(B(\alpha))}{\mathrm{Vol}_{\mathbb{H}^d}(B(R))} \approx \frac{1}{n}\,, \;\; \mathrm{Vol}_{\mathbb{H}^d}(B(\alpha)) \approx \frac{V_d(R)}{n}\,. \tag{3}$$

Assume for now that $\alpha \ll 1/\sqrt{d}$. In this case, we have (see Section 4.1)

$$\mathrm{Vol}_{\mathbb{H}^d}(B(\alpha)) \sim \mathrm{Vol}_{\mathbb{E}^d}(B(\alpha)) = \frac{\mathrm{Vol}(\mathbb{S}^{d-1})\alpha^d}{d}.$$

Therefore, from (3),

$$\alpha^d \approx \frac{V_d(R)\,d}{n\,\mathrm{Vol}(\mathbb{S}^{d-1})} = \frac{v_d(R)\,d}{n}.$$

Let us find an upper bound on the radius R such that the condition $\alpha \ll 1/\sqrt{d}$ is satisfied. Note that $v_d(R) = O\left(e^{R(d-1)} \cdot 2^{-d} \cdot d^{-1}\right)$ (see Appendix B). Thus, we need

$$\left(\frac{v_d(R)\,d}{n}\right)^{1/d} \ll \frac{1}{\sqrt{d}}, \;\; \left(\frac{e^{R(d-1)}\,2^{-d}}{n}\right)^{1/d} \ll \frac{1}{\sqrt{d}}, \;\; e^R \ll n^{1/(d-1)} \cdot d^{-1/2}\,.$$

Based on that, we further assume that $e^R \ll n^{1/(d-1)} \cdot d^{-1/2}$. In this case, the distance to the nearest neighbor is $\alpha = o\left(1/\sqrt{d}\right)$, and locally the graph-based search behaves similarly to the Euclidean case. This assumption is natural: we empirically show that larger values of R lead to much less efficient NNS.

4.3 Main results

In this section, we formally analyze the performance of graph-based NNS for uniform datasets in the hyperbolic space. As discussed above, to construct the nearest neighbor graph, we connect each point to its neighborhood located within a ball of a fixed radius. For any constant $M > 1$, let $G(M)$ be a graph obtained by connecting $\mathbf{x}_i$ and $\mathbf{x}_j$ iff

$$\rho(\mathbf{x}_i, \mathbf{x}_j) \leq M \left(\frac{d\,v_d(R)}{n}\right)^{1/d}.$$

This radius is chosen to get about M^d neighbors for each node. The following theorem holds.

Theorem 1. *Assume that $d = d(n)$ is such that $\log\log n \ll d(n) \ll \log n$ and $R = R(n)$ is such that $e^R \ll n^{\frac{1}{d-1}} \cdot d^{-1/2}$.*

For the exact NNS, let M be a constant s.t. $M > \sqrt{2}$. Then, with probability $1 - o(1)$, $G(M)$-based NNS finds the exact nearest neighbor. For c, r-ANN with some constant $c > 1$, let M be a constant s.t. $M > \sqrt{\frac{4c^2}{3c^2-1}}$. Then, with probability $1 - o(1)$, $G(M)$-based NNS solves c, r-ANN for any r.

In both cases, the time complexity is $O\left(M^d \cdot n^{1/d} \cdot R \cdot (v_d(R))^{-1/d}\right)$;

the space complexity is $O\left(n \cdot \log n \cdot M^d\right)$.

The formal proof of this theorem is given in Appendices A-C. The theorem covers several regimes, which we now discuss. First, assume that $R \ll 1/\sqrt{d}$. In this case, the geometry is approximately Euclidean. We have $v_d(R) \sim R^d$, so the following corollary holds.

Corollary 1. *If $R = R(n) \ll 1/\sqrt{d}$, then in Theorem 1 we obtain the time complexity $O\left(M^d \cdot n^{1/d}\right)$.*

As expected, this result is similar to the corresponding theorem in Prokhorenkova & Shekhovtsov (2020). However, as R becomes larger, time complexity changes. For instance, if $R \gg \log d$, then we have $v_d(R) \sim e^{R(d-1)}\,\Theta(d^{-1}2^{-d})$. Thus, we get the following corollary.

Corollary 2. *If $R = R(n) \gg \log d$, then in Theorem 1 we obtain the time complexity $O\left(M^d \cdot n^{1/d} \cdot R \cdot e^{-R(d-1)/d}\right)$.*

From this corollary we see that the time complexity decreases with the radius R. Thus, to make the complexity smaller, we should take larger values of R. According to Theorem 1, we can take R such that $e^R = n^{\frac{1}{d-1}}/(\sqrt{d}\,\varphi)$, where $\varphi = \varphi(n) \to \infty$. We obtain the following corollary.

Corollary 3. *If for an arbitrary $\varphi = \varphi(n) \to \infty$ we have $e^R = n^{\frac{1}{d-1}}/(\sqrt{d}\,\varphi) \to \infty$, then in Theorem 1 we get the time complexity $O\left(M^d \cdot \log n \cdot d^{-1/2} \cdot \varphi\right)$.*

Thus, in the hyperbolic space, we can reduce the number of steps from $n^{1/d}$ to about $\log n$. This shows that the NNS over plain nearest neighbor graphs is more efficient in the hyperbolic space under the conditions considered in this paper. Let us give an intuitive explanation of this result. The difference between Euclidean and hyperbolic regimes is due to the fact that the volume of a hyperbolic ball grows exponentially with its radius. Thus, we can faster reach any point from, e.g., the origin of the ball.

Note that in the Euclidean space, we can also reduce the number of steps to $\log n$ via adding long edges (Prokhorenkova & Shekhovtsov, 2020). In contrast, in hyperbolic space, this can be achieved without additional tricks. Our experiments on synthetic datasets confirm that without long edges, NNS is much more efficient in the hyperbolic space when dimension d is small.

Finally, let us note that Theorem 1 considers graphs constructed via a threshold for $\rho(\mathbf{x}_i, \mathbf{x}_j)$. In contrast, in practice, k-NN graphs or their approximations are used. For uniform datasets, we can prove the same theorem for k-NN graphs with $k = [M^d]$, see Appendix D.

5 Experiments

In this section, we first compare graph-based approaches to the algorithm proposed by Wu & Charikar (2020). Then, we compare the efficiency of graph-based approaches in Euclidean and hyperbolic spaces in the realistic setup of word embeddings; this experiment confirms that graph-based search in the hyperbolic space is not less efficient than in the Euclidean space. Finally, we illustrate our theoretical results given in Section 4.3 on synthetic datasets uniformly distributed within spaces of different curvatures. The code of our experiments supplements the submission.

5.1 Comparison with baseline

First, we compare graph-based approaches with an existing method of hyperbolic NNS. For this purpose, we collect the largest publicly available Poincaré GloVe vocabulary[2] of $189,533$ unique tokens. Poincaré GloVe was shown to outperform the Euclidean representation for tasks of similarity, analogy, and hypernymy detection (Tifrea et al., 2018). The dimensionality of the embeddings is 100. The set of tokens is randomly split into the base set of 180K elements and the query set of the remaining elements for evaluation.

On the base set, we construct the HNSW graph (Malkov & Yashunin, 2018) that is considered to be one of the current state-of-the-art similarity graphs for NNS. As for the search algorithm, we perform the best-first search. The parameter $efSearch$ determines the stopping criteria of the best-first search and allows us to vary the complexity versus accuracy tradeoff. For the baseline, the only practical algorithm we are aware of is proposed by Wu & Charikar (2020). The algorithm is called Spherical Shell: it is suggested to split the Poincaré ball into thin annuli and perform approximate Euclidean NNS (the authors use LSH) for some of them separately. Unfortunately, the implementation is not provided by the authors, so we use our implementation. To make the comparison fair, we count the number of distance computations (DCS) instead of the actual time, as the latter may depend on the efficiency of our implementation. The algorithm details and parameter tuning are discussed in Appendix E.

To evaluate the algorithms, we plot Complexity-versus-Accuracy curves. As a primary measure of the search accuracy, we consider `Recall@1`. The search complexity is the average number of DCS

[2] `https://github.com/alex-tifrea/poincare_glove`

per query. The results are shown in Figure 1. We see that HNSW significantly outperforms the baseline. This confirms that applying an algorithm directly to the hyperbolic space is more efficient than reducing the problem to Euclidean NNS.

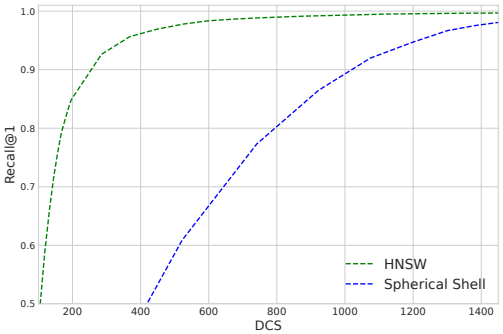

Figure 1: HNSW vs Spherical Shell on Poincaré GloVe embeddings

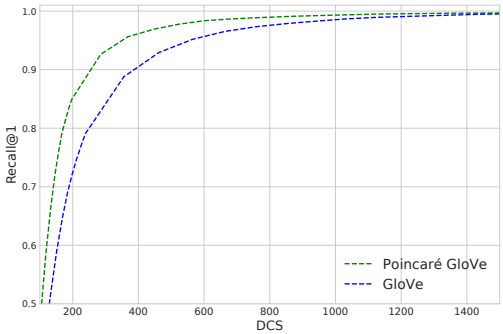

Figure 2: Efficiency of HNSW in hyperbolic space vs Euclidean space

5.2 Euclidean vs Poincaré GloVe

While our theoretical results give some intuition about why and how graph-based NNS works in hyperbolic spaces, the assumptions about uniform distribution and small dimension are quite strong. This section illustrates that graph-based methods are well suited for NNS by comparing Euclidean and hyperbolic spaces in a practical application. For this, we construct HNSW graphs for Euclidean GloVe (Pennington et al., 2014) and Poincaré GloVe (Tifrea et al., 2018) with the same tokens and perform NNS for each dataset. Note that the results cannot be compared directly: GloVe and Poincaré GloVe have different geometry, so nearest neighbors for the same queries may differ.

Figure 2 shows that HNSW built on embeddings in the hyperbolic space is *more efficient* than HNSW over Euclidean embeddings. This suggests that switching from Euclidean to hyperbolic embeddings does not make NNS less efficient.[3]

5.3 Illustrating theoretical results on synthetic datasets

Finally, we illustrate Theorem 1 and our corollary that for simple nearest neighbor graphs and sufficiently small dimension d, graph-based NNS is more efficient in the hyperbolic space. For this, we follow the setup of Prokhorenkova & Shekhovtsov (2020) and perform a synthetic experiment. We generate datasets uniformly distributed in different spaces: 1) on a sphere (Prokhorenkova & Shekhovtsov, 2020), 2) within a Euclidean ball, 3) within a ball of radius R in the hyperbolic space of curvature -1. For all spaces, we fix $n = 10^6$ and vary the dimension $d \in \{2, 4, 6\}$.

For the hyperbolic space, we also vary the radius R. Recall that this is equivalent to changing the curvature. To get an intuition on which values of R are meaningful, recall that Theorem 1 requires $e^R \ll n^{1/(d-1)}/\sqrt{d}$. Thus, roughly speaking, we obtain the following upper bound on R: $R_{max} = \frac{\log n}{d-1} - \log\sqrt{d}$. For $d = 2$, we get $R_{max} \approx 13.5$, for $d = 4$, we get $R_{max} \approx 3.9$, while for $d = 6$ we have $R_{max} \approx 1.9$. Thus, we see that even for $d = 6$ the bound on the radius is sufficiently small and the obtained geometry becomes similar to the Euclidean one (if we consider the theoretically analyzed parameter range). Thus, we do not consider $d > 6$ in this experiment.

First, we analyze the performance of greedy search over nearest neighbor graphs; this setup corresponds to our theoretical analysis. To get the Complexity-versus-Accuracy curves, we vary the graph degree. In Figure 3 we see that spherical and Euclidean spaces are very similar. Hyperbolic space on a small scale, i.e., when points are located inside a ball of a sufficiently small radius R, is similar to the Euclidean one. Then, as R increases, the performance improves. However, after some point, larger values of R reduce the quality of NNS. It is worth noting that this threshold agrees well with the dynamic of R_{max} (while being smaller, as expected).

[3]Note that computing the hyperbolic distance has the same complexity as computing the inner product, as follows from Equation (1).

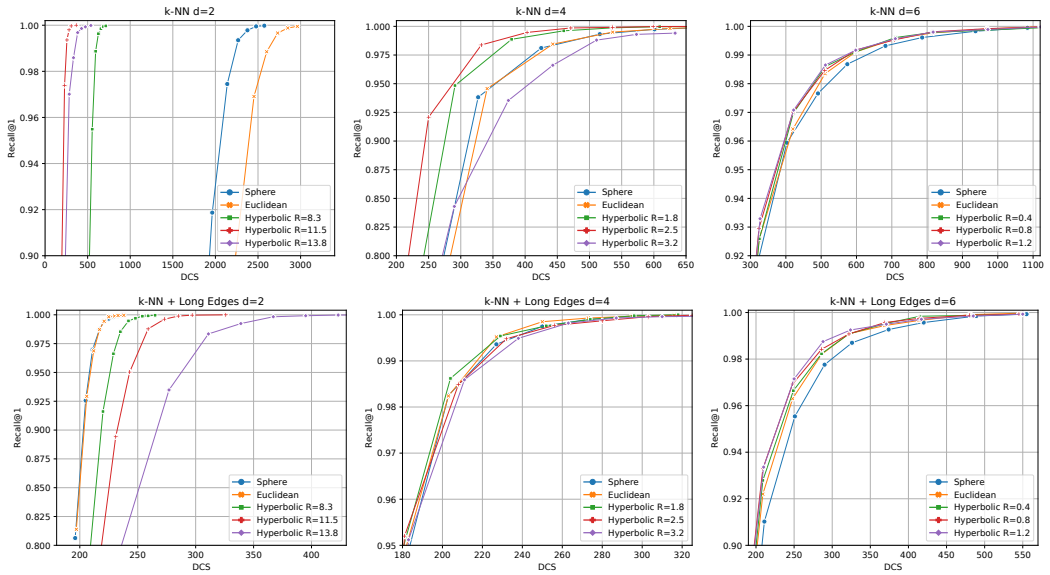

Figure 3: Greedy search over NN graphs without (top row) and with (bottom row) long edges

Then, we analyze what happens if we add long edges known to be essential for the NNS in spherical and Euclidean spaces when the dimension d is small. To incorporate long edges into NN graphs, we follow the procedure described in Prokhorenkova & Shekhovtsov (2020). As expected, long edges significantly boost the performance of NNS in spherical and Euclidean spaces. Note that they also improve performance in hyperbolic spaces, but the boost is smaller. As a result, the efficiency of NNS in all spaces becomes similar if R is sufficiently small, while larger values of R even lead to a performance downgrade.

We also conduct similar experiments with greedy search replaced by the best-first search, which is a standard technique for graph-based NNS performance improvement. The conclusions are the same; we include the figures in Appendix E.

6 Conclusion

This paper conducts a theoretical and empirical analysis of graph-based nearest neighbor search in hyperbolic spaces. First, we theoretically analyze the performance of greedy search over nearest neighbor graphs assuming that the dataset is uniformly distributed over a ball of radius R in the hyperbolic space. Assuming the dense regime ($d \ll \log n$) and that the absolute value of the curvature is not too large, we show that locally graph-based exploration is similar to the Euclidean case. However, globally, hyperbolic geometry allows for reducing the number of steps significantly. This theoretical result is also clearly illustrated by our synthetic experiments. On the other hand, long edges added to the NN graph boost the performance of NNS in the Euclidean space, so the performance becomes similar to the hyperbolic case.

From a practical perspective, we show that NNS for Poincaré embeddings is more efficient than for the corresponding Euclidean ones. Also, for the Poincaré GloVe dataset, graph-based methods significantly outperform the previously proposed approach for hyperbolic NNS.

We hope that our research will attract more attention to NNS in hyperbolic spaces and, in particular, to graph-based methods. Note that our theoretical analysis is focused on the dense setting, while our experiments on word embeddings suggest that graph-based NNS is also suitable for sparse datasets. Thus, a promising direction for future work is a theoretical analysis of the sparse setting.

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A AUXILIARY GEOMETRICAL RESULTS

In this section, we prove some auxiliary geometrical results that will be useful throughout the proofs. First, we analyze the properties of Euclidean balls and their intersections. Then, we obtain similar results for the hyperbolic space if the ball's radii are sufficiently small.

A.1 EUCLIDEAN BALLS AND THEIR INTERSECTIONS

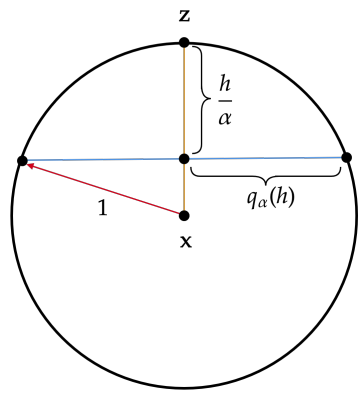
For a ball $B = B(1)$ of unit radius in a d-dimensional Euclidean space, we have that its volume satisfies

$$\mathrm{Vol}_{\mathbb{E}^d}(B) = \frac{\pi^{\frac{d}{2}}}{\Gamma\left(\frac{d}{2}+1\right)}.$$

In this section, we estimate volumes of spherical caps, and then use the obtained bounds to estimate the volumes of balls' intersections.

Let $B(\mathbf{x}, \alpha)$ be a ball of radius α centered at $\mathbf{x}$, and $C_\alpha(\mathbf{x}, \mathbf{z}, h) \subseteq B(\mathbf{x}, \alpha)$ be a d–dimensional spherical cap of height h centered at $\mathbf{z} \in \mathcal{S}_\alpha(\mathbf{x})$, i.e., $C_\alpha(\mathbf{x}, \mathbf{z}, h) = \{\mathbf{y} \in B(\mathbf{x}, \alpha) : \langle \mathbf{y}-\mathbf{x}, \mathbf{z}-\mathbf{x}\rangle \geq \alpha(\alpha - h)\}$. Let $C_\alpha(h) := \mathrm{Vol}_{\mathbb{E}^d}\left(C_\alpha(\mathbf{x}, \mathbf{z}, h)\right)$ be the volume of this spherical cap.

Definition 1. *Let $q_\alpha(h) := \left(1 - \left(1 - \frac{h}{\alpha}\right)^2\right)^{1/2}$ be the "relative radius" of a spherical cap (see $q_\alpha(h)$ in the figure).*



Lemma 2. *The volume $C_\alpha(h)$ of a spherical cap $C_\alpha(\boldsymbol{x}, \boldsymbol{z}, h)$ can be estimated as follows:*

$$\Theta(d^{-1}) \leq \frac{C_\alpha(h)}{\mathrm{Vol}_{\mathbb{E}^{d-1}}(B) \cdot \alpha^d \cdot q_\alpha(h)^{d+1}} \leq \Theta(d^{-\frac{1}{2}}).$$

Proof. For brevity, let $q = q_\alpha(h)$. Put $\gamma = \arccos(1 - h/\alpha)$, $0 \leq \gamma \leq \frac{\pi}{2}$. The volume of a spherical cap of height h is known to be:

$$C_\alpha(h) = \mathrm{Vol}_{\mathbb{E}^{d-1}}(B) \cdot \alpha^d \cdot \int_0^\gamma \sin^d(t)\, dt.$$

First, rewrite the integral:

$$\int_0^\gamma \sin^d(t)\, dt = |x = \sin^2 t| = \frac{1}{2}\int_0^{q^2} x^{\frac{d-1}{2}}(1-x)^{-\frac{1}{2}} dx$$

$$= |x = q^2 t| = \frac{1}{2} q^{d+1} \int_0^1 t^{\frac{d-1}{2}} \left(1 - q^2 t\right)^{-\frac{1}{2}} dt.$$

To prove the lemma, it remains to show that

$$\Theta(d^{-1}) \leq \int_0^1 t^{\frac{d-1}{2}} \left(1 - q^2 t\right)^{-\frac{1}{2}} dt \leq \Theta\left(d^{-\frac{1}{2}}\right).$$

Indeed,

$$\Theta(d^{-1}) = \int_0^1 t^{\frac{d-1}{2}} dt \leq \int_0^1 t^{\frac{d-1}{2}} \left(1 - q^2 t\right)^{-\frac{1}{2}} dt$$

$$\leq \int_0^1 t^{\frac{d-1}{2}} (1-t)^{-\frac{1}{2}} dt = \mathrm{B}\left(\frac{d+1}{2}, \frac{1}{2}\right) = \Theta\left(d^{-\frac{1}{2}}\right),$$

where $\mathrm{B}(\cdot,\cdot)$ denotes the beta function. This concludes the proof. □

Let us now estimate the volume of the intersection of two Euclidean balls. Let $W_{\mathbf{x}_i,\mathbf{x}_j}(\alpha,\beta)$ denote the intersection of $B(\mathbf{x}_i,\alpha)$ and $B(\mathbf{x}_j,\beta)$, i.e., $W_{\mathbf{x}_i,\mathbf{x}_j}(\alpha,\beta) = \{\mathbf{y} : \rho(\mathbf{x}_i,\mathbf{y}) \leq \alpha,\ \rho(\mathbf{x}_j,\mathbf{y}) \leq \beta\}$. Let $s := \rho(\mathbf{x}_i,\mathbf{x}_j)$ be the distance between the centers and $W(\alpha,\beta,s) := \mathrm{Vol}_{\mathbb{E}^d}\left(W_{\mathbf{x}_i,\mathbf{x}_j}(\alpha,\beta)\right)$ denote the volume of the intersection. The following lemma estimates the value $W(\alpha,\beta,s)$ under various conditions on α,β,s.

Lemma 3. *W.l.o.g., assume that $\alpha \leq \beta$. Define $A := \frac{(\alpha+\beta+s)(\alpha+\beta-s)(s+\alpha-\beta)(s+\beta-\alpha)}{4s^2}$.*

1. *If $\alpha+\beta < s$, then $W(\alpha,\beta,s) = 0$.*
2. *If $s-\alpha \leq \beta < \sqrt{\alpha^2+s^2}$, then*

$$\Theta\left(d^{-1}\right) \leq \frac{W(\alpha,\beta,s)\cdot\alpha\beta}{\mathrm{Vol}_{\mathbb{E}^{d-1}}(B)\cdot(\alpha+\beta)\cdot A^{\frac{d+1}{2}}} \leq \Theta\left(d^{-\frac{1}{2}}\right). \tag{4}$$

3. *If $\sqrt{\alpha^2+s^2} \leq \beta < s+\alpha$, then*

$$\frac{1}{2} \leq \frac{W(\alpha,\beta,s)}{\mathrm{Vol}_{\mathbb{E}^d}(B)\cdot\alpha^d} \leq 1, \tag{5}$$

$$\frac{\mathrm{Vol}_{\mathbb{E}^d}(B(\alpha)) - W(\alpha,\beta,s)}{\mathrm{Vol}_{\mathbb{E}^{d-1}}(B)\cdot A^{\frac{d+1}{2}}\cdot\alpha^{-1}} \leq \Theta\left(d^{-\frac{1}{2}}\right) \tag{6}$$

4. *If $s+\alpha \leq \beta$, then*

$$W(\alpha,\beta,s) = \mathrm{Vol}_{\mathbb{E}^d}(B)\cdot\alpha^d. \tag{7}$$

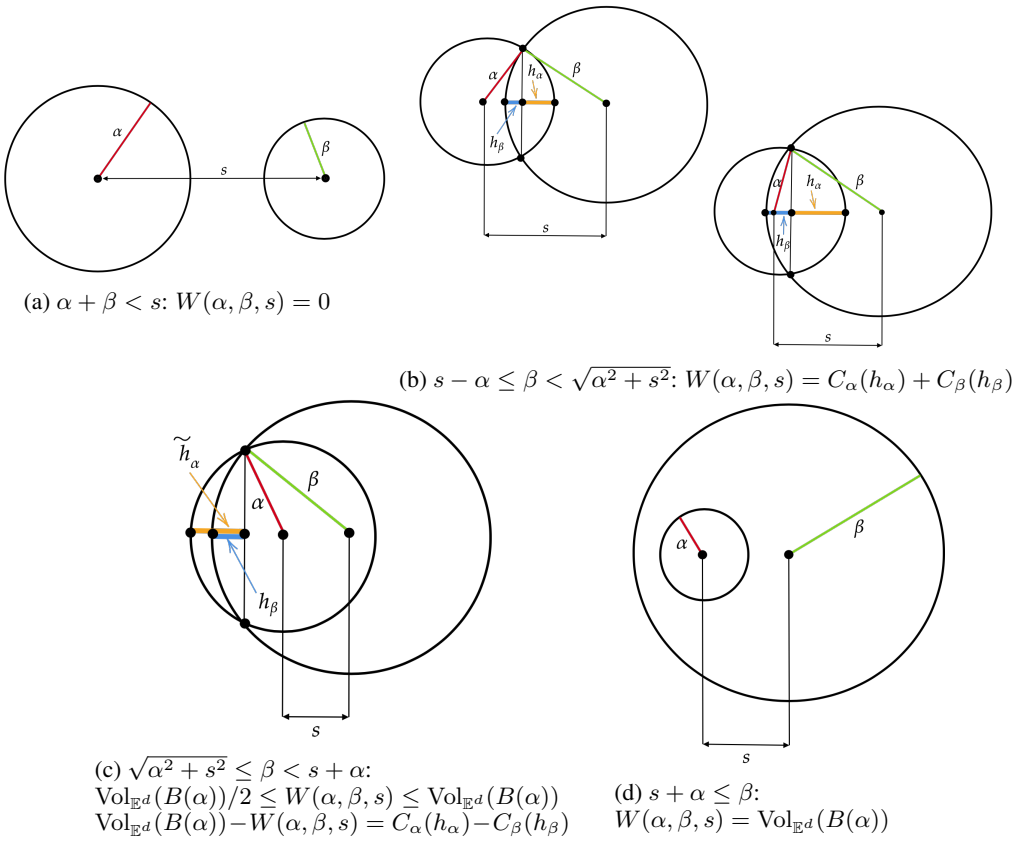
Proof. Let $h_\alpha := \frac{\beta^2-(s-\alpha)^2}{2s}$, $h_\beta := \frac{\alpha^2-(s-\beta)^2}{2s}$, $\widetilde{h}_\alpha := \frac{(\alpha+s)^2-\beta^2}{2s}$.

1. If $\alpha+\beta < s$, then the balls do not intersect and thus $W(\alpha,\beta,s) = 0$, see Figure 4a.
2. If $s-\alpha \leq \beta < \sqrt{\alpha^2+s^2}$, then, according to Figure 4b,

$$W(\alpha,\beta,s) = C_\alpha(h_\alpha) + C_\beta(h_\beta).$$

By Lemma 2, we have

$$\Theta\left(d^{-1}\right) \leq \frac{W(\alpha,\beta,s)}{\mathrm{Vol}_{\mathbb{E}^{d-1}}(B)\cdot\left(\alpha^d q_\alpha^{d+1}(h_\alpha) + \beta^d q_\beta^{d+1}(h_\beta)\right)} \leq \Theta\left(d^{-\frac{1}{2}}\right).$$



(a) $\alpha + \beta < s$: $W(\alpha, \beta, s) = 0$

(b) $s - \alpha \leq \beta < \sqrt{\alpha^2 + s^2}$: $W(\alpha, \beta, s) = C_\alpha(h_\alpha) + C_\beta(h_\beta)$

(c) $\sqrt{\alpha^2 + s^2} \leq \beta < s + \alpha$:
$\mathrm{Vol}_{\mathbb{E}^d}(B(\alpha))/2 \leq W(\alpha, \beta, s) \leq \mathrm{Vol}_{\mathbb{E}^d}(B(\alpha))$
$\mathrm{Vol}_{\mathbb{E}^d}(B(\alpha)) - W(\alpha, \beta, s) = C_\alpha(h_\alpha) - C_\beta(h_\beta)$

(d) $s + \alpha \leq \beta$:
$W(\alpha, \beta, s) = \mathrm{Vol}_{\mathbb{E}^d}(B(\alpha))$

Figure 4: Different cases in the proof of Lemma 3

Substituting $q_\alpha,\ q_\beta,\ h_\alpha,\ h_\beta$, we obtain that

$$\begin{aligned}
&\alpha^d q_\alpha^{d+1}(h_\alpha) + \beta^d q_\beta^{d+1}(h_\beta) \\
&\qquad = \alpha^d \left(\frac{\alpha^2 - (\alpha - h_\alpha)^2}{\alpha^2}\right)^{\frac{d+1}{2}} + \beta^d \left(\frac{\beta^2 - (\beta - h_\beta)^2}{\beta^2}\right)^{\frac{d+1}{2}} \\
&\qquad = \frac{1}{\alpha}\left(h_\alpha(2\alpha - h_\alpha)\right)^{\frac{d+1}{2}} + \frac{1}{\beta}\left(h_\beta(2\beta - h_\beta)\right)^{\frac{d+1}{2}} \\
&= \frac{1}{\alpha}\left(\frac{(\beta^2 - (s-\alpha)^2)((s+\alpha)^2 - \beta^2)}{4s^2}\right)^{\frac{d+1}{2}} + \frac{1}{\beta}\left(\frac{(\alpha^2 - (s-\beta)^2)((s+\beta)^2 - \alpha^2)}{4s^2}\right)^{\frac{d+1}{2}} \\
&\qquad = \left(\frac{1}{\alpha} + \frac{1}{\beta}\right) A^{\frac{d+1}{2}}.
\end{aligned}$$

3. If $\sqrt{\alpha^2 + s^2} \le \beta < s + \alpha$, then (see Figure 4c)

$$\frac{\mathrm{Vol}_{\mathbb{E}^d}(B(\alpha))}{2} \le W(\alpha, \beta, s) \le \mathrm{Vol}_{\mathbb{E}^d}(B(\alpha)),$$

Also, according to Figure 4c,

$$\mathrm{Vol}_{\mathbb{E}^d}(B(\alpha)) - W(\alpha, \beta, s) = C_\alpha(\widetilde{h}_\alpha) - C_\beta(h_\beta) \le C_\alpha\left(\widetilde{h}_\alpha\right).$$

By Lemma 2, we have

$$\frac{\mathrm{Vol}_{\mathbb{E}^d}(B) \cdot \alpha^d - W(\alpha, \beta, s)}{\mathrm{Vol}_{\mathbb{E}^{d-1}}(B) \cdot \alpha^d \cdot q_\alpha^{d+1}(\widetilde{h}_\alpha)} \le \Theta\left(d^{-\frac{1}{2}}\right).$$

Substituting q_α and $\widetilde{h}_\alpha$, we get

$$\begin{aligned}
\alpha^d q_\alpha^{d+1}(\widetilde{h}_\alpha) = \alpha^d \left(\frac{\alpha^2 - (\alpha - \widetilde{h}_\alpha)^2}{\alpha^2}\right)^{\frac{d+1}{2}} &= \frac{1}{\alpha}\left(\widetilde{h}_\alpha(2\alpha - \widetilde{h}_\alpha)\right)^{\frac{d+1}{2}} \\
&= \frac{1}{\alpha}\left(\frac{((s+\alpha)^2 - \beta^2)(\beta^2 - (s-\alpha)^2)}{4s^2}\right)^{\frac{d+1}{2}} = \frac{1}{\alpha} A^{\frac{d+1}{2}}.
\end{aligned}$$

4. If $s + \alpha \le \beta$, then $W(\alpha, \beta, s) = \mathrm{Vol}_{\mathbb{E}^d}(B(\alpha)) = \mathrm{Vol}_{\mathbb{E}^d}(B) \cdot \alpha^d$, see Figure 4d.

□

The following lemma will also be helpful in our proofs.

Lemma 4. *$W(\alpha, \beta, \alpha)$ and $W(\beta, \alpha, \alpha)$ are non-decreasing functions of α.*

Proof. Let us consider the configuration of balls shown in Figure 5. The d-dimensional ball centered at $\mathbf{q}'$ is contained within the ball centered at $\mathbf{q}$. Thus, the intersection $\mathbf{A}'\mathbf{B}'\mathbf{x}$ of the balls centered at $\mathbf{x}$ and $\mathbf{q}'$ is contained in the intersection $\mathbf{ABx}$ of the balls centered at $\mathbf{x}$ and $\mathbf{q}$. Clearly, the center $\mathbf{q}'$ of the ball which is closer to $\mathbf{x}$ can be taken on the geodesic between $\mathbf{q}$ and $\mathbf{x}$ without loss of generality. The same argument works when the ball centered at $\mathbf{x}$ contains the centers $\mathbf{q}$, $\mathbf{q}'$ of the other balls. □

A.2 Hyperbolic volumes

First, we briefly recall the basic properties of hyperbolic space, and then move towards the study of hyperbolic volumes and their Euclidean counterparts. It turns out that on the small scale hyperbolic volumes behave in an almost Euclidean way, while on larger scale their behaviour is fundamentally different.

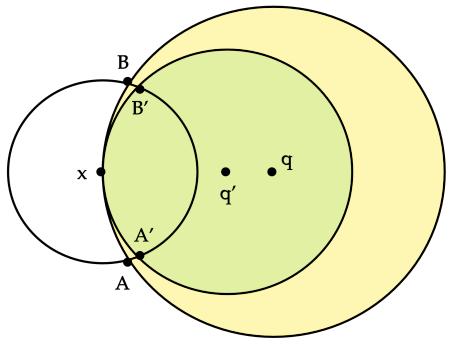


Figure 5: Monotonicity of $W(\alpha, \beta, \alpha)$ and $W(\beta, \alpha, \alpha)$

A.2.1 Background on hyperbolic space

Let $\mathbb{R}^{d,1}$ be the $(d+1)$-dimensional *Minkowski space*, i.e., the real vector space of dimension $(d+1)$ equipped with the inner product

$$\langle \mathbf{x}, \mathbf{y} \rangle_h = -x_0 y_0 + x_1 y_1 + \ldots + x_d y_d$$

of signature $(d, 1)$.

The *vector model* of the *d-dimensional hyperbolic Lobachevsky space* $\mathbb{H}^d$ is the connected component of the standard two-sheeted hyperboloid contained in the *future light cone*:

$$\mathbb{H}^d = \{\mathbf{x} \in \mathbb{R}^{d,1} \mid \langle \mathbf{x}, \mathbf{x} \rangle_h = -1, x_0 > 0\}. \tag{8}$$

The *hyperbolic metric* is given by

$$\cosh \rho(\mathbf{x}, \mathbf{y}) = -\langle \mathbf{x}, \mathbf{y} \rangle_h.$$

The coordinates $(x_0, x_1, \ldots, x_d)$ satisfy the following system of equations:

$$\begin{aligned} x_0 &= \cosh(t_1), \\ x_1 &= \sinh(t_1)\cos(t_2), \\ &\ldots \\ x_{d-1} &= \sinh(t_1)\sin(t_2)\ldots\sin(t_{d-1})\cos(t_d), \\ x_d &= \sinh(t_1)\sin(t_2)\ldots\sin(t_{d-1})\sin(t_d). \end{aligned}$$

This hyperbolic coordinate parameterization of $\mathbb{H}^d$ is the map

$$\chi\colon [0, +\infty) \times [0, \pi]^{d-2} \times [0, 2\pi] \to \mathbb{H}^d$$

defined by

$$\chi(t_1, \ldots, t_d) = (x_0, x_1, \ldots, x_d).$$

A subset $U \subset \mathbb{H}^d$ is called measurable if $\chi^{-1}(U)$ is measurable with respect to the standard Lebesgue measure on $\mathbb{R}^d$. Let $U \subset \mathbb{H}^d$ be a measurable set. Then, the hyperbolic volume of U is defined by

$$\mathrm{Vol}_{\mathbb{H}^d}(U) = \int\limits_{\chi^{-1}(U)} \sinh^{d-1}(t_1)\sin^{d-2}(t_2)\ldots\sin(t_{d-1})\, dt_1 dt_2 \ldots dt_{d-1} dt_d.$$

A.2.2 Approximating small hyperbolic volumes by their Euclidean counterparts

In this section, we show that small hyperbolic volumes can be approximated by Euclidean ones. This is very helpful for our analysis and will allow us to obtain analogs of Lemma 2 and 3 for small hyperbolic balls.

From the definition of the hyperbolic space (8), we see that $x_0 = \sqrt{1 + x_1^2 + \ldots + x_d^2}$. Let $U \subset \mathbb{H}^d$ be a measurable set containing the point $\mathbf{z} = (1, 0, \ldots, 0)$, and let U' be the projection of U along the x_0–coordinate from the hyperboloid onto the tangent space $T_{\mathbf{z}}\mathbb{H}^d = \{\mathbf{x} \in \mathbb{R}^{d,1} \mid x_0 = 1\} \simeq \mathbb{R}^d$ realised by the map $p : \mathbb{H}^d \to \mathbb{R}^d$. Let c be the central projection $c : \mathbb{H}^d \to T_{\mathbf{z}}\mathbb{H}^d \simeq \mathbb{R}^d$ from the origin $\mathbf{o} = (0, \ldots, 0)$. Let $F : U' \to c(U)$ be the map that satisfies $c = F \circ p$.

Let us note that the central projection c maps balls centered at $\mathbf{z}$ in $\mathbb{H}^d$ to balls centered at $p(\mathbf{z}) = \mathbf{z}$ in $\mathbb{R}^d$, and also spherical caps of such balls in $\mathbb{H}^d$ have spherical caps in $\mathbb{R}^d$ as their respective images, since every spherical cap is an intersection of some ball with a half-space, which is bounded by some hyperplane in $\mathbb{R}^{d,1}$ (the central projection of this hyperplane is also a hyperplane in $\mathbb{R}^d$).

According to Ratcliffe (2019),

$$\mathrm{Vol}_{\mathbb{H}^d}(U) = \int\limits_{U'} \frac{dx_1 \ldots dx_d}{\sqrt{1 + x_1^2 + \ldots + x_d^2}}.$$

We need to compare $\mathrm{Vol}_{\mathbb{H}^d}(U)$ to $\mathrm{Vol}_{\mathbb{E}^d}(c(U))$ in order to conclude that these quantities approximate each other in some appropriate regime.

Lemma 5. *Suppose that $U \subset \mathbb{H}^d$ is a measurable set such that $U \subset B(0, r)$. If $r \ll \frac{1}{\sqrt{d}}$ and $d \to \infty$, then we have*

$$\mathrm{Vol}_{\mathbb{H}^d}(U) = \mathrm{Vol}_{\mathbb{E}^d}(c(U)) \left(1 - O\left(d\, r^2\right)\right).$$

Proof. We have that $U' = p(U) \subset B_{\mathbb{R}^d}(0, \sinh(r))$, hence $x_1^2 + \ldots + x_d^2 \leq \sinh^2(r)$. Then,

$$\int\limits_{U'} \frac{dx_1 \ldots dx_d}{\cosh(r)} < \mathrm{Vol}_{\mathbb{H}^d}(U) = \int\limits_{U'} \frac{dx_1 \ldots dx_d}{\sqrt{1 + x_1^2 + \ldots + x_d^2}} < \int\limits_{U'} dx_1 \ldots dx_d = \mathrm{Vol}_{\mathbb{E}^d}(U').$$

By using Taylor series expansion, we obtain

$$\int\limits_{U'} \frac{dx_1 \ldots dx_d}{\cosh(r)} = \frac{1}{\cosh(r)} \mathrm{Vol}_{\mathbb{E}^d}(U') = \left(1 - \frac{r^2}{2} + \Theta\left(r^4\right)\right) \mathrm{Vol}_{\mathbb{E}^d}(U'),$$

and thus

$$\left(1 - \frac{r^2}{2} + \Theta\left(r^4\right)\right) \mathrm{Vol}_{\mathbb{E}^d}(U') < \mathrm{Vol}_{\mathbb{H}^d}(U) < \mathrm{Vol}_{\mathbb{E}^d}(U').$$

Now let us show that

$$\mathrm{Vol}_{\mathbb{E}^d}(U') = \mathrm{Vol}_{\mathbb{E}^d}(c(U)) \left(1 - O\left(dr^2\right)\right).$$

Indeed, the map $F : U' \to c(U)$ satisfies $c = F \circ p$ and is given by $F = (F_1, \ldots, F_d)$ with

$$F_i : x_i \mapsto \frac{x_i}{\sqrt{1 + x_1^2 + \ldots + x_d^2}}, \text{ for } i = 1, \ldots, d,$$

and thus the Jacobian of F satisfies

$$\det \left(\frac{\partial F_i}{\partial x_j}\right)_{i,j=1}^{d} = \frac{1}{(1 + x_1^2 + \ldots + x_d^2)^{\frac{d+2}{2}}} = 1 - O\left(dr^2\right),$$

whenever $x_1^2 + \ldots + x_d^2 \leq \sinh^2(r)$ and $dr^2 \to 0$. One can conveniently use spherical coordinates in order to perform the respective computation. The lemma now follows from standard Taylor series techniques. □

Let $B_d(\mathbf{x}, r)$ be a closed hyperbolic ball centered at a point $\mathbf{x} \in \mathbb{H}^d$ of radius $r > 0$. Then we can compute its volume as Ratcliffe (2019):

$$\mathrm{Vol}_{\mathbb{H}^d}(B_d(\mathbf{x}, r)) = \mathrm{Vol}\left(\mathbb{S}^{d-1}\right) \int\limits_0^r \sinh^{d-1}(t)\, dt.$$

For $r \gg \log d$, we have

$$\mathrm{Vol}_{\mathbb{H}^d}(B_d(\mathbf{x}, r)) \sim \mathrm{Vol}(\mathbb{S}^{d-1})\, \exp(r(d-1))\, \Theta(d^{-1} 2^{-d}).$$

For $r \ll 1/\sqrt{d}$, we have from Lemma 5 that

$$\mathrm{Vol}_{\mathbb{H}^d}(B_d(\mathbf{x}, r)) \sim \mathrm{Vol}_{\mathbb{E}^d}(B_d(\mathbf{x}, r)) \sim \mathrm{Vol}(\mathbb{S}^{d-1})\, d^{-1}\, r^d\, \Theta(1).$$

A.2.3 SMALL HYPERBOLIC BALLS AND THEIR INTERSECTIONS

Lemma 5 allows us to transfer our results for Euclidean balls and their intersections to the hyperbolic space when the radii of the balls are sufficiently small. Let $C_\alpha(h)$ be the volume of a spherical cap of height h in the hyperbolic space. The following lemma follows from Lemma 2 and Lemma 5.

Lemma 6. *For $\alpha \ll 1/\sqrt{d}$, the volume of a hyperbolic spherical cap can be estimated as follows:*

$$\Theta(d^{-1}) \leq \frac{C_\alpha(h)}{\mathrm{Vol}_{\mathbb{E}^{d-1}}(B) \cdot \alpha^d \cdot q_\alpha(h)^{d+1}} \leq \Theta(d^{-\frac{1}{2}}).$$

Let us now estimate the volume of the intersection of two hyperbolic balls. As before, denote by $W_{\mathbf{x}_i,\mathbf{x}_j}(\alpha,\beta)$ the intersection of $B(\mathbf{x}_i,\alpha)$ and $B(\mathbf{x}_j,\beta)$, i.e., $W_{\mathbf{x}_i,\mathbf{x}_j}(\alpha,\beta) = \{\mathbf{y} : \rho(\mathbf{x}_i,\mathbf{y}) \leq \alpha,\ \rho(\mathbf{x}_j,\mathbf{y}) \leq \beta\}$. Let $s := \rho(\mathbf{x}_i,\mathbf{x}_j)$ be the distance between the centers and $W(\alpha,\beta,s) := \mathrm{Vol}_{\mathbb{H}^d}\left(W_{\mathbf{x}_i,\mathbf{x}_j}(\alpha,\beta)\right)$ denote the volume of the intersection. The following lemma estimates the value $W(\alpha,\beta,s)$ for various relationships between α,β,s. Without loss of generality, we assume that $\alpha \leq \beta$.

Lemma 7. *Assume that $\alpha \ll 1/\sqrt{d}$, $\beta \ll 1/\sqrt{d}$. W.l.o.g., we may also assume that $\alpha \leq \beta$. Define $A := \frac{(\alpha+\beta+s)(\alpha+\beta-s)(s+\alpha-\beta)(s+\beta-\alpha)}{4s^2}$.*

1. *If $\alpha+\beta < s$, then $W(\alpha,\beta,s) = 0$.*
2. *If $s-\alpha \leq \beta < \sqrt{\alpha^2+s^2}$, then*
$$\Theta\left(d^{-1}\right) \leq \frac{W(\alpha,\beta,s)\cdot\alpha\beta}{\mathrm{Vol}_{\mathbb{E}^{d-1}}(B)\cdot(\alpha+\beta)\cdot A^{\frac{d+1}{2}}} \leq \Theta\left(d^{-\frac{1}{2}}\right). \tag{9}$$
3. *If $\sqrt{\alpha^2+s^2} \leq \beta < s+\alpha$, then*
$$\frac{1}{2} \leq \frac{W(\alpha,\beta,s)}{\mathrm{Vol}_{\mathbb{E}^d}(B)\cdot\alpha^d\cdot(1+o(1))} \leq 1, \tag{10}$$
$$\frac{\mathrm{Vol}_{\mathbb{H}^d}(B(\alpha)) - W(\alpha,\beta,s)}{\mathrm{Vol}_{\mathbb{E}^{d-1}}(B)\cdot A^{\frac{d+1}{2}}\cdot\alpha^{-1}} \leq \Theta\left(d^{-\frac{1}{2}}\right). \tag{11}$$
4. *If $s+\alpha \leq \beta$, then*
$$W(\alpha,\beta,s) = \mathrm{Vol}_{\mathbb{H}^d}(B(\alpha)) \sim \mathrm{Vol}_{\mathbb{E}^d}(B)\cdot\alpha^d. \tag{12}$$

Proof. To prove this lemma, we follow the proof of Lemma 3, and use Lemma 6 instead of Lemma 2. □

The following lemma is an analog of Lemma 4. Indeed, the argument uses only monotonicity of volumes under set-theoretic inclusions, which holds for both Euclidean and hyperbolic spaces.

Lemma 8. *$W(\alpha,\beta,\alpha)$ and $W(\beta,\alpha,\alpha)$ are non-decreasing functions of α.*

B PROOF OVERVIEW

In this section, we overview the proof of Theorem 1.

Recall that we assume that the distribution of the dataset is uniform over a d-dimensional ball $\mathcal{B}$ of radius $R = R(n)$ such that

$$e^R \ll \frac{n^{1/(d-1)}}{d^{1/2}}. \tag{13}$$

Then, the graph $G(M)$ is constructed by using balls of radius $\alpha_M = M\delta$ with

$$\delta = \left(\frac{dv_d(R)}{n}\right)^{1/d}. \tag{14}$$

Let us show that under the conditions of the theorem, we have $\delta \ll 1/\sqrt{d}$. First, note that

$$v_d(R) = \int\limits_0^R \sinh^{d-1}(t)\, dt \leq \int\limits_0^R \frac{e^{t(d-1)}}{2^{d-1}}\, dt \leq \frac{e^{R(d-1)}}{2^{d-1}(d-1)}\,.$$

Thus, we have

$$\delta \leq \left(\frac{de^{R(d-1)}}{2^{d-1}(d-1)n}\right)^{1/d} = \Theta\left(e^{R(d-1)/d} n^{-1/d}\right) \ll 1/\sqrt{d}.$$

The last inequality is due to the conditions of Theorem 1. Thus, we can apply Lemma 7 throughout the proof.

To prove that the algorithm succeeds w.h.p., we need to guarantee that it does not stop in a local optimum until we find the exact (or approximate) nearest neighbor of the query **q**. Given a point **x** such that $\rho(\mathbf{q}, \mathbf{x}) = \alpha_s$, the probability of making a step towards **q** is determined by $W(\alpha_s, \alpha_M, \alpha_s)$: the distance between the points is α_s, the neighbors of **x** are within the ball of radius α_M centered at **x**, and we accept those neighbors that are closer to **q** than **x**, i.e., within a ball of radius α_s centered at **q**. Lemma 9 analyzes the asymptotic behavior of $W(\alpha_s, \alpha_M, \alpha_s)$.

Lemma 4 states that $W(\alpha, \beta, \alpha)$ is a non-increasing function of α. Informally, it means that it is easier to make steps towards the query when $\rho(\mathbf{x}, \mathbf{q})$ is larger. In contrast, when **x** becomes closer to **q**, the probability of getting stuck in a local optimum increases. Therefore, to obtain lower bounds on $W(\alpha_s, \alpha_M, \alpha_s)$, we can consider only the case when α_s is small. Below we assume that $\alpha_s = s\delta$, where s is some constant.

Lemma 11 gives the following lower bounds on $W(\alpha_s, \alpha_M, \alpha_s)$:

1. if $M < s\sqrt{2}$, then $\frac{W(\alpha_s, \alpha_M, \alpha_s)}{V_d(R)} \geq \frac{1}{n} \cdot \left(M^2 - \frac{M^4}{4s^2}\right)^{\frac{d}{2}+o(d)}$;
2. if $M \geq s\sqrt{2}$, then $\frac{W(\alpha_s, \alpha_M, \alpha_s)}{V_d(R)} \geq \frac{1}{n} \cdot s^{d+o(d)}$.

Let us consider one step of the algorithm. We can move forward w.h.p. if $W(\alpha_s, \alpha_M, \alpha_s) \gg 1/n$. Formally speaking, Corollary 4 of Lemma 11 states that if M and s satisfy

$$s > 1 \text{ and either } M \geq s\sqrt{2} \text{ or } M^2 - M^4/4s^2 > 1, \tag{15}$$

then there exists a constant $S > 1$ such that we can make a step towards **q** with probability

$$1 - \left(1 - \frac{S^{d+o(d)}}{n}\right)^{n-1} = 1 - O\left(e^{-S^{d+o(d)}}\right)$$

since the expected number of nodes in the intersection of balls is much greater than 1.

We make steps of the greedy algorithm towards the query **q** as long as the probability of making the next step is large. Below we also prove that the overall probability of failure (taking into account all steps of the algorithm) is small. Now, let us show that under the conditions of the theorem, we reach some neighborhood of **q** and then either find the approximate near neighbor or find the exact nearest neighbor by making one more step.

First, let us consider the exact NNS. In this case, we assume that the nearest neighbor is located within a ball of radius r, $0 < r \leq 1$, centered at **q**. Our goal is to find the exact nearest neighbor. According to the statement of the theorem, we have $M > \sqrt{2}$. Observe that this implies

$$\frac{M}{\sqrt{2}} > \frac{M^2}{2\sqrt{M^2-1}}. \tag{16}$$

While we move towards the query, s becomes smaller. Let us figure out up to which s we can make steps. According to (15), we need either $1 < s \leq M/\sqrt{2}$ or $s > M^2/2\sqrt{M^2-1}$. According to (16), it reduces to $s > 1$. In other words, we can move forward to any $s > 1$. Then, according to Lemma 14, it is sufficient to have $M^2 > s^2 + r^2$ to reach the exact nearest neighbor of **q** in one step.

Thus, we can take any s s.t. $1 < s < \sqrt{M^2 - r^2}$: we can reach this distance with greedy search and then jump directly to the nearest neighbor with high probability.

Now, let us turn to the approximate near neighbor search c, r-ANN. In this case, we need to find an element that is within a distance rc from $\mathbf{q}$. According to the statement of the theorem, we have $M > \sqrt{4c^2/(3c^2 - 1)}$.

Note that $F(r) := 2r^2c^2\left(1 - \sqrt{1 - 1/r^2c^2}\right)$ decreases with r for $r > 1/c$ and equals 2 at $r = 1/c$, while $G(r) := \frac{2}{3}\left(r^2 + 1 + \sqrt{r^4 - r^2 + 1}\right)$ increases with r and equals 2 at $r = 1$. Both $F(r)$ and $G(r)$ attain $4c^2/(3c^2 - 1)$ at $r_0 = \sqrt{4c^2/(c^2 + 1)(3c^2 - 1)}$. Therefore, we either have

$$1 \geq r > r_0 \text{ and } M^2 > F(r) \tag{17}$$

or

$$r_0 \geq r > \frac{1}{c} \text{ and } M^2 > G(r). \tag{18}$$

To solve c, r-ANN, either we can reach s such that $rc > s$ or we can reach s such that at the next step we can find the exact nearest neighbor. Let us consider the first possibility. Note that

$$s > 1 \text{ and } M^2 > 2s^2\left(1 - \sqrt{1 - \frac{1}{s^2}}\right) \tag{19}$$

is equivalent to (15). In turn, since $2s^2(1 - \sqrt{1 - 1/s^2})$ is a decreasing function of s on $s > 1$, we get that (17) implies the existence of s such that $rc > s > 1$ and

$$M^2 > 2s^2\left(1 - \sqrt{1 - \frac{1}{s^2}}\right) > F(r).$$

Hence, since (15) holds, we can move forward to such s. Let us consider the second possibility. Observe that (18) is equivalent to

$$M^2 - r^2 > \frac{M^4}{4(M^2 - 1)}.$$

Therefore, there exists s such that the condition $s^2 < M^2 - r^2$ of Lemma 14 and (15) hold. Since (15) holds, we can move forward to such s and reach the exact nearest neighbor in one step as the condition of Lemma 14 is satisfied.

Above we show that under the conditions of the theorem, each step of the greedy search is successful with probability $1 - O\left(e^{-S^{d+o(d)}}\right)$. To formally prove that the algorithm succeeds with high probability, we need to limit the number of steps and estimate the overall probability of failure. For this, we show that at each step of the algorithm we become closer to the query by some fixed positive value. In Lemma 12, we prove that each step reduces the distance from $\mathbf{q}$ by at least $\varepsilon\delta$, where ε is some positive constant. Clearly, we start at a distance $O(R)$ from q. Hence, we are able to bound the number of steps by $O(R/\varepsilon\delta)$ which is $O\left(Rn^{1/d}(v_d(R))^{-1/d}\right)$.

To estimate the overall success probability, we have to consider the dependence of consecutive steps of the algorithm. Lemma 13 implies that consecutive steps are "almost independent" and the overall success probability is $1 - O\left(Rn^{1/d}(v_d(R))^{-1/d}e^{-S^{d+o(d)}}\right)$. The assumption $d \gg \log\log n$ and the fact that $v_d(R) = \Omega(R^d)$ yield $O\left(Rn^{1/d}(v_d(R))^{-1/d}e^{-S^{d+o(d)}}\right) = O\left(e^{\frac{\log n}{d} - S^{d+o(d)}}\right) = o(1)$.

While in most of the analysis we do not consider the cases when α_M-neighborhoods of the dataset elements intersect the boundary $\partial\mathcal{B}$, we need to show that possible intersections do not affect the result. The formal statement of this fact is given in Lemma 15.

Finally, let us discuss the time and space complexities of the algorithm. Let v be a fixed arbitrary node of $G(M)$ and let $N(v)$ denote the (random) number of its neighbors in $G(M)$. Let $f = f(n) = (n - 1)\mathrm{Vol}_{\mathbb{H}^d}\left(B(\alpha_M)\right)/\mathrm{Vol}_{\mathbb{H}^d}\left(\mathcal{B}\right)$ denote the upper bound for the expected number of neighbors of v (this is an upper bound due to possible boundary effects). In Lemma 16, we show that $N(v) \leq 3f/2$ with probability at least $1 - O(1/f)$.

To obtain the final time complexity of graph-based NNS, we sum up the complexity of all algorithm's steps. In Lemma 17, we show that if k steps of the NNS are made then the time complexity is $O(kfd)$ with probability $1 - O(1/kf)$.

In Lemma 18, we show that the number of edges in the graph is $E(G) \leq 3fn/4$ with probability $1 - O(1/fn)$. If we store the graph as the adjacency lists, then the space complexity is $O(E(G) \cdot \log n) = O(fn \log n)$.

Due to the choice of δ, we have $f = O\left(M^d\right)$. Hence, w.h.p. the space complexity is $O\left(n \cdot \log n \cdot M^d\right)$ and the time complexity is $O\left(R \cdot n^{1/d} \cdot (v_d(R))^{-1/d} \cdot M^d\right)$.

C RESULTS USED THROUGHOUT THE PROOF

In this section, we formulate supplemental statements used in the proof. We need these results for the hyperbolic space, but they are also true for the Euclidean one. Thus, we do not specify a particular space in $W(\cdot, \cdot, \cdot)$.

C.1 ANALYSIS OF CONVERGENCE

Recall that $\alpha_M = M\delta$ and $\alpha_s = s\delta$, where M and s are some constants and δ is defined in (14). Recall that $\delta \ll 1/\sqrt{d}$.

Lemma 9. *Define* $A := \frac{\alpha_M^2(4\alpha_s^2 - \alpha_M^2)}{4\alpha_s^2}$.

If $\alpha_M \leq \alpha_s\sqrt{2}$, *then*

$$\Theta\left(d^{-1}\right) \leq \frac{W(\alpha_s, \alpha_M, \alpha_s) \cdot \alpha_M \alpha_s}{\mathrm{Vol}_{\mathbb{E}^{d-1}}(B) \cdot (\alpha_M + \alpha_s) \cdot A^{\frac{d+1}{2}}} \leq \Theta\left(d^{-\frac{1}{2}}\right). \tag{20}$$

If $\alpha_M > \alpha_s\sqrt{2}$, *then*

$$\frac{W(\alpha_s, \alpha_M, \alpha_s)}{\mathrm{Vol}_{\mathbb{E}^d}(B)\, \alpha_s^d} = \Theta(1). \tag{21}$$

Proof. We apply Lemma 7. First, consider the case $\alpha_M \leq \alpha_s$. Then, the case 2 applies to $W(\alpha_M, \alpha_s, \alpha_s)$. From (9) we obtain

$$\Theta\left(d^{-1}\right) \leq \frac{W(\alpha_s, \alpha_M, \alpha_s) \cdot \alpha_M \alpha_s}{\mathrm{Vol}_{\mathbb{E}^{d-1}}(B) \cdot (\alpha_M + \alpha_s) \cdot A^{\frac{d+1}{2}}} \leq \Theta\left(d^{-\frac{1}{2}}\right). \tag{22}$$

Now, consider the case $\alpha_s < \alpha_M$.

1. If $\alpha_s < \alpha_M \leq \alpha_s\sqrt{2}$, then from (9) we obtain
$$\Theta\left(d^{-1}\right) \leq \frac{W(\alpha_s, \alpha_M, \alpha_s) \cdot \alpha_M \alpha_s}{\mathrm{Vol}_{\mathbb{E}^{d-1}}(B) \cdot (\alpha_M + \alpha_s) \cdot A^{\frac{d+1}{2}}} \leq \Theta\left(d^{-\frac{1}{2}}\right).$$
2. If $\alpha_s\sqrt{2} < \alpha_M < 2\alpha_s$, then (10) yields
$$W(\alpha_s, \alpha_M, \alpha_s) = \Theta\left(\mathrm{Vol}_{\mathbb{E}^d}(B) \cdot \alpha_s^d\right).$$
3. If $2\alpha_s \leq \alpha_M$, then (12) gives
$$W(\alpha_s, \alpha_M, \alpha_s) = \mathrm{Vol}_{\mathbb{E}^d}(B) \cdot \alpha_s^d\,(1 - o(1)).$$

This concludes the proof of the lemma. □

Lemma 10. *Denote by* $A = \delta^2 \cdot \frac{(M+r+s)(M+r-s)(s+M-r)(s+r-M)}{4s^2}$. *If* $\alpha_s - \alpha_r < \alpha_M < \sqrt{\alpha_s^2 + \alpha_r^2}$, *then*

$$\Theta\left(d^{-1}\right) \leq \frac{W(\alpha_r, \alpha_M, \alpha_s) \cdot \delta}{\mathrm{Vol}_{\mathbb{E}^{d-1}}(B) \cdot A^{\frac{d+1}{2}}} \leq \Theta\left(d^{-\frac{1}{2}}\right). \tag{23}$$

If $\alpha_M > \sqrt{\alpha_s^2 + \alpha_r^2}$*, then*

$$\frac{\mathrm{Vol}_{\mathbb{H}^d}(B(\alpha_r)) - W(\alpha_r, \alpha_M, \alpha_s)}{\mathrm{Vol}_{\mathbb{E}^{d-1}}(B) \cdot A^{\frac{d+1}{2}} \cdot \delta^{-1}} \leq \Theta\left(d^{-\frac{1}{2}}\right). \tag{24}$$

Proof. The result follows directly from Lemma 7. □

Lemma 11. *If* $M > s\sqrt{2}$*, then*

$$W(\alpha_s, \alpha_M, \alpha_s) \geq \frac{V_d(R)}{n} \cdot s^{d+o(d)}.$$

If $M \leq s\sqrt{2}$*, then*

$$W(\alpha_s, \alpha_M, \alpha_s) \geq \frac{V_d(R)}{n} \cdot \left(M^2 - \frac{M^4}{4s^2}\right)^{\frac{d}{2}+o(d)}.$$

Proof. If $M > s\sqrt{2}$, then we can apply (21) to obtain

$$\begin{aligned} W(\alpha_s, \alpha_M, \alpha_s) \geq \Theta\left(d^{-1} \cdot (s\delta)^d \cdot \mathrm{Vol}_{\mathbb{E}^d}(B)\right) &= \Theta\left(d^{-1} \cdot s^d \cdot \frac{dv_d(R)}{n} \cdot \mathrm{Vol}_{\mathbb{E}^d}(B)\right) \\ &= \Theta\left(s^d \cdot \frac{V_d(R)}{n} \cdot \frac{\mathrm{Vol}_{\mathbb{E}^d}(B)}{\mathrm{Vol}(\mathbb{S}^{d-1})}\right) = \frac{V_d(R)}{n} s^{d+o(d)}. \end{aligned}$$

If $M \leq s\sqrt{2}$ then we can apply (20) to obtain

$$\begin{aligned} W(\alpha_s, \alpha_M, \alpha_s) &\geq \mathrm{Vol}_{\mathbb{E}^{d-1}}(B) \cdot \delta^{-1} A^{\frac{d+1}{2}} \Theta(d^{-1}) \\ &= \mathrm{Vol}_{\mathbb{E}^{d-1}}(B) \cdot \delta^{-1} \cdot \alpha_M^{d+1} \cdot \left(1 - \frac{\alpha_M^2}{4\alpha_s^2}\right)^{\frac{d+1}{2}} \cdot \Theta(d^{-1}) \\ &= \mathrm{Vol}_{\mathbb{E}^{d-1}}(B) \cdot \delta^d \cdot M^{d+1} \left(1 - \frac{M^2}{4s^2}\right)^{\frac{d+1}{2}} \cdot \Theta(d^{-1}) \\ &= \frac{\mathrm{Vol}_{\mathbb{E}^{d-1}}(B)}{\mathrm{Vol}(\mathbb{S}^{d-1})} \cdot \frac{V_d(R)}{n} \cdot M^{d+1} \left(1 - \frac{M^2}{4s^2}\right)^{\frac{d+1}{2}} \cdot \Theta(1) \\ &= \Theta\left(d^{-1}\right) \cdot \frac{V_d(R)}{n} \cdot \left(M^2 - \frac{M^4}{4s^2}\right)^{\frac{d+1}{2}} = \frac{V_d(R)}{n} \cdot \left(M^2 - \frac{M^4}{4s^2}\right)^{\frac{d}{2}+o(d)}. \end{aligned}$$

□

Corollary 4. *If* $s > 1$ *and either* $M > s\sqrt{2}$ *or* $M^2 - M^4/4s^2 > 1$*, then there exists a constant* $S > 1$ *such that* $W(\alpha_s, \alpha_M, \alpha_s) \geq \frac{V_d(R)}{n} S^{d+o(d)}$.

Lemma 12. *Assume that* $s > 1$*. If*

$$M > s\sqrt{2} \text{ or } M^2 - \frac{M^4}{4s^2} > 1, \tag{25}$$

then there exist constants $S > 1$ *and* $\varepsilon > 0$*, such that*

$$W\left(\alpha_M, \alpha_s, \alpha_s + \varepsilon\delta\right) \geq \frac{V_d(R)}{n} S^{d+o(d)}.$$

Proof. If $M > s\sqrt{2}$, then we can choose a sufficiently small $\varepsilon > 0$ such that $M^2 \geq s^2 + (s+\varepsilon)^2$. Then, the result follows from Lemma 11 and the fact that $s > 1$. Otherwise $M^2 < s^2 + (s+\varepsilon)^2$, and instead of the condition $M^2 - \frac{M^4}{4s^2} > 1$ from (23) we have

$$\frac{4s^2(s+\varepsilon)^2 - (M^2 - s^2 - (s+\varepsilon)^2)^2}{4(s+\varepsilon)^2} > 1.$$

As it holds for $\varepsilon = 0$, we can choose a small enough $\varepsilon > 0$ that it is still satisfied. □

Lemma 13. *The dependence of consecutive steps is negligible.*

Proof. First, consider the case $M \leq s\sqrt{2}$. It suffices to show that $W_1 = W(\alpha_M, \alpha_s, \alpha_s + 2\varepsilon\delta)$ is negligible in comparison with $W_1 + W_2 = W(\alpha_M, \alpha_s, \alpha_s + \varepsilon\delta)$ and the same for $W_1 = W(\alpha_s, \alpha_M, \alpha_s + 2\varepsilon\delta)$ compared to $W_1 + W_2 = W(\alpha_s, \alpha_M, \alpha_s + \varepsilon\delta)$. From (23) we can write their ratio

$$\frac{W_1}{W_1 + W_2} = \left(\frac{4(s+\varepsilon)^2}{2\left(M^2 s^2 + s^2(s+\varepsilon)^2 + M^2(s+\varepsilon)^2\right) - \left(M^4 + s^4 + (s+\varepsilon)^4\right)} \right.$$
$$\left. \cdot \frac{2\left(M^2 s^2 + s^2(s+2\varepsilon)^2 + M^2(s+2\varepsilon)^2\right) - \left(M^4 + s^4 + (s+2\varepsilon)^4\right)}{4(s+2\varepsilon)^2} \right)^{\frac{d+1}{2}} = o(1).$$

Since at each step we reduce the radius of the ball centered at $\mathbf{q}$ which contains the current position by at least $\varepsilon\delta$, any ball encountered in the current iteration intersects only a constant number of other balls, so their overall effect is negligible.

In the case when $M > s\sqrt{2}$ and $s > 1$ with probability $1 - o(1)$ we find the nearest neighbor in one step. □

Lemma 14. *If for some constants M, s, r we have $M^2 > s^2 + r^2$, then*

$$\mathrm{Vol}_{\mathbb{H}^d}\left(B(\alpha_r)\right) - W\left(\alpha_r, \alpha_M, \alpha_s\right) \leq \mathrm{Vol}_{\mathbb{H}^d}\left(B(\alpha_r)\right) \cdot \beta^d$$

with some $\beta < 1$.

Proof. It follows from (24) that

$$\mathrm{Vol}_{\mathbb{H}^d}\left(B(\alpha_r)\right) - W\left(\alpha_r, \alpha_M, \alpha_s\right) \leq \Theta\left(d^{-\frac{1}{2}}\right) \cdot \mathrm{Vol}_{\mathbb{E}^{d-1}}(B) \cdot A^{\frac{d+1}{2}} \cdot \delta^{-1}.$$

It remains to bound from above the following ratio:

$$\frac{\Theta\left(d^{-\frac{1}{2}}\right) \cdot \mathrm{Vol}_{\mathbb{E}^{d-1}}(B) \cdot A^{\frac{d+1}{2}} \cdot \delta^{-1}}{\mathrm{Vol}_{\mathbb{H}^d}\left(B(\alpha_r)\right)} = \frac{\Theta\left(d^{-\frac{1}{2}}\right) \cdot \mathrm{Vol}_{\mathbb{E}^{d-1}}(B) \cdot A^{\frac{d+1}{2}}}{\mathrm{Vol}_{\mathbb{E}^d}(B) \cdot r^d \cdot \delta^{d+1}} = \Theta(1) \cdot \left(\frac{A}{\delta^2 r^2}\right)^{\frac{d+1}{2}}$$
$$= \Theta(1) \cdot \left(\frac{(M+r+s)(M+r-s)(s+M-r)(s+r-M)}{4r^2 s^2}\right)^{\frac{d+1}{2}} =$$
$$\Theta(1) \cdot \left(1 - \frac{(M^2 - s^2 - r^2)^2}{4s^2 r^2}\right)^{\frac{d+1}{2}} \leq \beta^{d+1}$$

for some $\beta < 1$. □

C.2 Analysis of the boundary effect

Lemma 15. *The boundary effect is negligible and does not affect our results.*

Proof. Consider the worst-case scenario when the current element is located on the boundary of the ball $\mathcal{B}$ (see Figure 6). First, consider the Euclidean space. Let us show that $W(\alpha, R, R)$ converges to $\frac{1}{2}\mathrm{Vol}_{\mathbb{E}^d} B(\alpha)$ if $\alpha = \Theta(\delta)$. Note that $W(\alpha, R, R) = C_\alpha(h) + C_R(\alpha - h) < \frac{1}{2}\mathrm{Vol}_{\mathbb{E}^d} B(\alpha)$. We have

$$h = \frac{R^2 - (R-\alpha)^2}{2R} = \alpha - \frac{\alpha^2}{2R}; \quad \frac{h}{\alpha} = 1 - \frac{\alpha}{2R}; \quad \frac{\alpha - h}{R} = \frac{\alpha^2}{2R^2}.$$

On the other hand,

$$C_\alpha(h) = \frac{1}{2}\mathrm{Vol}_{\mathbb{E}^{d-1}}(B)\alpha^d \mathrm{B}\left(\frac{d+1}{2}, \frac{1}{2}; 1 - \frac{\alpha^2}{4R^2}\right) \to$$
$$\frac{1}{2}\mathrm{Vol}_{\mathbb{E}^{d-1}}(B)\alpha^d \mathrm{B}\left(\frac{d+1}{2}, \frac{1}{2}\right) = \frac{1}{2}\mathrm{Vol}_{\mathbb{E}^d} B(\alpha),$$

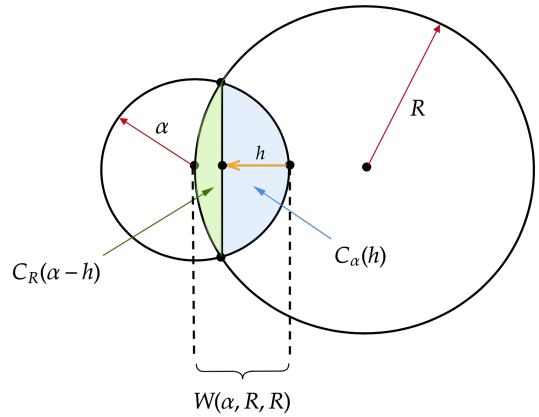


Figure 6: Boundary effect is negligible

if $\alpha \ll 1/\sqrt{d}$. Indeed,

$$\mathrm{B}\left(\frac{d+1}{2}, \frac{1}{2}\right) - \mathrm{B}\left(\frac{d+1}{2}, \frac{1}{2}; 1 - \frac{\alpha^2}{4R^2}\right) = \int_0^{\frac{\alpha^2}{4R^2}} t^{(d-1)/2}(1-t)^{-1/2} dt$$
$$\leq \frac{1}{\sqrt{1 - \frac{\alpha^2}{4R^2}}} \int_0^{\frac{\alpha^2}{4R^2}} t^{(d-1)/2} dt = \frac{\left(\frac{\alpha}{2R}\right)^{d+1}}{\sqrt{1 - \frac{\alpha^2}{4R^2}}} \to 0$$

for $(\alpha/R)^d \to 0$, which is the case since $(\alpha/R)^d = \frac{\Theta(1)^d dv_d(R)}{nR^d} \to 0$ for $d \ll \log n$.

In the hyperbolic case, the "small" ball of radius α is small enough ($\alpha \ll 1/\sqrt{d}$) so that its geometry can be considered Euclidean, and thus we can apply Lemma 5 to estimate the volume of $C_\alpha(h)$. The "large" hyperbolic ball of radius R in this case can be though of as a Euclidean ball (of radius $\sim \log R$) in the upper half–space model, and then we can carry out the same analysis on the Euclidean scale of the "small" radius α ball. □

C.3 Time and space complexity

In this section, we estimate time and space complexity. Recall that $N(v)$ denotes the number of neighbors of an element v in $G(M)$ and $f = (n-1)\mathrm{Vol}_{\mathbb{H}^d}(B(\alpha_M))/\mathrm{Vol}_{\mathbb{H}^d}(\mathcal{B})$. The proofs of the lemmas below follow the corresponding proofs by Prokhorenkova & Shekhovtsov (2020). We keep the proofs here for completeness.

Lemma 16. *The probability of the event "$N(v)$ satisfies $N(v) \leq \frac{3}{2}f$" is at least $1 - \frac{4}{f}$.*

Proof. First, let us note that we may neglect the boundary effect as we are interested in the upper bound on complexity. Indeed, the random variable $N(v)$ is upper bounded by the random variable $N'(v)$ having the binomial distribution $\mathrm{Bin}\left(n-1, \frac{\mathrm{Vol}_{\mathbb{H}^d}(B(\alpha_M))}{\mathrm{Vol}_{\mathbb{H}^d}(\mathcal{B})}\right)$ with expected value f. Thus, via the Chebyshev's inequality, we obtain

$$\mathsf{P}\left(N(v) > \frac{3}{2}f\right) \leq \mathsf{P}\left(|N(v) - f| > \frac{f}{2}\right) \leq \frac{4\,\mathsf{Var}\left(N(v)\right)}{f^2} \leq \frac{4}{f}.$$

□

Lemma 17. *The time complexity of k steps of the graph-based NNS is $O(kfd)$ with probability $1 - O\left(\frac{1}{kf}\right)$.*

Proof. We can upper bound the number of distance computations by the random variable distributed according to $\mathrm{Bin}\left(k(n-1), \frac{\mathrm{Vol}_{\mathbb{H}^d}(B(\alpha_M))}{\mathrm{Vol}_{\mathbb{H}^d}(\mathcal{B})}\right)$ and proceed as in the proof of Lemma 16. Finally, note that one distance computation takes $\Theta(d)$. □

Lemma 18. *The probability of the event "$E(G)$ satisfies $E(G) \leq \frac{3}{4}fn$" equals $1 - O\left(\frac{1}{fn}\right)$.*

Proof. The proof directly follows Prokhorenkova & Shekhovtsov (2020). The only modification that we have is that the probability p of an edge between two nodes can be bounded as (see Lemma 15)

$$\frac{\mathrm{Vol}_{\mathbb{H}^d}\left(B(\alpha_M)\right)}{2\mathrm{Vol}_{\mathbb{H}^d}\left(\mathcal{B}\right)} \lesssim p \leq \frac{\mathrm{Vol}_{\mathbb{H}^d}\left(B(\alpha_M)\right)}{\mathrm{Vol}_{\mathbb{H}^d}\left(\mathcal{B}\right)}.$$

□

D k-NN GRAPHS

Theorem 2. *Assume that $d = d(n)$ is such that $\log\log n \ll d(n) \ll \log n$ and $R = R(n)$ is such that $e^R \ll n^{\frac{1}{d-1}} \cdot d^{-1/2}$.*

For the exact NNS, let M be a constant s.t. $M > \sqrt{2}$ and let $k = [M^d]$. Then, with probability $1 - o(1)$, NNS based on k-NN graph finds the exact nearest neighbor. For c, r-ANN with some constant $c > 1$, let M be a constant s.t. $M > \sqrt{\frac{4c^2}{3c^2-1}}$ and $k = [M^d]$. Then, with probability $1 - o(1)$, NNS based on k-NN graph solves c, r-ANN for any r.

In both cases, the time complexity is $O\left(M^d \cdot n^{1/d} \cdot R \cdot (v_d(R))^{-1/d}\right)$;

the space complexity is $O\left(n \cdot \log n \cdot M^d\right)$.

To prove this theorem, let us note that the number of neighbors at distance at most r from v has binomial distribution $\mathrm{Bin}\left(n-1, \frac{\mathrm{Vol}(B(r))}{\mathrm{Vol}(\mathcal{B})}\right)$. From this, we can show that the radius of a ball containing M^d nearest neighbors is between $M(1-\varepsilon)\delta$ and $M(1+\varepsilon)\delta$ for any $\varepsilon > 0$ w.h.p. for all nodes. This can be done via the union bound and the Chernoff's bound. Thus, w.h.p., the neighborhoods considered in the theorem are asymptotically $M\delta$, so the arguments from the proof of Theorem 1 can be applied.

E EXPERIMENTS

Implementation Our implementation supplements the submission.

Best-first search In the main text, for the synthetic experiments, we use the greedy search. However, in graph-based NNS algorithms, the greedy search is often replaced by the best-first search (a.k.a. beam search). In this case, instead of keeping track of only the best candidate, we maintain a dynamic list of several candidates. In particular, this technique is used in HNSW (Malkov & Yashunin, 2018), and the size of the candidate list is controlled by the parameter $efSearch$.

Hyperparameters Recall that to plot Figure 3, we vary the graph degree to control the complexity and accuracy of NNS. In Figures 1 and 2, we use the best-first search, so we vary the parameter $efSearch$ and fix the graph degree. In this case, we tune M and $efConstruction$ HNSW hyperparameters, which are responsible for the graph degree and quality of the graph construction, respectively. For both GloVe and Poincaré GloVe databases, we get M=10 and $efConstruction$=300.

Spherical Shell implementation As a baseline, we implement Spherical Shell proposed by Wu & Charikar (2020). As in the original paper, we split the elements into 25 bands such that $w^{i-1} \leq \frac{1}{1-\|x\|^2} \leq w^i$. To achieve this, we take $w = 1.05$. For each band, we construct LSH with 50 tables. Each table has $[\log(m)] - 1$ bins, where m is the number of elements in the band. The number of

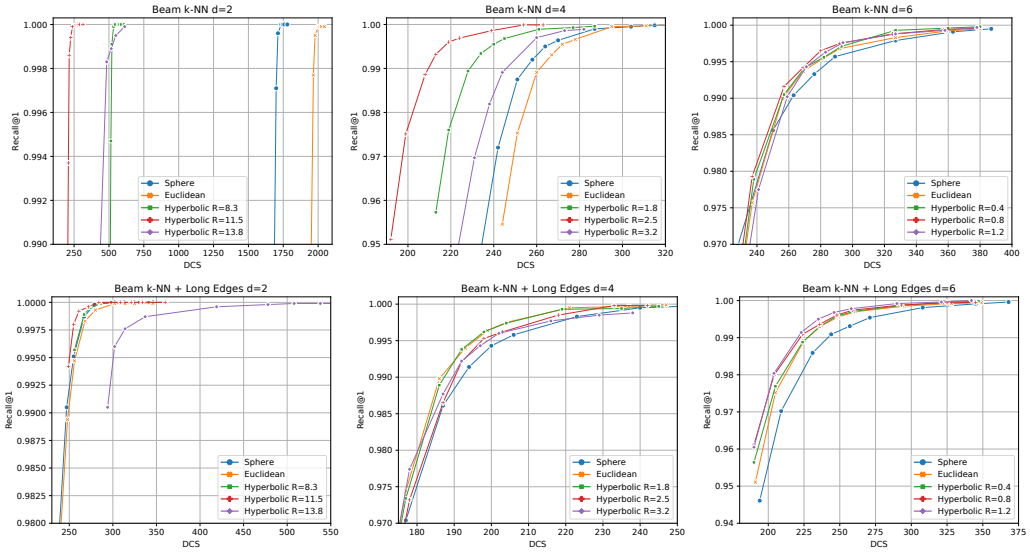


Figure 7: Best-first search over NN graphs without (top row) and with (bottom row) long edges

probes is tuned for each band to achieve 0.95 recall (this value has been chosen to achieve better results). When searching for the nearest neighbor for a query q, we compute the nearest neighbors within l bands closest to q and take the best one according to the hyperbolic distance. The number of bands l is varied from 1 to 10, thus giving the curve on Figure 1.

Additional experiments Figure 7 is similar to Figure 3, but now we use the best-first search instead of the greedy search. We see that the conclusions are the same.